

INFORME FINAL

Código del proyecto: 7973			
Título del proyecto: Teoría de Floquet para el estudio de correlaciones en sistemas atómicos dependientes periódicamente en el tiempo			
Facultad o Instituto Académico: Ciencias Naturales y Exactas			
Departamento o Escuela: Física			
Grupo (s) de investigación: Física Teórica del Estado Sólido / QuanTIC			
Investigadores	Nombre	Tiempo asignado	Tiempo dedicado
Investigador Principal	Karem Cecilia Rodríguez Ramírez	10	10
Coinvestigadores	Javier Madroñero Pabón	10	10
	Alejandro González Melán (Estudiante de Doctorado)	40	40
Otros participantes	Manuel Humberto Muñoz Arias (Estudiante de pregrado) Isabel Guzmán Naranjo (Estudiante de Pregrado) Jhoan Sebastián Ortiz Girón (Estudiante de Pregrado)		

CONTENIDO

Informe Final

ANEXOS

1. Artículo A2
2. Acta de sustentación y tesis de pregrado de Manuel Muñoz
3. Acta de sustentación y tesis de pregrado de Isabel Guzman
4. Proyecto para Colciencias
5. Vinculación de monitores
6. Actas de propiedad intelectual
7. Anexos "Few-level model for helium"



Fecha de presentación del Informe: Día Mes Año

Datos generales del Proyecto

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1. Resumen ejecutivo:

Se espera que describa el proyecto, planteamiento del problema, objetivos, metodología, principales resultados obtenidos y las conclusiones. La extensión debe ser de máximo de 500 palabras (en español y en inglés).

Resumen: Los conceptos de correlaciones y complejidad van de la mano en sistemas atómicos. Incluso sistemas relativamente "pequeños" pueden ser extremadamente

¹ Todas las personas relacionadas en el informe y que participen en el proyecto deben haber suscrito el acta de propiedad intelectual de acuerdo con los formatos establecidos.

complejos debido a las fuertes correlaciones entre sus constituyentes. En este proyecto se estudiaron las correlaciones y sus consecuencias en dos clases de sistemas atómicos con dependencia periódica en el tiempo: el átomo de helio forzado periódicamente y átomos fríos en redes ópticas que incluyen modulaciones periódicas en el tiempo.

En el primer sistema la interacción interelectrónica es la causa de su no integrabilidad, de su alta complejidad y de las correlaciones electrónicas que combinadas con un forzamiento externo periódico en el tiempo son responsables de la formación de paquetes de onda no dispersivos, es decir, objetos cuánticos que se propagan a lo largo de órbitas clásicas del sistema sin dispersión. A pesar de su posible impacto en el campo de la información cuántica y del control coherente no existe aún evidencia experimental a cerca de los paquetes de onda no dispersivos y tampoco se habían diseñado mecanismos para preparar al átomo de helio en los estados altamente excitados que los generan. Nuestros resultados – basados en sofisticados algoritmos computacionales elaborados a partir de la teoría de Floquet – dan lugar a una propuesta para preparar y detectar estos estados a partir del estudio de sus acoples con estados ligados del átomo. Igualmente, se encontraron y caracterizaron las vidas medias y algunas propiedades de localización de los paquetes de onda no dispersivos.

La teoría de Floquet es igualmente adecuado para el tratamiento de gases bosónicos en redes ópticas con modulaciones periódicas en el tiempo. Problemas fundamentales de sumo interés en la comunidad científica internacional están relacionadas por ejemplo con procesos de transporte y dinámica fuera del equilibrio. En particular, usamos el modelo inclinado (tilted) de Bose-Hubbard de dos bandas para la descripción de gases bosónicos en redes ópticas, el cual se transforma en un sistema periódico en el tiempo en el marco de interacción. Con ayuda de este método fue posible construir un simulador cuántico para magnetismo usando redes ópticas, diseñar protocolos para la preparación de estados en sistemas minimalistas de dos partículas en dos sitios de red y explorar procesos de difusión en el espacio de Hilbert en regímenes caóticos del sistema. Esto último nos permitió verificar la hipótesis de termalización de estados propios que es fundamental para la formulación de una teoría consistente de termalización cuántica.

Los productos mas importantes obtenidos son dos tesis de pregrado, un artículo A2, una ponencia nacional e importantes avances en el desarrollo de una tesis doctoral.

Abstract: Correlations and complexity are two concepts that come together in atomic systems. Apparently simple “small” systems can be highly complex due to the strong correlations between their components. In this project we studied the correlations and their consequences in two kinds of atomic systems with periodic time dependence: the driven helium atom and cold atoms in optical lattices.

In the first system, the inter-electronic interaction is the cause of its non-integrability, of its high complexity, and of the electronic correlations. The latter, combined with an external periodic driving, gives rise to non-dispersive wave packets, that is, quantum

objects that propagate along classical periodic orbits without dispersion. Despite their possible impact in quantum information and coherent control, there is no experimental evidence of their existence. There had been neither designed mechanisms for the preparation and detection of the highly excited states the generate this objects. Our results – based on sophisticated computational algorithms developed starting from the Floquet theory – give rise to a proposal for the preparation and detection of these states. This proposal is originated from the study of the coupling of the so called frozen planet states to bound states of helium. Furthermore, we were able to find and quantitatively caracterize the energies, lifetimes and some localization properties of non-dispersive wave packets.

Floquet theory is equally appropriate for the treatment of bosonic gases in optical lattices with time-periodic modulations. Fundamental problemas fundamentales of great interest for the international scientific community are related to transport processes and dynamics out of equilibrium. In particular, we used the Bose-Hubbard model for tilted optical lattices, which is transformed into a periodic time-dependent system in the interaction picture.

With the help of this method it was possible to build a quantum simulator of magnetis using optical lattices, to design protocols for the preparation of some states of interest in minimal systems of two particles in two sites, and to explore diffusion in Hilbert space in chaotic regimes of the system. The latter allowed us to verify the eigenstate thermalization hypothese, which is fundamental for the formulation of a consistent theory of quantum thermalization.

The most relevant products obtained within this proyect are two undergraduate thesis, an A2 article, a poster in a national event, and significant advances for a doctoral thesis.

2. Síntesis del proyecto:

En una extensión máxima de 5 páginas, se debe mostrar el cumplimiento de los objetivos del proyecto y debe incluir:

Tema: Teoría de Floquet para el estudio de correlaciones en sistemas atómicos dependientes periódicamente en el tiempo

Objetivo general

El objetivo general de este proyecto consiste en estudiar la dinámica tanto de átomos de helio en presencia de campos electromagnéticos como de bosones en redes ópticas con dependencia periódica del tiempo usando teoría de Floquet.

Objetivos específicos

- Estudio de los acoples dipolares y canales de decaimiento de estados de planeta congelado (EPC) de helio.

- Estudio de los canales y tasas de decaimiento de paquetes de onda no dispersivos (POND) en el átomo de helio forzado.
- Detección de POND en sistemas bosónicos ultrafríos en redes ópticas unidimensionales.
- Estudio de transiciones cinéticas a través de diferentes fases cuánticas obtenidas por la variación bien sea adiabática o súbita de parámetros.

Metodología

La parte fundamental para el éxito del presente proyecto consistió en la implementación del formalismo de Floquet tanto en el átomo de helio forzado como en sistemas de átomos fríos en redes ópticas.

Estados de planeta congelado y paquetes de onda no dispersivos en helio:

Se usó un modelo planar que permite la implementación relativamente simple de la representación matricial del hamiltoniano del sistema para su posterior diagonalización. La construcción de los elementos de matriz del hamiltoniano y del operador de dipolo se puede conseguir eficientemente usando lenguaje simbólico (por ejemplo, con Mathematica), para su implementación posterior en FORTRAN. Las matrices resultantes son de tipo escaso (sparse matrices) y tienen una estructura de banda.

Los EPC son estados resonantes inmersos en el continuo del espectro de helio. Los estados resonantes se pueden identificar usando el método de rotación compleja, por medio del cual las coordenadas de posición se rotan en el plano complejo en un ángulo dado dando lugar a un problema de valores propios que ya no es hermítico sino simétrico complejo. La implementación de este método nos permitió identificar tanto las energías como las tasas de decaimiento de EPC. El análisis de los acoples de estos estados con estados ligados del átomo se hizo estudiando sus proyecciones en el espacio de configuración y las secciones transversales de fotoionización desde estados simpletados excitados hasta regiones de energía donde se encuentran dichos estados. Desde el punto de vista numérico las matrices diagonalizadas mas grandes alcanzaron a ocupar aproximadamente 30GB de RAM.

De otro lado, para el átomo forzado la estructura de bandas y el carácter escaso de las matrices en el problema de valores propios para el operador de Floquet se mantiene. Sin embargo la diagonalización completa de este problema en las regiones donde aparecen los paquetes de onda no dispersivos define un problema computacional de grandes proporciones (matrices a diagonalizar requieren una memoria RAM del orden de 500GB) fuera del alcance de nuestros recursos. Alternativamente en procesos multifotónicos que involucran estados altamente excitados y campos electromagnéticos de baja frecuencia e intensidad (como es el caso en la formación de POND) interviene típicamente un número relativamente pequeño de resonancias del átomo no perturbado. Es decir, filtrando inteligentemente los estados del átomo fue posible reducir significativamente (aproximadamente en un factor 20 o más) las dimensiones

del problema de valores propios y caracterizar las energías y tiempos de vida de los POND.

Gases bosónicos en redes ópticas:

Para estudio de correlaciones y transporte en sistemas de átomos fríos en redes ópticas se usó el modelo inclinado (tilted) de Bose-Hubbard de dos bandas. El hamiltoniano correspondiente es independiente del tiempo, pero se puede transformar en uno dependiente periódicamente del tiempo en el marco de interacción. A partir de aquí se usa el formalismo de Floquet para estudiar la evolución temporal del sistema. El problema numérico asociado es algo exigente pero con los recursos adquiridos a través del proyecto (estación de trabajo de alta capacidad, entre otros) fue posible resolverlo.

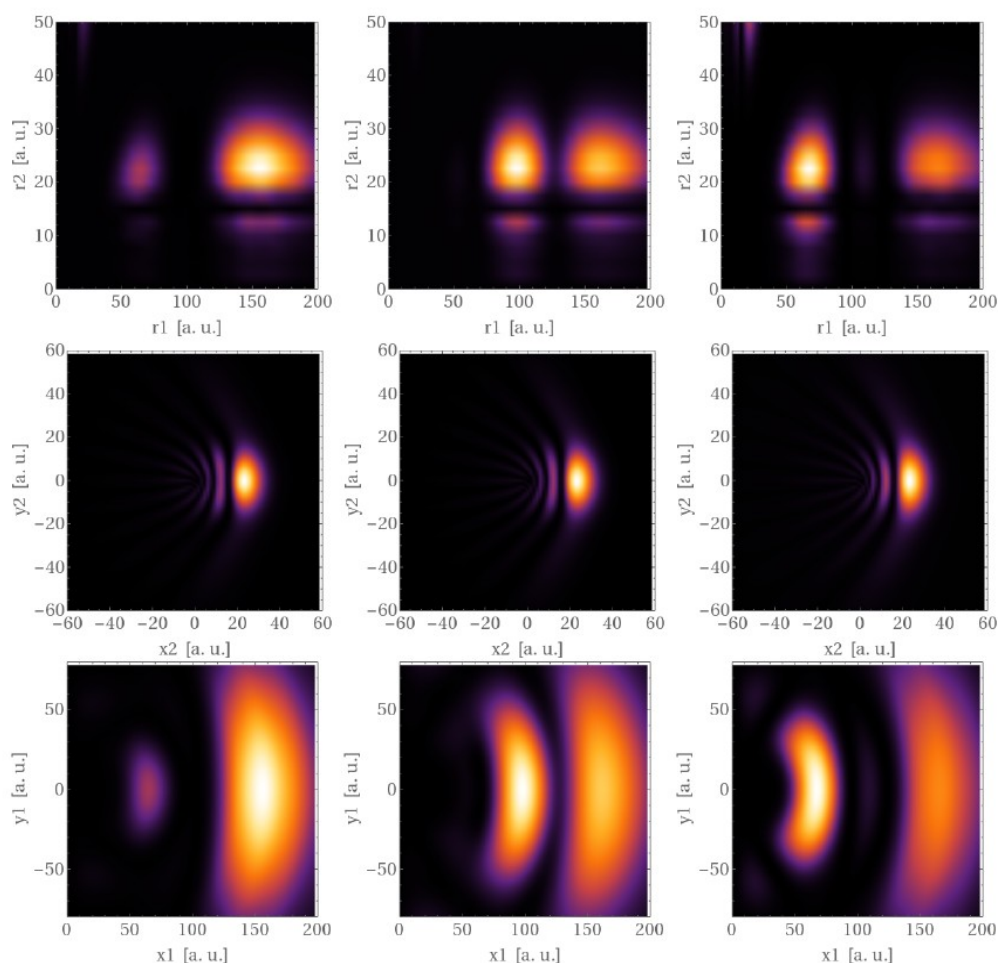
Resultados obtenidos

La investigación en el marco del presente proyecto ha culminado. Los resultados obtenidos se encuentran en su mayoría consignados en los trabajos de grado (anexos) de los estudiantes Manuel Muñoz e Isabel Guzmán y en el artículo (anexo) *Chaotic level mixing in a two-band Bose-Hubbard model* [C. Parra-Murillo, J. Madroñero, y S. Wimberger, *Annalen der Physik* **527**, 656 (2015)]. Además de esto aún hay resultados no publicados, obtenidos en el marco del doctorado del estudiante Alejandro González.

Isabel Guzmán mostró que los EPC están fuertemente acoplados con algunos estados simplemente excitados del átomo de helio. La caracterización de estos acoples se consiguió a través de un estudio exhaustivo de las secciones transversales de ionización y de las proyecciones de los estados en el espacio de configuración. El resultado más importante de este estudio es la formulación de un posible mecanismo para la detección de EPC usando procesos de excitación con dos láseres a partir del estado base y usando estados simplemente excitados como puente de transición hacia EPC.

Alejandro González desarrollo un sofisticado código para obtener y caracterizar paquetes de ondas no dispersivas de helio. Este código incorpora la diagonalización numéricamente exacta de la representación del átomo de helio no perturbado en términos de cuatro osciladores acoplados y hace uso del método de rotación compleja para resolver las resonancias del sistema (estados doblemente excitados) que de otra manera están inmersos en el continuo. Los estados resonantes y del continuo obtenidos allí se usan para construir la representación matricial del operador de Floquet. Detalles sobre este método se encuentran en el anexo *Few-level model for the driven 2D helium*, el cual es parte de un artículo en proceso de redacción. La ventaja de esta representación es la reducción significativa del tamaño del problema de valores propios: nuestros estimativos indican que las matrices involucradas en problema de valores propios del operador de Floquet ocuparían una memoria superior a 1TB usando la representación en osciladores armónicos. En cambio, en esta nueva representación las matrices a diagonalizar no sobrepasan los 15GB.

Con ayuda de este método se encontraron POND por debajo de los umbrales de ionización $N=4$, 5, 6 y 7 para estados triplete de helio. La figura siguiente muestra diferentes proyecciones de un POND por debajo de $N=6$.



La cuasienergía y su tasa de decaimiento en unidades atómicas (ua) son respectivamente -0.07317 y $-6.8E-07$. Las columnas corresponden a proyecciones para $t=0$, $T/4$ y $T/2$, respectivamente, siendo T el periodo del forzamiento externo. En la primera fila se observa la proyección del estado a lo largo de la configuración colineal, es decir, cuando el ángulo entre los radios r_1 y r_2 (distancia de los electrones al núcleo) es 0. En la segunda fila se observa la proyección del electrón interno cuando el electrón externo se localiza en una posición fija alrededor del máximo de la densidad total de probabilidad ($r_2 \approx 150 \text{ ua}$). Las proyecciones del electrón externo para una posición fija

Elaborado por: Vicerrectoría de Investigaciones

($r_1 \approx 20a$) del electrón interno se muestran en la tercera fila. Se observa que el electrón interno no se ve afectado por el campo externo mientras el electrón externo oscila periódicamente con el campo alrededor de su posición de equilibrio.

De otro lado, los resultados de Manuel Muñoz se enmarcan en el contexto de simulación y control cuántico usando redes ópticas. Primero, se estableció una conexión entre el sistema de átomos fríos en redes ópticas y cadenas de espines usadas para el estudio de magnetismo cuántico. Concretamente, se construyó un simulador cuántico basado en una cadena de espines de Heisenberg para caracterizar procesos de segundo orden en el modelo de Bose-Hubbard. Estos procesos consisten en la propagación de cuasipartículas (par de ocupación hueco-doblón). El resultado fundamental es que la propagación de estas cuasipartículas puede ser interpretada como un paquete de ondas de espines en la cadena de Heisenberg. Segundo, se exploró la dinámica entre bandas que se puede establecer mediante la inclusión de un término que acople éstas a partir de ocupaciones dobles de los sitios de red en la banda inferior. Para el sistema minimal (dos partículas en una red de dos pozos) el resultado principal es el acceso a estados que se asemejan a estados de Bell (importantes para computación cuántica). Sin embargo, este resultado no es robusto al escalar el tamaño del sistema.

Finalmente, el modelo de Bose-Hubbard de dos bandas nos permitió investigar procesos de difusión caótica y termodinámica cuántica. El modelo usado exhibe un régimen caótico. La evolución temporal a través de esta región genera un complejo proceso de mezcla de estados que evita la generación de estados ocupando exclusivamente la segunda banda que son de interés en la comunidad de óptica e información cuántica. Esto se debe al acople no local entre las dos bandas. Una forma de caracterizar la mezcla caótica de estados consiste en estudiar la termalización de observables con la ayuda la hipótesis de termalización de estados propios (el valor esperado de un observable y su promedio temporal se acercan a la aproximación diagonal). Los observables estudiados para los cuales se verificó esta hipótesis son (i) interacción de partículas de un mismo sitio de la red en una banda definida, (ii) interacción de partículas en bandas distintas de un mismo sitio de la red, y (iii) número de ocupación de la banda superior. Los detalles de estos resultados se encuentran en el artículo anexo *Chaotic level mixing in a two-band Bose-Hubbard model*.

Principales conclusiones y/o recomendaciones

La teoría de Floquet nos permitió tratar sistemas atómicos de uno o varios átomos. En ambos casos las correlaciones bien sean intra-atómicas o entre los átomos dan lugar a una gran cantidad de efectos, como la generación de POND, difusión en el espacio de Hilbert y termalización cuántica. La comprensión de estos efectos es de gran interés en el contexto de control cuántico, información cuántica, simulación cuántica, entre otros.

Se demostró la generación de POND en el átomo de helio a partir de EPC, para los cuales, además, se propuso un método para su detección usando un proceso bicromático de dos fotones para excitar el estado base.

Para el sistema de átomos fríos en redes ópticas se mostró que

(i) puede ser usado como simulador de sistemas del estado sólido, como cadenas de espines;

(ii) hasta cierto punto se puede controlar su dinámica, por ejemplo, para generar estados de interés como estados de Bell, sin embargo la alta complejidad del espectro de cuasi-energías produce un complicado proceso de mezcla de estados que impiden controlar el sistema mediante protocolos sencillos. Esta misma complejidad, sin embargo, nos permite verificar la hipótesis de termalización de estados propios, lo cual se enmarca dentro del muy actual contexto de termalización cuántica.

3. Productos:

Tabla No. 1. **Cantidad y tipo de productos pactados en el Acta de Trabajo y Compromiso y productos finalmente presentados**

TIPO DE PRODUCTOS	No. de PRODUCTOS PACTADOS	No. de PRODUCTOS PRESENTADOS
Productos de nuevos conocimientos		
Artículo completo publicado en revistas A1 o A2	1	1
Artículo completo publicados en revistas B	0	
Artículo completo publicados en revistas C	0	
Libros de autor que publiquen resultados de investigación	0	
Capítulos en libros que publiquen resultados de investigación	0	
Productos o procesos tecnológicos patentados o registrados	0	
• Prototipos y patentes	0	
• Software	0	

TIPO DE PRODUCTOS	No. de PRODUCTOS PACTADOS		No. de PRODUCTOS PRESENTADOS	
Productos o procesos tecnológicos usualmente no patentables o protegidos por secreto industrial	0			
Normas basadas en resultados de investigación	0			
Formación de recursos humanos	No. de estudiantes vinculados	No. de tesis	No. De estudiantes Vinculados	No. De tesis
Estudiantes de pregrado	4	2	2	2
Semillero de Investigación	1		1	
Estudiantes de maestría	0		0	
Estudiantes de doctorado	1	0	1	0
Productos de divulgación				
Publicaciones en revistas no indexadas	0		0	0
Ponencias presentadas en eventos (congresos, seminarios, coloquios, foros)	No. de ponencias nacionales	No. de ponencias internacionales	No. de ponencias nacionales	No. de ponencias internacionales
Ponencias presentadas en eventos (congresos, seminarios, coloquios, foros)	1	0	1	0
Propuesta de investigación				
Propuestas presentadas en convocatorias externas para búsqueda de financiación.	1		1	

Tabla No. 2. Detalle de productos.

Para cada uno de los productos obtenidos y relacionados en la tabla anterior, indique la información solicitada para cada uno, anexando copia de las respectivas constancias. Como anexo a esta guía encontrará el instructivo para la revisión de informes finales y productos

Tipo de producto:	Artículo A1
Nombre General:	Annalen der Physik 527 , 656 (2015)].
Nombre Particular:	Chaotic level mixing in a two-band Bose-Hubbard model
Ciudad y fechas:	Publicado online el 11 de febrero de 2015
Participantes:	C. Parra-Murillo, J. Madroñero, y S. Wimberger
Sitio de información:	
Formas organizativas:	Grupo QuanTIC

Tipo de producto:	Tesis de pregrado
Nombre General:	
Nombre Particular:	Study of doublon dynamics in optical lattices: spin chains and perspectives on quantum control
Ciudad y fechas:	Cali, 7 de enero de 2016
Participantes:	Manuel Humberto Muñoz Arias
Sitio de información:	Biblioteca Central
Formas organizativas:	Grupo QuanTIC

Tipo de producto:	Tesis de pregrado
Nombre General:	
Nombre Particular:	Planetary States in Two-electron Atomic Systems
Ciudad y fechas:	Cali, 29 de octubre de 2015



fechas:	
Participantes:	Isabel Guzmán Naranjo
Sitio de información:	Biblioteca Central
Formas organizativas:	Grupo QuanTIC

Tipo de producto:	Semillero de Investigación
Nombre General:	
Nombre Particular:	
Ciudad y fechas:	Cali, 18 de febrero de 2015
Participantes:	Jhoan Sebastian Ortiz Girón
Sitio de información:	
Formas organizativas:	Grupo QuanTIC

Tipo de producto:	Monitor de investigación
Nombre General:	
Nombre Particular:	
Ciudad y fechas:	
Participantes:	Jhoan Sebastian Ortiz Girón
Sitio de información:	10 de septiembre de 2015
Formas organizativas:	Grupo QuanTIC



Tipo de producto:	Monitor de investigación
Nombre General:	
Nombre Particular:	
Ciudad y fechas:	
Participantes:	Juan Pablo Villada
Sitio de información:	13 de marzo de 2015
Formas organizativas:	Grupo de Física Teórica del Estado Sólido

Tipo de producto:	Estudiante de doctorado vinculado
Nombre General:	
Nombre Particular:	
Ciudad y fechas:	Todo el proyecto
Participantes:	Alejandro González Melán
Sitio de información:	
Formas organizativas:	Grupo QuantIC

Tipo de producto:	Ponencia nacional
Nombre General:	Poster en el XIV Encuentro Nacional de Óptica y V Conferencia Andina y del Caribe y sus Aplicaciones
Nombre Particular:	Cuopling of frozen planet states of helium to its bound states: towards the preparation of two-electron nondispersive wave packets



Ciudad y fechas:	Cali, del 16 al 20 de noviembre de 2015
Participantes:	Isabel Guzmán
Sitio de información:	
Formas organizativas:	Grupo QuanTIC

Tipo de producto:	Proyecto Colciencias (Convocatoria externa)
Nombre General:	
Nombre Particular:	Formation and control of cold molecules
Ciudad y fechas:	18 de junio de 2014
Participantes:	Beatriz Elena Londoño Flórez Karem Cecilia Rodríguez Ramírez Carlos Alberto Arango Mambuscay Julio César Arce Clavijo José Guillermo López Sotelo
Sitio de información:	
Formas organizativas:	Grupos Óptica Cuántica, Física Teórica del Estado Sólido y Química Teórica y Computacional

4. Impactos actual o potencial:

Haga una descripción y/o relacione los impactos que tenga el proyecto en los diferentes ámbitos: académico, productivo, social, educativo, entre otros.

Si posee información acerca de los impactos actuales o potenciales de la investigación, preséntela en máximo una página. Se refiere a los aportes que ofrece en el campo de investigación al que corresponde. Incluye las tecnologías y resultados de IDi que puedan transferirse a los sectores productivos y de servicios, tanto nacionales como internacionales.



Los resultados e impactos científicos, así como los desarrollos tecnológicos derivados del desarrollo y adaptación de software que se ha realizado pueden verificarse a través del artículo y tesis publicadas.

Como producto de recurso humano a nivel profesional se introdujeron cuatro estudiantes de pregrado en el campo de gases fríos y física atómica, de lo cual resultaron dos tesis de pregrado. También trabajó activamente un estudiante de doctorado.

Los medios divulgativos del proyecto fueron basados principalmente en charlas científicas de orden institucional como el seminario del Grupo d Física Teórica del Estado Sólido y el seminario del grupo QuantIC, ambos del Departamento de Física de la Universidad del Valle. Igualmente se presentó una charla nacional (ver productos).

Finalmente, cabe resaltar que las líneas de investigación en gases fríos y en física atómica eran prácticamente inexistentes en el Departamento de Física de la Univerisdad del Valle.

La presente versión del informe contiene las observaciones de los evaluadores:

Firma del investigador principal

VoBo. Vicedecano de Investigaciones

Por favor presente su informe impreso y en formato digital en hoja tamaño carta, letra arial 11, con espacios de 1 1/2

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Para consultar la homologación de una revista extranjera puede ingresar el ISSN (completo o parcial) o el título de la revista (completo o parcial).

Recuerde que si tiene los datos completos su búsqueda será más precisa. Al terminar haga clic en Buscar o Enter.

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Chaotic level mixing in a two-band Bose-Hubbard model

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A two-band Bose-Hubbard model is presented which is shown to be minimal in the necessary coupling terms at resonant tunneling conditions. The dynamics of the many-body problem is studied by sweeping the system across an avoided level crossing. The linear sweep generalizes Landau-Zener transitions from single-particle to many-body realizations. The temporal evolution of single- and two-body observables along the sweeps is investigated in order to characterize the non-equilibrium dynamics in our complex quantum system.

1 Introduction

Describing stationary ground states and transport dynamics in real solid-states is notoriously difficult because of the too many degrees of freedom involved. It is the merit of simplified models, which nevertheless take into account the relevant physical mechanisms, to allow analytical and numerical predictions for such complex quantum systems. A celebrated model is the Hubbard model first introduced for fermions, whose main approximations are that it is discrete describing a lattice system and that interactions are typically short ranged [1].

The realization of lattice models with ultracold atoms has given new impetus to the theoretical study of many-body models, be it for fermions or bosons. Neglecting the spin degree of freedom, the simplest Hubbard model in one spatial dimension is integrable for fermions, while its counterpart for bosons is shown to be non-integrable [2]. This originates in the fact that too many combinations exist of distributing bosons on a lattice. The Bose-Hubbard model we are referring to now and in the following is given by the many-body Hamiltonian [3]

$$\hat{H}_{\text{BHM}} = \sum_l \left[-\frac{J}{2} (\hat{a}_{l+1}^\dagger \hat{a}_l + h.c.) + \frac{W}{2} \hat{a}_l^{\dagger 2} \hat{a}_l^2 \right]. \quad (1)$$

Here $\hat{a}_l$ and $\hat{a}_l^\dagger$ are the bosonic annihilation and creation operators in the lattice mode l , W denotes the

interaction strength and J the tunneling coupling between the wells. This model is only integrable for either $W = 0$ (non-interacting case) or $J = 0$ (no dynamics) as one may easily verify. If both energy scales J and WN_{fill} , where N_{fill} is the average filling, are comparable, the Bose-Hubbard model is a paradigm for a quantum chaotic system [2]. The Hamiltonian above well describes an ultracold atomic gas in sufficiently deep lattices where the ground band is very flat and decoupled from higher lying energy bands of the periodic lattice [3].

Many extensions of the basic model of Eq. (1) have been recently studied [3, 4]. To be more specific, models with more than the usual single-band approximation were investigated in references [5–8], additional gravitational forces in [9, 10], or non-local interactions in [11–15]. Our goal is here to present a model including two coupled energy bands. Such a system is implemented in ongoing experiments, for instance at Innsbruck [16–18], Harvard [19, 20] and Munich [11, 21], and finds application in other realizations of Wannier-Stark lattice systems with ultracold bosons [22, 23]. Because of the non-local interband couplings, our minimal two-band model has similar quantum chaotic properties as its simplest version (1), see also refs. [24, 25]. We will show now how these properties can be used to steer many-body Landau-Zener dynamics [26] and to investigate the quantum (thermo)dynamics of the isolated many-body quantum system.

2 Minimal two band model

Our two band model, considerably extending the Hamiltonian of Eq. (1), for locally interacting bosons is given by

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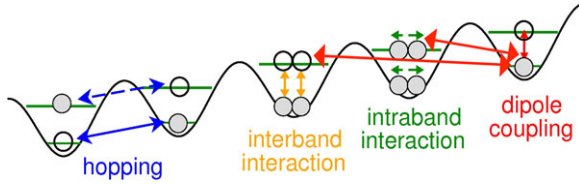


Figure 1 Sketch of the system we model by the Hamiltonian (2). The hopping terms represent J_a (solid blue arrow) and J_b (dashed blue arrow). Intraband and interband interactions correspond to the terms with $W_{a,b}$, W_x , respectively. The field induced dipole couplings are shown by the red arrows for C_μ , with $\mu = -2, -1, 0$. All the latter turn out to be relevant at the corresponding resonant tunneling conditions as the next two figures report.

the following Hamiltonian

$$\begin{aligned} \hat{H}_{2B} = & \sum_{l,\beta} \left[-\frac{J_\beta}{2} (\hat{\beta}_{l+1}^\dagger \hat{\beta}_l + h.c.) + \frac{W_\beta}{2} \hat{\beta}_l^{\dagger 2} \hat{\beta}_l^2 + 2\pi F l \hat{n}_l^{(\beta)} \right] \\ & + 2\pi F \sum_{l,\mu} [C_\mu \hat{a}_{l+\mu}^\dagger \hat{b}_l + h.c.] + \frac{W_x}{2} \sum_l [\hat{b}_l^{\dagger 2} \hat{a}_l^2 + h.c.] \\ & + 2W_x \sum_l \hat{n}_l^{(a)} \hat{n}_l^{(b)} + \frac{\Delta}{2} \sum_l (\hat{n}_l^{(b)} - \hat{n}_l^{(a)}). \end{aligned} \quad (2)$$

This model preserves the total number N of bosons on L lattice sites. Then the full dimension of the state space (Fock space) is given by

$$D = \frac{(N + 2L - 1)!}{N!(2L - 1)!}. \quad (3)$$

The operators $\hat{\beta}_l$ and $\hat{\beta}_l^\dagger$ represent the annihilation and creation operators. $\hat{n}_l^{(\beta)} = \hat{\beta}_l^\dagger \hat{\beta}_l$ is the number operator, with band index $\beta \in \{a, b\}$ for the lower and the upper band, respectively. The parameter space is defined by the parameters $(J_\beta, W_\beta, W_x, C_\mu, \Delta)$. Most of the terms are sketched schematically in Fig. 1. J_β is the kinetic energy scale, characterizing the nearest neighbor hopping matrix elements. The W 's represent the on-site, intra- and inter-band interaction strengths. $2\mu + 1$ dipole coupling coefficients C_μ are induced by the constant gravity or Stark field F , with $\mu \in \mathbb{Z}$. The Stark force itself is given by the third term in the first line of Eq. (2). The average energy band gap is given by Δ . Two-body interactions between the local onsite single-particle energy band levels lead to the interband exchange term in the second line of Eq. (2).

In contrast to previous versions of the above model [10, 27], we explicitly include here more cross-band couplings with $|\mu| \leq 2$, for which $\mu = \{-2, -1, 0, 1, 2\}$. At least for resonant tunneling restricted to the next two neighboring sites, more terms are not necessary since the

corresponding coupling coefficients go fast to zero with increasing $|\mu|$ [24]. Yet, as we shall see non-onsite cross terms are very relevant to describe, for instance, resonant tunneling between the two energy bands induced by the Stark field. Resonant tunneling finds important applications in solid-state devices [28] and is studied experimentally with ultracold atoms in the mean-field [22, 23] and many-particle regime [16–18]. In our sketch of Fig. 1, resonant tunneling is almost realized between the upper level of the middle well and the lower level of the rightmost site. The resonance conditions are given for specific values of the Stark force, which is well controllable experimentally [16–18, 22, 23]. From Fig. 1 it should be clear that the addition of the coupling terms $C_{\pm 1}$ and $C_{\pm 2}$ is crucial for investigating, in particular, first and second-order resonant tunneling, i.e. resonant tunneling to the nearest or next nearest neighbor well, respectively.

The non-integrability of Hamiltonian (2) makes necessary a numerical treatment based on exact diagonalization or explicit integration schemes. For the former, we actually transform the static Stark terms into periodically time-dependent phase factors for the hopping parameters and diagonalize the corresponding time-independent Floquet matrix. The temporal evolution for non-periodic time-dependence is done with a highly optimized Runge-Kutta scheme taking into account only the non-zero elements for matrix-vector multiplications. More details on numerical procedures are discussed elsewhere [29]. Here we focus on the physical consequences of the strong coupling in dynamical simulations. In this regime, the actual finite size of the system expressed in number of atoms N and lattice sites L is not really crucial since the total size D of the accessible Hilbert space is anyway large for $N, L \geq 4$ [24, 25, 29]. Hence we can restrict to rather small $L = 4$ and $L = 5$ with filling of order one for numerically expensive time-dependent computations.

The importance of including the interband non-local couplings $C_{\pm 1, \pm 2}$ close to resonant tunneling conditions is highlighted in Figs. 2 and 3.

First, we study the temporal evolution of the upper-band population for an initial state with filling one and all atoms in the ground band. The upper-band occupation number is given by the expectation value

$$M(t) = \sum_l \langle \phi(t) | n_l^{(b)} | \phi(t) \rangle, \quad (4)$$

with $|\phi(t)\rangle$ being the time evolved state starting from an initial Fock state. Figure 2(a) shows this number for $N = 4 = L$ versus time for no interactions $W_{a,b,x} = 0$. While for the case with only C_0 nonzero almost perfect interband

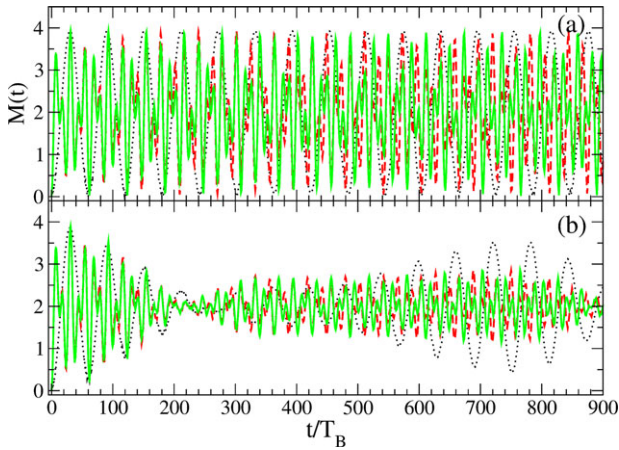


Figure 2 The temporal evolution of the initial state $|\psi_0\rangle = |1111; 0000\rangle$ ($N = 4 = L$) in time units of the Bloch period $T_B = 1/F$. Shown are the upper band populations $M(t)$ for (a) $W_{a,b,x} = 0$ and (b) weak interactions $W_a = 2.1 \times 10^{-3}$, $W_b = 2.6 \times 10^{-3}$, $W_x = 2.3 \times 10^{-3}$. The different curves are computed including only $C_0 = -0.09$ (black dotted lines), C_0 and $|C_{\pm 1}| = 0.039$ (red dashed lines), and finally the full model dynamics with all coupling elements $C_{0,\pm 1,\pm 2}$ with $|C_{\pm 2}| = 2.1 \times 10^{-3}$ (green solid lines). The almost perfect oscillations in (a) and the revival in (b) around $t/T_B = 750$ are heavily affected by the additional coupling terms. In particular, the phase of the inter-band oscillations depends on the specific model and the revival in (b) disappears in the background when including $C_{\pm 1,\pm 2}$. The remaining parameters are $F = 0.19$, $\Delta = 1.16$, $J_a = 0.08$, $J_b = -0.12$.

oscillations occurs, the addition of the terms with $|\mu| > 0$ complicates the dynamics. Hence, the results are different even for the non-interacting problem. Here the simplified theory of ref. [27] predicts an oscillation period which is independent of the system size, here in particular of N and L at constant $N/L = 1$. Taking into account the terms C_μ , with $\mu = \pm 1, \pm 2$, the oscillations show additional periods and the specific result depends on the system size L instead (not shown). The situation is even more dramatic if we look at an interacting case in Fig. 2(b), for which the revivals, seen if only C_0 is considered (dotted line), are degraded once we include the $C_{\pm 1,\pm 2}$ coupling terms (see solid line for the full model for instance). This means that the periodic revivals seen for the non-interacting case and just C_0 couplings disappear not only because of stronger interactions, but also due to the additional couplings $C_{\pm 1,\pm 2}$. This implies that – even in the non-interacting case – the two-band system cannot be mapped any more onto a simple quantum spin Ising model, as done e.g. in [19, 30].

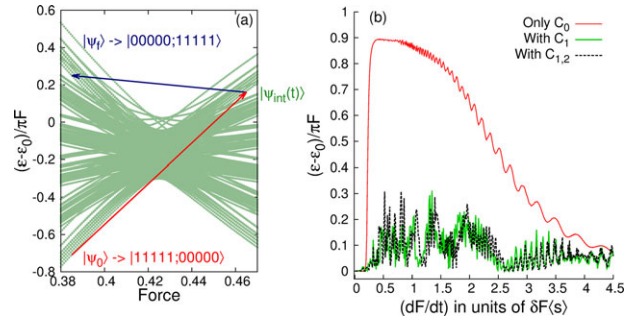


Figure 3 Dynamical numerical experiment to prove the importance of field inter band cross terms C_μ with $\mu \neq 0$. (a) Typical many-body energy spectrum across resonant tunneling characterized by a single-particle avoided crossing (filled by dense lying many-body levels). We try to transfer an initial state $|\psi_0\rangle$ via a fast (adiabatic) evolution to an intermediate state $|\psi_{\text{int}}\rangle$ via a sweep with the rates shown on the x axis in (b) into the final state $|\psi_f\rangle$. The arrows indicate the start of the protocol at $F_0 \approx 0.385$ over the intermediate value $F_{\text{int}} \approx 0.465$ back to $F_f = F_0$. (b) The success probability of transferring a large population from a Mott-like lower band state into a corresponding upper band state as a function of the slope of the force sweep (in units of $\delta F(s)$ as defined in the main text). In the case of $C_\mu = 0$ for $\mu \neq 0$ the success is high (red/upper solid line). The inclusion of more relevant couplings $C_{\pm 1}$ (green/lower solid line) and both $C_{\pm 1,\pm 2}$ (black dashed line) destroys this possibility. While the details depend on the specific model used for the computation, we observe that the crucial additional term is $C_{\pm 1}$ for the first-order resonance studied here for $L = 5 = N$. Our realistic parameters are [24]: $\Delta = 0.32$, $J_a = 0.041$, $J_b = -0.046$, $W_a = 0.027$, $W_b = 0.029$, $W_x = 0.028$, $C_0 = -0.096$, $|C_{\pm 1}| = 0.046$, $|C_{\pm 2}| = 0.007$.

Secondly, we investigate the temporal evolution of an eigenstate of the two band system which has again the form $|\psi_0\rangle \approx |1111; 00000\rangle$ at a specific value of the force $F = F_0$. Then we sweep the force linearly in time $F(t) = \dot{F}t + F_0$ and follow the dynamics of the corresponding many-body state $|\psi(t)\rangle$. The goal of our optimization procedure is to realize a final state close to $|00000; 11111\rangle$, which would correspond to transferring a Mott-like state from the ground band to the second band. The following protocol turned out to be feasible, see panel (a) in Fig. 3:

- (i) the initial and the intermediate state are chosen around but slightly outside the resonant tunneling region of width δF in the spectrum (see panel (a) in Fig. 3); more precisely, the initial state on the left at F_0 and the intermediate state at F_{int} on the right at of this region. The final state is obtained at the same force value where we started from $F_f = F_0$.
- (ii) we diabatically evolve, i.e. with large sweeping rate $\dot{F} \gg \delta F(s)$, the initial condition from left to right.

Here δF is the width of the resonant tunneling region and $\langle s \rangle$ the mean level spacing. This procedure ensures that the intermediate state $|\psi_{\text{int}}\rangle$ is of a similar form in the Fock basis as the initial one, yet its energy is increased.

- (iii) Now we invert the evolution, i.e., the state $|\psi_{\text{int}}\rangle$ is evolved backwards decreasing the force again. We compute the success probability, i.e., the probability of obtaining as a final state $|\psi_f\rangle = |00000; 11111\rangle$ as a function of the slope $\dot{F}$.

In panel (b) of Fig. 3 we show the success probability (solid red line). The latter shows a clear stable maximum over a sufficiently broad range of slopes (plateau region), while for too large slopes Rabi-like oscillations occur. The plateau region is obtained for sweeping rates values which are close to but smaller than the product of the effective width δF of the many avoided crossing and $\langle s \rangle$. Hence, if only the coefficient C_0 is included the protocol above would produce reliably the target state. Including higher order couplings, our protocol becomes unstable and useless for a production of this particular state with high fidelity. For nearest-neighbor resonant tunneling, the main contribution with respect to the naive model (red/upper solid line) arises from $C_{\pm 1}$, while the next order $C_{\pm 2}$ will become important for longer-range resonant tunneling along the lattice (not shown here, but studied in the mean-field regime experimentally in [22, 23]).

The two examples shown in Figs. 2 and 3 show that we cannot neglect non-local band exchange terms C_μ , with $\mu = \pm 1, \pm 2$, in particular at resonant tunneling conditions [22, 23]. On the one hand, it denies the possibility to prepare interesting higher-band states, if not very sophisticated protocols for optimizing the transport across the interband avoided crossing region are found. On the other hand, only the inclusion of next-nearest neighbor cross couplings leads to a complex mixing of the states corresponding to the instantaneous spectra for fixed forces F , respectively. This chaotic level mixing and its consequences will now be characterized further in the next section.

3 Quantum thermodynamics

Since our model conserves the particle number N , the sum of the lower and upper band population obviously is $\sum_l (n_l^{(a)} + n_l^{(b)}) = N$. In the limit of vanishing interactions $W_\beta, W_x \rightarrow 0$, the spectrum of (2) can be split into sets of states with the same upper-band occupation number [25, 29], see Eq. (4). These sets of states, we call them M manifolds in the following, are very useful also

for the characterization of the complex spectra of interacting systems. As shown in detail in ref. [25], close to resonant interband tunneling, these manifolds lose their property of being good quantum numbers due to strong interactions. This indicates that the spectra are strongly mixed due to the interactions *and* the avoided crossing, which squeezes the levels close together (see Fig. 3(a)).

Other useful quantities for the characterization of strong level mixing are

$$\theta_{\beta=a,b} = \left\langle \frac{1}{2} \sum_l \hat{\beta}_l^{\dagger 2} \hat{\beta}_l^2 \right\rangle_\phi \quad (5)$$

and

$$\theta_x = 2 \left\langle \sum_l n_l^{(a)} n_l^{(b)} \right\rangle_\phi \quad (6)$$

They represent the onsite intraband particle interactions and the onsite interband interactions, respectively. Obviously, both quantities are zero in the interaction-free case.

We want to study now better the non-equilibrium dynamics in the presence of interactions comparable to the hopping strength. As in the previous section, we drive an initial state across the resonant tunneling regime, where many non-adiabatic transitions take place. For this, we use a linear sweeping function, which is indeed inspired by Landau-Zener transition models for our system [31]: $F(t) = \dot{F}t + F_0$, $t > 0$. The rate $\dot{F}$ is chosen in such a way to be similar to the product of the mean level spacing $\langle s \rangle$ and the total width δF in the parameter F of the strongly coupled region in the spectrum. This guarantees an optimal sweeping rate for strong level coupling in the dynamics, avoiding too diabatic (direct crossing of the region without level spreading) or too adiabatic (following essentially one level only) evolutions. The scan starts slightly before the avoided crossing at resonant tunneling and stops slightly afterwards. The presence of avoided crossings in the spectrum, see Fig. 3(a), generates then a spreading of the initially localized wave packet in the instantaneous eigenbasis of states $|\epsilon_i\rangle$ with eigenenergies $\epsilon_i(F(t))$. The local density of states (LDOS), defined by

$$P_\psi(\epsilon, g) = \sum_i |C_i|^2 \delta(\epsilon - \epsilon_i), \quad (7)$$

with $C_i \equiv \langle \psi | \epsilon_i \rangle$, characterizes this spreading. For strong interactions, a nearly flat distribution is reached. Here $|C_i|^2 \sim 1/D$, i.e. the system obeys an equipartition condition. The spreading may also be analyzed using the

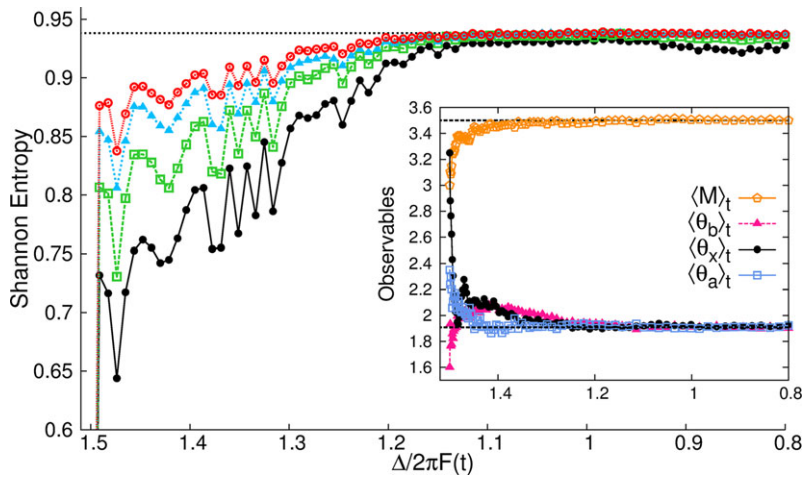


Figure 4 Shannon entropy in the instantaneous basis, see Eq. (8), in units of $\ln D$ for $N = 6$, $L = 5$. The different colors represent different M manifolds of the initial state: $M = 0$ (black line with circles), $M = 1$ (green dashed line with squares) and $M = 2$ (light/blue dashed line with triangles) and $M = 3$ (red dashed line with open circles). The inset shows the temporal evolution of the single and two-body observables $\{\hat{M}, \hat{\theta}_{\beta,x}\}$. All of them relax quickly to their equilibrium value given in Eq. (9) and plotted as constant black dashed lines. The other parameters are identical to the ones of Fig. 3 and correspond for our filling $N/L = 6/5$ to a regime of strong level mixing due to interparticle interactions.

Shannon information entropy [32]

$$S_{\text{sh}} = - \sum_i |C_i|^2 \ln |C_i|^2, \quad (8)$$

which approaches $S_{\text{sh}} \approx \ln D$ in statistical equilibrium. The evolution of the entropy is shown for typical system parameters in Fig. 4. The entropy starts out from a small value, which is zero when we start exactly with an eigenstate of the system for $F = F_0$. Then it systematically increases saturating after crossing the minimum of the avoided crossing. The saturation values are all identical and close to one (actually 0.94 as predicted by random matrix theory for fully chaotic level mixing [33, 34]).

The thermalization of observables in a complex quantum system can be investigated with the help of the eigenstate thermalization hypothesis [35–37]. For this, we check whether the expectation value of our operator $\hat{O}$ of interest and its time average approach the diagonal approximation:

$$\langle \hat{O} \rangle_t \equiv \langle \psi_t | \hat{O} | \psi_t \rangle, \quad \overline{O} \equiv \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \langle \hat{O} \rangle_{t'} dt' \longrightarrow \sum_i |C_i|^2 O_{ii}, \quad (9)$$

where $O_{ij} = \langle \varepsilon_i | \hat{O} | \varepsilon_j \rangle$. Since we are treating a closed system, the density matrix is represented by the pure state $|\psi_t\rangle$ for the full system. In the regime of strong chaotic level mixing, the distribution of the coefficients $|C_i|$ after the sweep is essentially flat confirming the statistical relaxation in our isolated system (see the discussion of the Shannon entropy above). This regime can indeed be characterized by an effective temperature of the size of the spectral width divided by the Boltzmann constant, see ref. [38] for the somewhat subtle definition of temperature in our isolated system of interacting particles in

terms of the instantaneous Floquet bases at fixed forces F .

The coherent dephasing arises from passing the zone with many avoided crossings with a broad distribution of widths as expected from random matrix theory, see e.g. [39]. The passing of this chaotic zone close to resonant tunneling conditions makes the off-diagonal elements O_{ij} go to zero quickly and the evolution can be well approximated by the diagonal contributions only. We study the time evolution of the set of observables $\{\hat{M}, \hat{\theta}_{\beta,x}\}$ introduced above. Optimal thermalization in the instantaneous eigenbases is obtained for a sweeping parameter $\dot{F}/\delta F(s)$ of order 1. This condition corresponds to the strong mixing condition mentioned already in the previous section. All the expectation values shown in the inset of Fig. 4 converge to their microcanonical averages (in our case identical to the diagonal ensemble on the right hand side of Eq. (9)) via quantum chaotic diffusion across the instantaneous spectrum. Hence, the right hand side of Eq. (9) is, in practice, not any more dependent on the initial state because of the strong level mixing and the resulting irreversibility of the quench dynamics (see [38] for details).

4 Conclusions and perspectives

We presented a model of two energy bands coupled by internal particle-particle interactions and by an external Stark force. Our model may be realized with ultracold bosons in periodic optical lattices [16–18]. The non-intergrability of our quantum many-body system can be used to engineer complex dynamics. The temporal evolution of the system across a region of strong level clustering (avoided crossings) highlights the relevance of additional interband coupling terms. Furthermore,

it allows us to investigate the chaotic diffusion and non-equilibrium properties of single and two-body observables within the instantaneous quantum spectra. An advantage of our system is that the sweep across the chaotic spectral region at resonant tunneling conditions can be done rather fast (also because the region is small in parameter space, see e.g. Fig. 3(a)), and one does not have to wait asymptotically long for reaching thermalization. Together with possible experimental implementations with ultracold atoms, our results shed light on the understanding of thermalization in closed non-integrable systems through the eigenstate thermalization hypothesis [35–37]. Other applications include the study of reversibility properties [38, 40] and the deterministic production of entanglement [41] in driven many-body quantum systems.

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Key words. Bose-Hubbard model, quantum transport, ultracold atoms, Wannier-Stark, quantum chaos.

References

- [1] M. Rasatti (ed.), *The Hubbard model: Recent results* (World Scientific, 1991); W. Nolting, *Grundkurs Theor. Phys., Vielteilchentheorie Vol. 7* (Springer, 2009).
- [2] A. R. Kolovsky and A. Buchleitner, *Europhys. Lett.* **68**, 632 (2004).
- [3] D. Jaksch and P. Zoller, *Ann. Phys.* **315**, 52 (2005); M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen De, and U. Sen, *Adv. Phys.* **56**, 243 (2007); I. Bloch, J. Dalibard, and W. Zwerger, *Rev. Mod. Phys.* **80**, 885 (2008).
- [4] P. Jason and M. Johansson, *Phys. Rev. A* **85**, 011603 (2012), and references therein.
- [5] V. W. Scarola and S. Das Sarma, *Phys. Rev. Lett.* **95**, 033003 (2005).
- [6] J.-P. Martikainen and J. Larson, *Phys. Rev. A* **86**, 023611 (2012).
- [7] F. Hebert, Z. Cai, V. G. Rousseau, C. Wu, R. T. Scalettar, and G. G. Batrouni, *Phys. Rev. B* **87**, 224505 (2013).
- [8] S. Takayoshi, H. Katsura, N. Watanabe, and H. Aoki, *Phys. Rev. A* **88**, 063613 (2013).
- [9] A. Buchleitner and A. R. Kolovsky, *Phys. Rev. Lett.* **91**, 253002 (2003).
- [10] A. Tomadin, R. Mannella, and S. Wimberger, *Phys. Rev. Lett.* **98**, 130402 (2007).
- [11] S. Fölling, S. Trotzky, P. Cheinet, M. Feld, R. Saers, A. Widera, T. Müller, and I. Bloch, *Nature* **448**, 1029 (2007); S. Trotzky, P. Cheinet, S. Fölling, M. Feld, U. Schnorrberger, A. M. Rey, A. Polkovnikov, E. A. Demler, M. D. Lukin, and I. Bloch, *Science* **319**, 295 (2008).
- [12] T. Lahaye, C. Menotti, L. Santos, M. Lewenstein, and T. Pfau, *Rep. Prog. Phys.* **72**, 126401 (2009).
- [13] C. Albrecht and S. Wimberger, *Phys. Rev. B* **85**, 045107 (2012).
- [14] A. Kolovsky, J. Link, and S. Wimberger, *New J. Phys.* **14**, 075002 (2012).
- [15] N. Bartolo, D. J. Papoular, L. Barbiero, C. Menotti, and A. Recati, *Phys. Rev. A* **88**, 023603 (2013).
- [16] F. Meinert, M. J. Mark, E. Kirilov, K. Lauber, P. Weinmann, A. J. Daley, and H.-C. Nägerl, *Phys. Rev. Lett.* **111**, 053003 (2013).
- [17] F. Meinert, M. J. Mark, E. Kirilov, K. Lauber, P. Weinmann, M. Gröbner, and H.-C. Nägerl, *Phys. Rev. Lett.* **112**, 193003 (2014).
- [18] F. Meinert, M. J. Mark, E. Kirilov, K. Lauber, P. Weinmann, M. Gröbner, A. J. Daley, and H.-C. Nägerl, *Science* **344**, 1259 (2014).
- [19] J. Simon, S. Bakr, M. Ruichao, M. E. Tai, M. Preiss and M. Greiner, *Nature* **472**, 307 (2011).
- [20] W. S. Bakr, P. M. Preiss, M. E. Tai, M. Ruichao M, J. Simon, and M. Greiner, *Nature* **480**, 500 (2011).
- [21] Y.-A. Chen, S. Huber, S. Trotzky, I. Bloch, and E. Altman, *Nat. Phys.* **7**, 61 (2011); C. Kasztelan, S. Trotzky, Y.-A. Chen, I. Bloch, I. P. McCulloch, U. Schollwöck, and G. Orso, *Phys. Rev. Lett.* **106**, 155302 (2011).
- [22] C. Sias, A. Zenesini, H. Lignier, S. Wimberger, D. Ciampini, O. Morsch, and E. Arimondo, *Phys. Rev. Lett.* **98**, 120403 (2007).
- [23] A. Zenesini, C. Sias, H. Lignier, Y. Singh, D. Ciampini, O. Morsch, R. Mannella, E. Arimondo, A. Tomadin, and S. Wimberger, *New J. Phys.* **10**, 053038 (2008).
- [24] C. A. Parra-Murillo, PhD Thesis, Heidelberg University (2013).
- [25] C. A. Parra-Murillo, J. Madroñero, and S. Wimberger, *Phys. Rev. A* **88**, 032119 (2013).
- [26] T. Oka and H. Aoki, *Phys. Rev. B* **81**, 033103 (2010).
- [27] P. Plötz, J. Madroñero, and S. Wimberger, *J. Phys. B* **43**, 081001(FTC) (2010).
- [28] L.L. Chang, L. Esaki, and R. Tsu, *Appl. Phys. Lett.* **24**, 593 (1974); L. Esaki, *IEEE J. Quantum Electron.* **22**, 1611 (1986).
- [29] C. A. Parra-Murillo, J. Madroñero, and S. Wimberger, *Comp. Phys. Comm.* **186**, 19 (2015).
- [30] P. Plötz, P. Schlagheck, and S. Wimberger, *Eur. Phys. J D* **63**, 47 (2011).
- [31] G. Tayebirad, A. Zenesini, D. Ciampini, R. Mannella, O. Morsch, E. Arimondo, N. Lörch, and S. Wimberger, *Phys. Rev. A* **82**, 013633 (2010).
- [32] R. Blümel and U. Smilansky, *Phys. Rev. Lett.* **58**, 2531 (1987).
- [33] V. Zelevinsky, B. A. Brown, N. Frazier, and M. Horoia, *Phys. Rep.* **276**, 85 (1996).
- [34] L. F. Santos, F. Borgonovi, and F. M. Izrailev, *Phys. Rev. Lett.* **108**, 094102 (2012).
- [35] J. M. Deutsch, *Phys. Rev. A* **43**, 2046 (1991).
- [36] M. Srednicki, *Phys. Rev. E* **50**, 888 (1994).

- [37] M. Rigol, V. Dunjko, M. Olshanii, *Nature* **452**, 854 (2008); A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, *Rev. Mod. Phys.* **83**, 863 (2011); J. Eisert, M. Friesdorf, and C. Gogolin, arXiv:1408.5148; T. Langen, R. Geiger, J. Schmiedmayer, arXiv:1408.6377.
- [38] C. A. Parra-Murillo, J. Madroño, and S. Wimberger, *Phys. Rev. A* **89**, 053610 (2014).
- [39] J. Zakrzewski and M. Kuś, *Phys. Rev. Lett.* **67**, 2749 (1991); P. Plötz, M. Lubasch, and S. Wimberger, *Physica A* **390**, 1363 (2011).
- [40] T. Engl, J. Dujardin, A. Argüelles, P. Schlagheck, K. Richter, and D. Urbina, *Phys. Rev. Lett.* **112**, 140403 (2014).
- [41] M. Lubasch, F. Mintert, and S. Wimberger, *Phys. Rev. A* **84**, 063615 (2011).



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Study of doublon dynamics in optical lattices: spin chains and perspectives on quantum control



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Manuel Humberto Muñoz

Trabajo de grado
(Proyecto de investigación)

Facultad de Ciencias Naturales y Exactas
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Santiago de Cali, Octubre 22 del 2015

To my parents.

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Resumen

Motivados por los recientes experimentos en simulación cuántica y los avances en control coherente, ambos haciendo uso de gases cuánticos ultrafríos en redes ópticas, hemos estudiado temáticas particulares dentro de cada una de estas dos grandes áreas de la física cuántica moderna. Hemos dedicado la primer parte de esta tesis al estudio de modelos de magnetismo cuántico en una dimensión, especialmente la cadena XXZ, esto usando un modelo de Bose-Hubbard en la aproximación de una sola banda energética para bosones ultrafríos en una red óptica unidimensional. Establecimos una conexión entre el sistema atómico y el sistema magnético gracias a la propagación de una excitación, denominada dipolo (par ocupación doblón-hueco) del sistema atómico en el contexto de una red inclinada. En un segundo capítulo hemos explorado, con un modelo de Bose-Hubbard en la aproximación de dos bandas energéticas, la dinámica entre bandas que se puede establecer mediante la inclusión de un término que acople éstas a partir de ocupaciones dobles de los sitios de red en la banda inferior.

Abstract

Motivated by state-of-the-art experiments related to quantum simulation with ultra cold quantum gases and by the advances in the coherent control of ultracold matter, we theoretically address issues encircling two large areas of quantum physics: quantum simulation and coherent control. We devote the first chapter of this thesis to the study of one dimensional quantum magnetism, especially in the case of a XXZ Heisenberg model, by means of a single band Bose-Hubbard Hamiltonian. This research, based in the issue of ultracold quantum gases, clearly shows how the Feynmann's idea of quantum simulation works. As it will be shown a fundamental physical entity is the quasiparticle known as dipole, a pair of doublon-holon. A second chapter consider a similar type of dynamics but extending our model by including a second Bloch band to our Bose-Hubbard Hamiltonian. Here we explore possibilities of coherent control of the inter-band dynamics estrictly induced by the creation of doublons in the lowest energy Bloch band.

Chapter 1

Introduction

Since the beginning of quantum theory in the 1900's one of its major applications has been the study of matter. Nowadays we call it quantum matter and is one of the fields with the larger activity in both theory and experiment. The field had a boost with the development of modern techniques of cooling and trapping atoms that gave the Nobel prizes in physics to Steven Shu, John Phillips and Cohen-Tannoudji in 1997, followed by the successful achievement of the Bose-Einstein condensation [1–3] that was recognized with the Nobel price of 2001 to Eric Cornell, Wolfgang Ketterle, and Carl Wieman. That gave birth to a field known today as ultracold matter or ultracold atoms physics, which has had great success thanks to the possibilities of trapping and controlling quantum matter. Perhaps the first experimental proof of this high controllability was realized by Greiner *et al.* in 2002 [4] by showing how a sample of Rubidium atoms loaded in an optical lattice can undergo a phase transition between superfluid and Mott-insulator phases, and the reversibility of the process. Since then there have been extensive developments in this field, many of those are summarized and can be found in [5].

Since ultracold atoms loaded in optical lattices present the most cleanest setup available today, physicists have taken advantage of this to study complex condensed matter systems in regimes that are usually unreachable. This thanks to the implementation of today-called quantum simulators [6–9]. In addition, it is possible to study quantum matter dynamically, where usually this evolution mixes a large number of accessible states and it results in diffusion in the large Hilbert space of the problem [10]. However the high controllability of ultracold matter has allowed physicists to propose and test protocols for the coherent control of the time evolution of quantum systems, see for example [11–13].

1.1 Quantum simulation

The high difficulty of studying quantum systems by means of the computational tools available today has open a whole new field in quantum physics: Quantum simulation: As Richard Feynman said “Nature is not classical, dammit, and if you want to make a simulation of nature, you would better make it quantum mechanical, and by golly it is a wonderful problem, because it does not look so easy” [14]. At the core of this field we found a simple idea. As Feynman said, you can mimic the behavior of a quantum system with another more controllable one. The main objective

of having a more controllable system is to extract useful information about the behavior of the original system, information that can otherwise be screened or destroyed by noise or the influence of impurities and defects when studying the original system.

Although quantum simulation is a nice and simple idea, its implementation is not an easy task. First, a good system to be used as quantum simulator has to be found. Fortunately, modern techniques of cooling and trapping atoms even at the level of single ions [6], perfected superconducting cavities [15], photonic crystals [16], quantum dot and quantum circuits [17] form a set of possibilities for a choice of which is the best suited quantum simulator.

In this work we explore quantum simulation of one dimensional spin chains. Among the different systems that can be used as quantum simulators we will focus our attention on trapped ultracold quantum gases, for which a high degree of controllability has been reached, and in fact they have already been used to simulate some complex quantum systems as the Hofstadter Hamiltonian [8] and frustration in a spin system [9].

1.2 Ultracold atoms and optical lattices

Atomic systems cooled near to the absolute zero and periodic lattices made up by the superposition of counterpropagating laser beams offer one of the cleanest experimental setups we have today. The system is characterized by a high degree of control over the parameters of the systems, as was proven by the achievement of the Bose-Einstein condensation [1–3] and the phase transition between Mott insulator and superfluid states [4]. The possibilities for a system of ultracold atoms loaded in an optical lattice are huge. This can be seen from the active and dynamic growth this field has had over the last decade [5], and it has found its place in modern physics as an independent field of research rather than a branch of a larger field.

In the present section we want to introduce some basic notions related to ultracold atoms and optical lattices that are going to be helpful for understanding further developments presented in this thesis.

1.2.1 Bose-Einstein condensation

For many years the limit of how low the temperature of a sample can be reduced was placed at the temperature of liquid nitrogen. However, with the understanding of the statistical nature of temperature that barrier could be overcome. Nowadays we frequently hear of ultracold temperatures that goes up to hundredths of Kelvin's as near to the absolute zero as never before. All this thanks first to modern techniques of trapping matter as Magneto Optical Traps (MOT), optical lattices, or optical molasses. And some modern cooling techniques as Doppler cooling [18, 19], Sisyphus cooling (see Sec. 8.8 in [20]), and evaporative cooling [21]. The temperatures that have been reached with these techniques have been low enough to achieve and observe some exotic and novel phenomena. For example, Bose-Einstein condensation (BEC) [1–3] which occurs around 10^{-5} K in diluted gases, though this temperature depends on the confinement potential (chapter 1 of [22]).

As predicted by Bose and Einstein [23], a collection of bosons cooled near the absolute zero

undergoes a phase transition characterized by a massive occupation of one quantum state. This can be seen either from the singularity that appears in the occupation number when described by Bose-Einstein statistics, or when one or more eigenvalues $n_i(t)$ of the reduced single-particle density matrix is of the order of the total number of particles N

$$\rho(\mathbf{r}\alpha, \mathbf{r}'\alpha'; t) \equiv \langle \hat{\phi}^\dagger(\mathbf{r}, \alpha) \hat{\phi}(\mathbf{r}', \alpha') \rangle = \sum_i n_i(t) \chi_i^*(\mathbf{r}, \alpha; t) \chi_i(\mathbf{r}', \alpha'; t), \quad (1.1)$$

where $\hat{\phi}(\mathbf{r}, \alpha)$ represents bosonic field operators, with α denoting additional degrees of freedom, and $\chi_i(\mathbf{r}, \alpha; t)$ are single particle eigenfunctions of $\rho(\mathbf{r}\alpha, \mathbf{r}'\alpha'; t)$. Although BEC is not the main subject of the present work it helps us to understand up to what extend ultracold temperatures have allowed physics to advance in the study of quantum matter.

1.2.2 Optical lattices

An optical lattice can be understood as a periodic chain of atomic traps or potential wells in which atoms can be confined due to the interaction between their atomic dipolar momentum and the electric field. Periodic potentials are generated by the interference of counter-propagating laser beams, where the resulting standing wave has a period equal to $\lambda/2$ with λ the wavelength of the used laser. If the electric field of the laser varies spatially, then it generates an electric force on the atoms [24]

$$\mathbf{F}_{\text{dip}} = \frac{1}{2} \alpha(\omega_L) \nabla [|\mathbf{E}(\mathbf{r})|^2], \quad (1.2)$$

where $\alpha(\omega_L)$ is the atomic polarizability and ω_L is the field frequency. The interaction with the electric field makes the atoms experience a dipole potential given by [24]

$$V_{\text{dip}}(\mathbf{r}) = \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} \langle |\mathbf{E}(\mathbf{r})|^2 \rangle, \quad (1.3)$$

with $\Delta = \omega_L - \omega_0$ the detuning between the frequency of the field and the atomic transition frequency ω_0 . In the semi-classical treatment (particles are quantized and the radiation is treated classically), the atom is treated as a two level system with decay rate Γ . An optical potential exerts a repulsive force on the atoms if we have blue detuning $\Delta > 0$ and an attractive one if we have red detuning $\Delta < 0$ [5]. Periodic potentials in 2D and 3D can be realized by including extra pairs of counterpropagating laser beams and varying the angles between the pairs, typically those angles are set such that the pairs are orthogonal. Here, we are interested in a one dimensional profile created by the interference of two laser beams one with half the periodicity of the other. Thus, our dipole potential reads

$$V_{\text{dip}}(\mathbf{r}) = -V_0 [\cos(2k_L x) + s_0 \cos(4k_L x + \phi)], \quad (1.4)$$

with $s_0 = \frac{V_1}{V_0}$ and ϕ the phase difference between the two cosinusoidal waves of amplitudes V_0 and V_1 , respectively. With this potential profile we can effectively isolate the first two Bloch bands, that is, eigenenergy bands of a free particle in a periodic potential, and thus neglect the influence of higher bands on the system. Usually this set up is called a bichromatic potential or miniband structure, and its properties can be controlled by means of the parameters s_0 and ϕ [25]. In addition we can introduce an external field $V_{\text{WS}}(x) = Fx$ to define the known Wannier-Stark system [26].

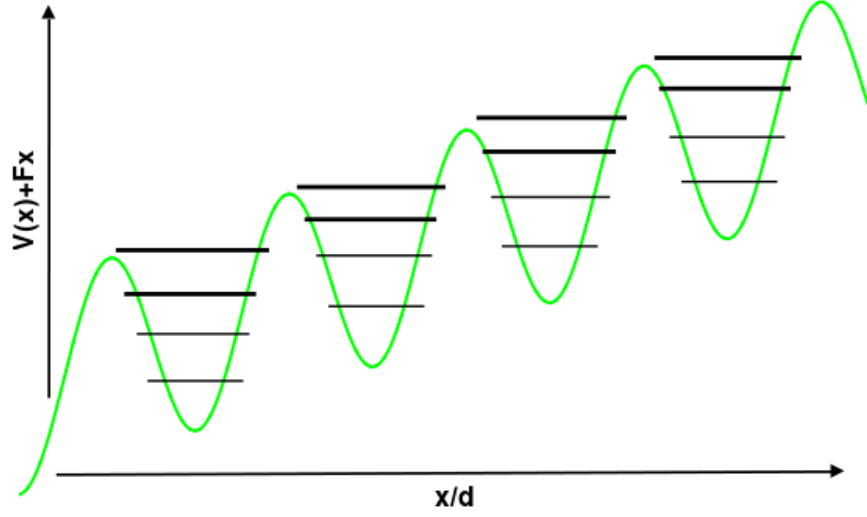


Figure 1.1: Schematic representation of a Wannier-Stark ladder in a monochromatic potential, including the first and second energy bands, the extra levels correspond to the raising in each band energy when there is more than one particle in a site. With $d = d_L$.

1.3 The Wannier-Stark system

1.3.1 Generalities

As mentioned in Sec. 1.2.2 by introducing an external field of the form $V_{\text{WS}}(x) = Fx$, we obtain the Wannier-Stark system. The Hamiltonian for the tilted lattice reads

$$\hat{H}_0 = -\frac{\hbar^2}{2m_0} \frac{\partial^2}{\partial x^2} + V(x) + Fx, \quad \text{with} \quad V(x + d_L) = V(x), \quad (1.5)$$

where F is a static external force that can be treated as a control parameter. The energies of the system are given by $\epsilon_l = E_0 + l d_L F$ [27], that is, the energies are obtained after translation over l wells of the lattice starting from the untilted system energy E_0 (see Fig. 1.1). On the other hand, the eigenstates of the system, commonly known as Wannier-Stark states are given by

$$|w_l\rangle = \sum_m J_{m-l} \left(\frac{J}{2d_L F} \right) \hat{a}_m^\dagger |0\rangle, \quad (1.6)$$

where J_{m-l} is a Bessel function of the first kind, and d_L is site separation distance or lattice constant. These states are localized functions in the coordinate space at the l th well of the lattice. Schematically, in presence of a fixed force, the energy levels of the Wannier-Stark system represent a set of equidistant states, called the Wannier-Stark ladder. For every energy band one can build the respective Wannier-Stark ladder and they are going to be separated by an energy gap, say $\Delta_{\beta\beta'}$ which varies as we go up in the band index β . The Hamiltonian in Eq. (1.5) is unbounded and with a continuum spectrum, *i.e.*, it does not have discrete eigenvalues [26]. Such contradiction finds its solution in the following argument, the spectrum is complex and the discrete

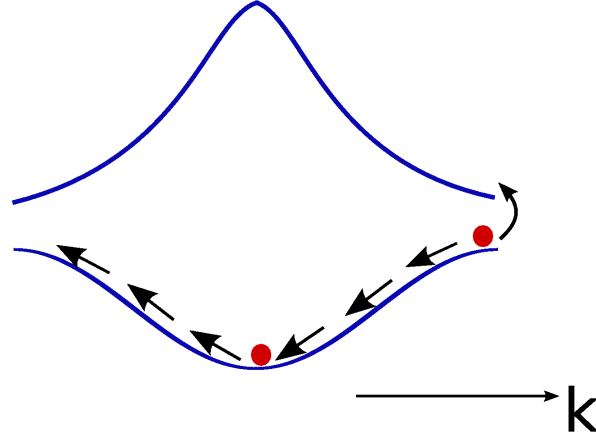


Figure 1.2: Schematic representation of the two main processes taking place in the Wannier-Stark system. Bloch oscillations within the first Brillouin zone and Landau-Zener tunneling to higher bands [26].

energies presented above are resonances embedded in the complex continuum

$$\epsilon_l^\beta = E_\beta + ld_L F - i \frac{\Gamma_\beta}{2}, \quad (1.7)$$

where Γ_β stands for the decay rate of each band that appears as a consequence of the unbounded spectrum and the Wannier-Stark states being metastable. Among the effects that arises as consequences of the external force, Bloch oscillations [28] are one of the most interesting. When we place a particle on a given lattice site it will get accelerated but without escaping from the lattice confinement. Instead it will undergoes Bloch oscillations with a period $T_B = 2\pi\hbar/d_L F$, known as the Bloch period. The other interesting process is Landau-Zener tunneling characterized by the promotion of particles lying in the lower band to higher energy bands, as we can see in Fig. 1.2: when the particle is undergoing Bloch oscillations there is a non-zero probability for it to get promoted to the upper band as it gets closer to the boundary of the first Brillouin zone. This effect gets naturally enhanced when two different Wannier-Stark ladders get maximally coupled via interband resonant tunneling at values of the force approximately given by

$$F_{|l-l'|} \approx \frac{\Delta_{\beta,\beta'}}{d_L |l-l'|}, \quad (1.8)$$

where $\Delta_{\beta,\beta'}$ is the energy separation between Bloch bands β, β' , and l, l' are the lattice sites whose lower(upper) and upper(lower) single particle levels become degenerate respectively. Following the notation of ref [29], we define $r = |l - l'|$ as the order of the resonance with $r \in \mathbb{Z}$. In the following, the vicinity of the Stark force F_r will be referred as the resonant regime.

1.4 The Bose-Hubbard model

In this work we will be dealing mainly with the single-band Bose-Hubbard model. However, here we are going to present some short passage on the derivation of the whole model for the many body problem (a more complete treatment can be found in chapter 3 of [30]). To do so, the general

Hamiltonian we need to study is [31],

$$H = \int \hat{\phi}^\dagger(x)[H_0(x) + Fx]\hat{\phi}(x)dx + g_{1D} \int \int \hat{\phi}^\dagger(x)\hat{\phi}^\dagger(x)\delta(x-x')\hat{\phi}(x')\hat{\phi}(x')dx dx', \quad (1.9)$$

where the second term stands for the allowed interaction between particles, which is reduced only to contact ones described by a pseudo-potential $g_{1D}\delta(x)$ [32]. In order to compute the transformation of each of the terms in Eq. (1.9) we need to define the proper field operators for our description. These operators can be defined in the following way. It is known that the periodic problem has its solution in the Bloch theorem, therefore $\psi_k^\alpha(x) = e^{ikx}u_k^\alpha(x)$ known as Bloch waves are solutions of

$$H_0\psi_k^\alpha(x) = E_k^\alpha\psi_k^\alpha(x), \quad \text{with} \quad H_0(x) = \frac{P^2}{2m} + V_0 \cos(2k_L x), \quad (1.10)$$

where k represents the quasi-momentum restricted to first Brillouin zone $-\pi/d_L \leq k \leq \pi/d_L$, α labels the band, and $u_k^\alpha(x)$ are functions with the same period as the lattice $u_k^\alpha(x + d_L) = u_k^\alpha(x)$. Here E_k^α are the eigenenergies, the so-called Bloch energy bands since k is continuous. Since the Bloch waves are periodic functions of the quasimomentum they can be expanded in a Fourier series. The expansion can be written as

$$\psi_k^\alpha(x) = \sqrt{\frac{d_L}{2\pi}} \sum_{x_l} w^\alpha(x - x_l) e^{ikx_l},$$

with expansion coefficients $w^\alpha(x - x_l) = \sqrt{\frac{d_L}{2\pi}} \int_{BZ} \psi_k^\alpha(x) e^{-ikx_l} dx, \quad (1.11)$

where the expansion coefficients are the known Wannier Functions [33]. In Eq. (1.11) $x_l = d_L l$ and l labels the lattice site. Some properties of the wannier functions are that they form an orthonormal set, and their parity is band dependent as follows

$$\int w^\alpha(x - x_l) w^{\alpha'}(x - x_{l'}) = \delta_{\alpha\alpha'} \delta_{ll'}, \quad (1.12)$$

$$w^\alpha(-x) = (-1)^{\alpha-1} w^\alpha(x). \quad (1.13)$$

The maximal localized Wannier functions that drop exponentially for $x < |d_L|$ [34] can be obtained once we have guaranteed the analyticity of the Bloch waves (for a deeper discussion on Bloch and Wannier functions see App. 1 of [35]). We write the field operators in terms of the Wannier functions to obtain a description of local single-particle states,

$$\hat{\phi}(x) = \sum_{\alpha=1}^{\infty} \sum_{l \in \mathbb{Z}} w^\alpha(x - x_l) \hat{a}_l^\alpha, \quad (1.14)$$

where the operator $\hat{a}_l^{\alpha\dagger}$ creates a boson in well l on band α . For short, we will speak site l and band α .

In the following and throughout this work we set $\hbar = 1$ and the energy unit is given by the recoil energy $E_r = k_L^2/2m$. Additionally, we use the rescaling

$$k \rightarrow k/k_L, \quad x \rightarrow x/d_L, \quad V_i \rightarrow V_i/E_r. \quad (1.15)$$

Now that we have a clear definition of the field operators we can proceed by writing down the explicit form of each of the terms in Eq. (1.9). The part corresponding to the periodic problem reads

$$\int \hat{\phi}^\dagger(x) [H_0(x) \hat{\phi}(x)] dx = \sum_{\alpha} \sum_{l,l'} J_{l-l'}^{\alpha} \hat{a}_l^{\alpha\dagger} \hat{a}_{l'}^{\alpha},$$

$$\text{with} \quad J_{l-l'}^{\alpha} \equiv \int w^{\alpha}(x - x_l) H_0(x) w^{\alpha}(x - x_{l'}) dx = \epsilon_{l-l'}^{\alpha}, \quad (1.16)$$

where $\epsilon_{l-l'}^{\alpha}$ represents the Fourier transformation of the eigenenergies. Here the contribution mediated by $J_{l-l'}^{\alpha}$ is referred as hopping because it destroys a particle in a site l and creates it on a site l' . Although there is a possibility for hopping between different bands by computing an expansion of the Bloch hamiltonian in terms of the creation (annihilation) operators, the coefficients for such transitions are zero due to the orthonormality of the Wannier functions (see Chap. 3 of [30]).

The term containing the external Stark force transforms under the field operators defined in Eq. (1.14) as

$$F \int \hat{\phi}^\dagger(x) x \hat{\phi}(x) dx = d_L F \sum_{\alpha,l} l \hat{a}_l^{\alpha\dagger} \hat{a}_l^{\alpha} + d_L F \sum_{\alpha,\alpha'} \sum_{l,l'} C_{l-l'}^{\alpha\alpha'} \hat{a}_l^{\alpha\dagger} \hat{a}_{l'}^{\alpha'},$$

$$\text{where} \quad C_{l-l'}^{\alpha\alpha'} \equiv \int w^{\alpha}(x - x_l) x w^{\alpha'}(x - x_{l'}) dx. \quad (1.17)$$

We see that the external field has the following effects: first it tilts the lattice, and second it couples different sites and bands. Here, the parity property in Eq. (1.12) implies that the external force does not couple different sites in the same band. Finally, the term of the interparticle interaction in Eq. (1.9) takes the form

$$g_{1D} \int \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \hat{\phi}(x) dx = \sum_{\alpha_1, \dots, \alpha_4} \sum_{l_1, \dots, l_4} M_{l_1 \dots l_4}^{\alpha_1 \dots \alpha_4} \hat{a}_{l_1}^{\alpha_1\dagger} \hat{a}_{l_2}^{\alpha_2\dagger} \hat{a}_{l_3}^{\alpha_3} \hat{a}_{l_4}^{\alpha_4},$$

$$\text{with} \quad M_{l_1 \dots l_4}^{\alpha_1 \dots \alpha_4} \equiv g_{1D} \int w^{\alpha_1}(x - x_{l_1}) w^{\alpha_2}(x - x_{l_2}) w^{\alpha_3}(x - x_{l_3}) w^{\alpha_4}(x - x_{l_4}) dx. \quad (1.18)$$

Since the Wannier functions are maximally localized on the lattice sites the dominant contributions to the interaction are on-site ones given by $M_{llll}^{\alpha_1 \dots \alpha_4}$. However, the parity of the Wannier functions force many of these coefficients to vanish. A more broad discussion on the Bose-Hubbard coefficients can be found in Chap. 1 of [36].

As stated at the beginning of this section our main object of study is the single-band Bose-Hubbard Hamiltonian. This model is a reduction of the full many-body problem presented here when we truncate the number of energy bands to one, and in terms of the previous expressions it reads,

$$H = \sum_{l,l'} J_{l-l'} \hat{a}_l^\dagger \hat{a}_{l'} + d_L F \sum_l l \hat{a}_l^\dagger \hat{a}_l + \sum_l M_{llll}^{1111} \hat{a}_l^\dagger \hat{a}_l^\dagger \hat{a}_l \hat{a}_l, \quad (1.19)$$

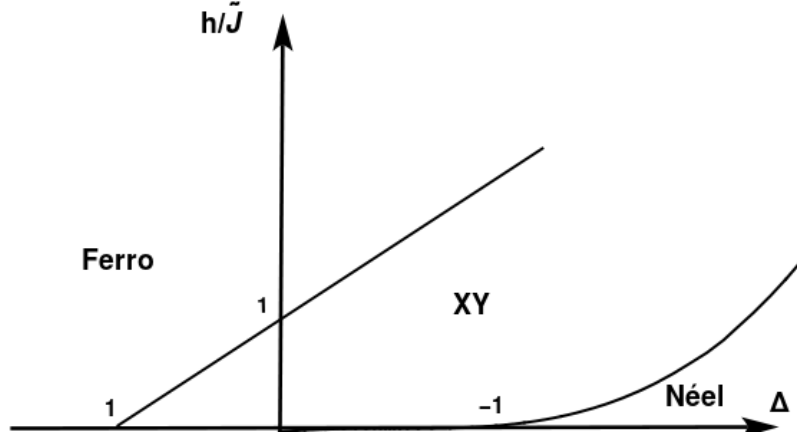


Figure 1.3: Phase diagram of the XXZ-model for $S = 1/2$ in presence of an external field in z -direction [37].

1.5 Some properties of the XXZ-chain model

The study of one-dimensional quantum magnetism is one of the more prolific areas in condensed matter physics. Both, because it provides physicists with a better understanding of strong correlated systems and because it has direct application on the study of real materials. One paradigmatic model in the study of these quantum systems is known as the Heisenberg XXZ-chain model. This model features two different phases. The ferromagnetic phase and the anti-ferromagnetic phase or Néel phase.

Here, we have special interest in a $S = 1/2$ XXZ chain in presence of an external field in the z -direction. The specific Hamiltonian reads

$$H = \tilde{J} \sum_n (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z) + h \sum_n \sigma_n^z, \quad (1.20)$$

where σ_n^i , $i = x, y, z$ are the usual Pauli matrices, $\tilde{J}$ the super exchange coupling, Δ the anisotropy parameter, and h the strength of the magnetic field. Additionally, the most important feature of this model is that the longitudinal coupling between spins interchanges up and down spins, $|\uparrow\downarrow\rangle \rightarrow |\downarrow\uparrow\rangle$. This coherent exchange of the positions of two spins in adjacent sites is known as superexchange (see [37]).

The phase diagram of the XXZ-Heisenberg model in presence of a z -external Zeeman field can be viewed in Fig. 1.3, where the regions for each of the three main phases, ferromagnet, antiferromagnet and XY are delimited. A more deep presentation of this phase diagram can be found in [38].

We have special interest in the two opposed phases of the model, both presented in Fig. 1.3. The ferromagnetic phase appears for $\Delta < -1$. In this phase the XXZ chain exhibits a ground state where all spins point either up or down, with total magnetization different from zero. The introduction of the external Zeeman field does not alter the system because the total spin component σ_{tot}^z commutes with the Hamiltonian leading only to an increment in the energy without

altering the wave functions. However, it does stabilize the ground state and lift the broken spin inversion symmetry. Here the basic excitations of the ground state are called magnons. They are single impurities that breaks the large order of the ferromagnet and can, as a consequence of the superexchange, travel along the chain.

The Néel or antiferromagnetic phase appears for $\Delta > 1$. This phase features, in the thermodynamic limit, a two-fold degenerated ground state with zero total magnetization but finite sublattice magnetization, $N^z = \sum_n (-1)^n \sigma_n^z$. In contrast with the Ferromagnetic phase quantum fluctuations prevent the order from being complete since the sublattice magnetization does not commute with the XXZ Hamiltonian.

The excitations of these phase can be understand thinking on the ground states at the thermodynamic limit. One starts there from either of the two degenerated ground states and breaks only one bond one will end up with a cluster of three spins oriented in the same fashion. Later the superexchange will change this configuration by another one where the cluster has recovered its alternating order but on each side of the cluster there will be two small clusters of two spins oriented in the same fashion. These are known as two-domain walls and as for the magnons in the ferromagnet they can propagate along the chain. One can see that for a finite system depending on how many bonds you break in the antiferromagnetic ground state you could arrive to a similar state where a single spin impurity propagates.

There is an additional phase that lies just in the middle of the two previously mentioned phases. However, for the sake of keeping the discussion in this thesis simple and related to what will be presented in incoming chapters we are not dealing with the XY phase here. Nevertheless we recommend [37] for the interested reader.

1.6 The rest of this work

In Chap. 1 we presented some necessary concepts for the later developments of this work. Mainly, they are ultracold atoms and optical lattices in Sec. 1.2, the one-dimensional Bose-Hubbard model in Sec. 1.4, and the Heisenberg XXZ-chain model in Sec. 1.5. The subsequent chapters are devoted to the study of two main areas. First, quantum simulation, in particular the construction of bridges between one dimensional ultracold atomic systems and one dimensional magnetism. Second, coherent control, taking advantage of the controllability of ultracold atomic systems to propose and test routes towards the achievement of some states of interest. To do that the rest of this work is divided as follows.

In Chap. 2 we present one already proposed and tested quantum simulation of the antiferromagnetic Ising chain in transverse and longitudinal fields, and the link between second order processes in the single-band Bose-Hubbard model and spin transport in the form of spin waves in the Heisenberg XXZ-model. Later, in Chap. 3 we introduced the two-band Bose-Hubbard Hamiltonian with a doublon-mediated interband coupling, and the respective dynamical study was done using two different techniques, shaking the lattice and parametric evolution. All this looking forward to the achievement of some specific states. We include three appendices. App. A deals with some generalities of the Schrieffer-Wolff transformation and its application to the models studied in the two core chapters of this thesis. App. B presents a collection of results from Chap. 3 with the parametric evolution. App. C presents two different issues: In Sec. C.1 a more extensive ex-

planation of the procedure we used to study the interference time in Chap. 2 is presented, and in Sec. C.2 the situation of having an initial state with a dipole in the middle of the lattice is studied.

Chapter 2

Quantum simulation with the single-band Bose-Hubbard model

2.1 From the single-band Bose-Hubbard model to a Ising chain

One big question that arises when you want to simulate a spin system with bosons is how to restrict the otherwise large number of degrees of freedom allowed to bosonic particles. To find the proper regime in which the Hilbert spaces of the spin system and the bosonic system have commensurable dimensions is usually a hard task. However, it has been shown [39] and proven experimentally [7] that in the single band approximation of the Bose-Hubbard model, as presented in the previous chapter (Eq. (1.19)), it is indeed possible to find a proper regime in which the situation mentioned above occurs for the spin and bosonic systems. In the following sections we will present this regime and the quantum simulation that can be built working on it.

2.1.1 Mott insulator in a strong tilted lattice

The single-band Bose-Hubbard model was presented in Eq. (1.19). This model features two phenomenologically distinct phases, a superfluid one and an insulator one referred to as Mott insulator. This phase features negligible hopping amplitude (which translates to deep potential wells) and a definite average density of particles, with the site occupation number fixed. This is the phase we have interest to work with in the present chapter.

Our study is based on the B-H Hamiltonian but written in a slightly different form, where the operators accounting for the interaction part are written such that they stand for the double occupation of individual lattice sites. Such Hamiltonian reads

$$\hat{H} = -J \sum_l (\hat{a}_{l+1}^\dagger \hat{a}_l + \text{h.c.}) + \frac{U}{2} \sum_l \hat{n}_l (\hat{n}_l - 1) + F \sum_l l \hat{n}_l, \quad (2.1)$$

where J is the hopping amplitude between next neighboring sites, U is the interparticle energy interaction, F is the strength of the external field, $\hat{a}_l^\dagger$ ($\hat{a}_l$) are bosonic creation (annihilation) operators, and $\hat{n}$ is the boson number operator. In particular, we set $d_L = 1$. Usually the dynamics of this Hamiltonian is rather complex and can lead to chaotic behavior [30].

Here we are interested in the strong Stark forces regime and by that we mean

$$J, \quad |U - E| \ll U, \quad E. \quad (2.2)$$

We will focus our study in a initial state given by a Mott insulator with unitary filling ($n_0 = 1$), that is, we will work with deep wells such that $U \gg J$ and a mean density of particles per well equal to one. In other words the filling factor N/L (number of particles over number of sites) is going to be fixed at one. Even though we are in presence of a strong external field the Mott phase is stable [39]. The stability of the Mott state under the presence of the tilt is justified as long as the transition between untilted system and the tilted one is done via a sudden quench. In this case we can energetically lock the Mott state regardless the presence of the tilt.

In the strong Stark forces regime we basically turned the external force to a point in which it is comparable with the energy given by the interparticle interaction. In other words the external force is bringing the energy level of a site into an energy degeneracy with the energy level of two particles in a next neighboring site. Then, the large Hilbert space of our problem can be effectively reduced to a manifold of states that are resonantly coupled to the Mott state. The reduction is way advantageous and we can see it from the calculation of the dimension of the Hilbert space for the resonant manifold given by,

$$\dim(H_{n+1}) = \dim(H_n) + \dim(H_{n-1}), \quad \text{with} \quad \dim(H_1) = 1, \quad \text{and} \quad \dim(H_2) = 3, \quad (2.3)$$

where n stands for the number of lattice sites. This expression can be figured out by thinking on the number of different resonant states available from the Mott state for unitary filled lattices ($N/L = 1$) of length $L = 1, 2, 3, \dots$ with periodic boundary conditions. We have to remember that the expression presented in Eq. (2.3) works only for the case of unitary filling.

The states that belong to the resonant manifold are accessible from the Mott state by means of a resonant transition [39, 40]. Those states given by the movement of a particle from one site to the next neighboring site when the energy levels of a single particle and two particles respectively are degenerated due to the external force. In Fig. 2.1 we present an example of such a transition. These resonant transitions are called dipole transitions, because in the process we have created a pair holon-doublon (a vacancy and two particles in next neighboring sites) as a consequence of the resonance. These dipoles are the only allowed deformations of the Mott state in our regime of interest [39] and together they constitute a good subspace of accessible states of our system.

The restriction on having further transitions once we have created the dipole is given by the fact that the external force does not couple the energy level of two particles with any other energy level in the direction of the tilt. Hence, we can treat the dipole as a whole entity in itself. To write an effective Hamiltonian it is convenient to introduce an operator that stands for the process of create or destroy a dipole. We define it as

$$\hat{d}_l^\dagger = \frac{\hat{a}_{l+1}^\dagger \hat{a}_l}{\sqrt{n_0(n_0 + 1)}}, \quad (2.4)$$

where n_0 is the average occupation that we set to one [39]. By introducing this operators we have reduced our problem to work in the subspace of dipole states and in such a scenario we can write

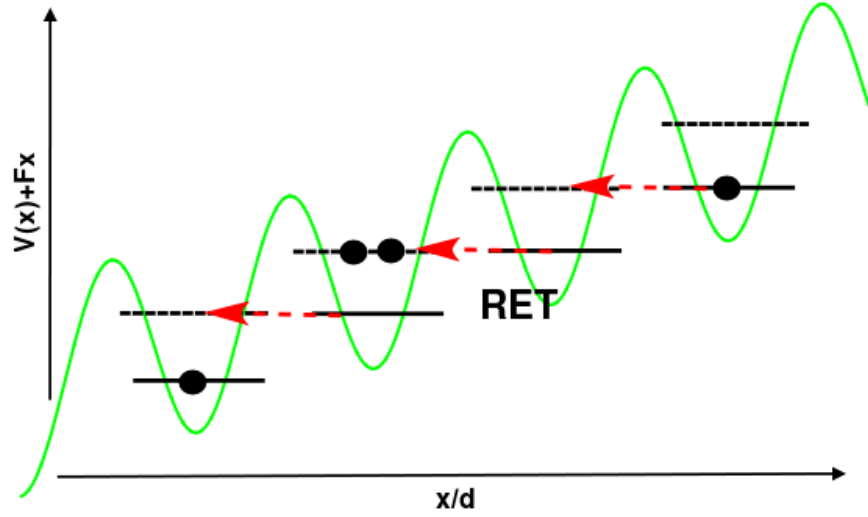


Figure 2.1: Schematic representation of a resonant transition as a consequence of the strong Stark force bringing close in energy the levels of a single particle (solid line) and two particles (dashed line) in next neighboring sites, such transitions happened usually at $U \approx E$. This process is known as resonant enhance tunneling (RET). With $d = d_L$.

an effective Hamiltonian for the Bose-Hubbard model in Eq. (2.1). It reads

$$\hat{H}_d = -J\sqrt{2} \sum_l (\hat{d}_l^\dagger + \hat{d}_l) + (U - E) \sum_l \hat{d}_l^\dagger \hat{d}_l, \quad (2.5)$$

where we can either create or destroy a dipole with an amplitude J and once we have created it, it will have an energy $U - E$. We may notice that a single site of the lattice can support only one dipole and once we have a dipole in a given site we cannot create a dipole in the next neighboring site. Therefore, the Hamiltonian in Eq. (2.5) has the following restrictions:

$$\hat{d}_l^\dagger \hat{d}_l \leq 1 \quad \text{and} \quad \hat{d}_{l+1}^\dagger \hat{d}_{l+1} \hat{d}_l^\dagger \hat{d}_l = 0. \quad (2.6)$$

The reduction of the Hilbert space of our system to the dipole subspace and the restrictions in Eq. (2.6) will allow us to build a spin chain simulator.

2.1.2 Antiferromagnetic Ising model in transverse and longitudinal fields

From the restrictions on the process of dipole creation we can extract the following information: (1) the number of dipoles per site is either one or zero. Therefore, this can be related to a system with two occupation values that can be understood in terms of spins. (2) The second restriction is reminiscent of a next neighboring interaction, since we cannot have dipoles in next neighboring sites. With this two statements in mind we define the following mapping between dipoles and spins:

$$\sigma_l^z = 1 - 2\hat{d}_l^\dagger \hat{d}_l, \quad \sigma_l^x = \hat{d}_l^\dagger + \hat{d}_l, \quad \text{and} \quad \sigma_l^y = i(\hat{d}_l^\dagger - \hat{d}_l). \quad (2.7)$$

An schematic representation of the spin mapping is presented in Fig. 2.2.

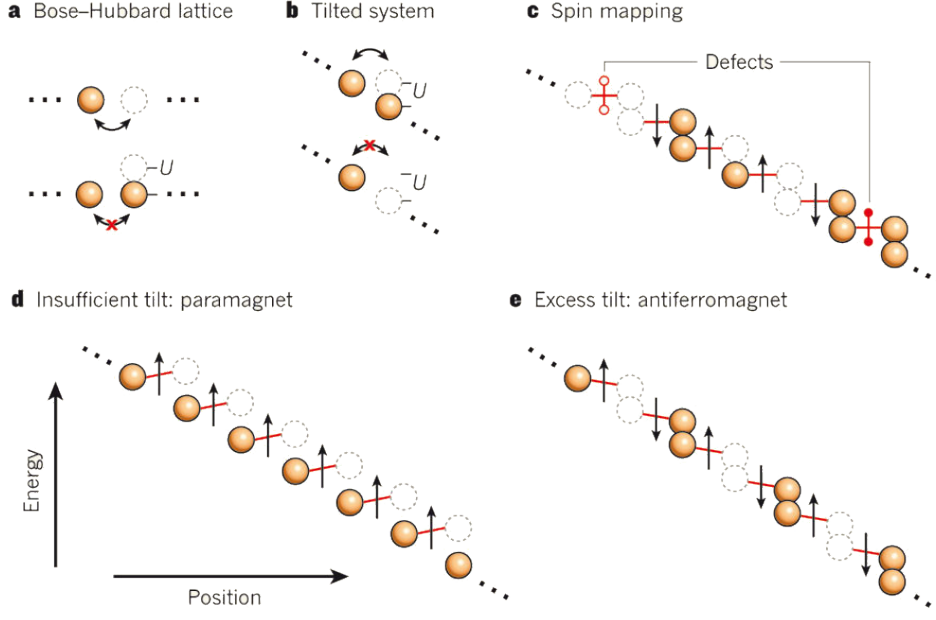


Figure 2.2: (a) Schematic representation of the different processes that take place within the single-band Bose-Hubbard model. (b) Representation of the allowed processes for the tilted single band system. (c) Spin mapping. (d) and (e) Two different phases exhibited by the Ising model in transverse and longitudinal field Eq. (2.8); for insufficient tilt (d) we have a paramagnetic phase and for excess of tilt (e) we have an antiferromagnetic phase [41].

We can thus write our dipole Hamiltonian in terms of spin operators, but for that it is useful to implement the constraint forbidding dipoles in next neighboring sites in the Hamiltonian such that we will have a next neighbor interaction. To do that we will include an energy term of the form $W \hat{d}_{l+1}^\dagger \hat{d}_{l+1} \hat{d}_l^\dagger \hat{d}_l = \frac{W}{4} (1 - 2\sigma_l^z + \sigma_{l+1}^z \sigma_l^z)$. After some algebra the Hamiltonian can be brought into the following form in terms of spin operators:

$$\hat{H}_s = \tilde{W} \sum_l \left(\frac{1}{2} \sigma_{l+1}^z \sigma_l^z - h_x \sigma_l^x - h_z \sigma_l^z \right). \quad (2.8)$$

This model is usually referred to as the Ising model in a transverse and longitudinal fields [42]. Here, $h_x = 2\sqrt{2} \frac{J}{\tilde{W}}$ and $h_z = 1 - \frac{\Delta}{\tilde{W}}$, with $\Delta = E - U$, are the strengths of the longitudinal and transverse fields, respectively, and $\tilde{W} = \frac{W}{2}$. It is known that the interplay between the magnitude of the two fields drives a phase transition between a paramagnetic phase and an antiferromagnetic phase. Interestingly this phase transition can be in general classified as a second order phase transition [42]. However, there is a special point (multi critical point) at which the phase transition is a first order one. This is precisely the point where the parameters h_x , h_z and Δ take the values given above. That means, our simulation works precisely at the critical point [7].

To see a little bit clearer how the simulation we have presented in the last and present sections works, let us take a look at the dipole Hamiltonian, but first we define a control parameter given

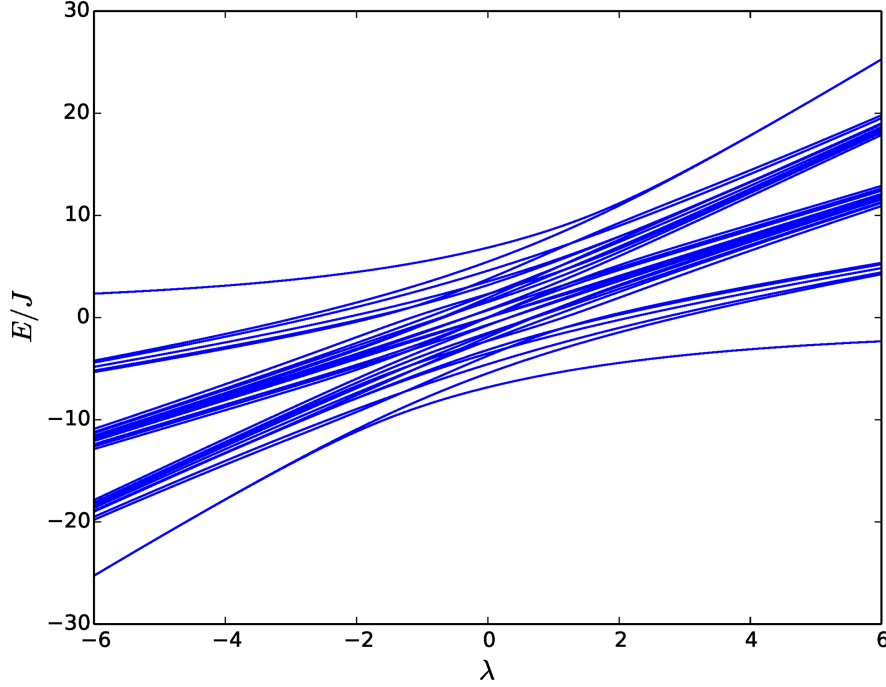


Figure 2.3: Energy spectrum for a chain with eight sites and unitary filled as a function of λ . We can see that the ground state exhibits two different behaviors, one for $\lambda \ll 1$ and for $\lambda \gg 1$, that we relate with a paramagnetic phase and an antiferromagnetic phase of the spins model. Here the dimension of the Hilbert space is $\dim(\hat{H}) = 47$.

by $\lambda = \frac{U-E}{J}$ that varies continuously. With that change the Hamiltonian now reads

$$\hat{H}_d = -\sqrt{2} \sum_l (\hat{d}_l^\dagger + \hat{d}_l) + \lambda \sum_l \hat{d}_l^\dagger \hat{d}_l. \quad (2.9)$$

The explicit λ dependence of this Hamiltonian allows us to apply the definition of quantum phase transition given in [43]. In Fig. 2.3 we have computed the spectrum of the Hamiltonian in Eq. (2.9) for a chain of eight sites and unitary filling as a function of λ . If we focus our attention to the ground state we see that it exhibits two different behaviors (for further details see [43]). For $\lambda \gg 1$ the system is in a state with no dipoles and one particle per site, which corresponds to a paramagnetic phase according to the mapping presented in Fig. 2.2. For values of $\lambda \ll 1$ the ground state is two-fold degenerated, where these states are one with dipoles in every odd site and one with dipoles in every even site. Either of them corresponds to an antiferromagnetic phase, hence we can see that as we vary λ by changing the external force we drive the system from a paramagnet to an antiferromagnet.

The quantum simulation we have just presented was verified experimentally in 2011 in Greiner's ultracold atoms laboratory at Harvard University [7]. There, they could observe the transition from a paramagnet to an antiferromagnet and backwards as they ramp up and down the magnitude of the external field. For some clarifying comments on the methods implemented in [7] we recommend [41].

2.2 Signatures of spin-waves and interference in the single-band B-H model

In Sec. 2.1.2 we saw how it is possible to map a Bose-Hubbard model to a Quantum Ising chain in presence of both transverse and longitudinal fields. That was done by taking advantage of the natural resonant excitations of the Mott state once we energetically lock it in the tilted system. However, we have not provided further insights on this excitations. The objective of the present section is to explore the dynamics of those excitations.

As we have seen those excitations are a pair of holon-doublon called dipoles [39]. The first fact that was known is that dipoles are a whole structure on itself and they can move as such [39]. Therefore, a natural question that arises is whether one can have propagation of such an excitation when starting from a state with one dipole on one edge. Besides the time evolution of the system, the incoming sections are focused on the study of the particular situation outlined above when open boundary conditions are taken into account.

2.2.1 Second order processes in the single-band B-H model

As stated above we performed the time evolution of our system with an initial condition given by $|11\dots1120\rangle$, where the lattice was tilted upwards ($F > 0$), and far from any resonance. We take $F = xU + \delta$, where $x \in [3, 4)$, and δ a proper offset to guarantee that the system was outside of any kind of resonance. This last constraint was imposed in order to look for phenomena not considered so far in this work (notice that the case $F \approx U$ was studied in Sec. 2.1). In Fig. 2.4 we have plotted the population along the lattices sites, $\langle \hat{n}_l \rangle = \langle \psi(t) | \hat{n}_l | \psi(t) \rangle$, for the time evolution performed.

All the simulations where performed for different sets of Bose-Hubbard parameters. In particular the results presented in this section were obtained with the parameters of [44]. Regarding the range of values we have chosen for x it was a range where we are away of the situation presented in Sec. 2.1 and with a not to large tilt such that the wells were completely isolated one from another.

From Fig. 2.4 we can see that the time evolution has two major characteristics. First, it allows the dipole to propagate all along the lattice, though the initial information about the localization of it is not completely preserved through the propagation. Second, once the dipole has completed one transit it starts to propagate backwards but before completing the second transit it interferes with itself. That manifested itself as the splitting of the probability distribution of single site occupation, as can be seen in Fig. 2.4. This sort of behavior can be linked to the so called quantum carpets [45]. The link is more easily done in the limit of lattices with a large number of sites (as we will see in Sec. 2.2.4). Let us talk first about the dipole propagation. If we take a look to the Bose-Hubbard Hamiltonian in Eq. (2.1) it is easy to see that this model does not allow transport of particles beyond hopping and resonant tunneling. However, we are seeing that the dipole as whole jumps from one site to the next-neighboring one and so on until it has reach the opposite edge of the chain. Actually it evolves as $|111120\rangle \rightarrow |111201\rangle \rightarrow |112011\rangle \rightarrow |120111\rangle \rightarrow |201111\rangle$. Here the movement of the dipole can only be realized by two successive hoppings. Hence, we have a second order tunneling process. At this point one can be wondering, how to extract the relevant

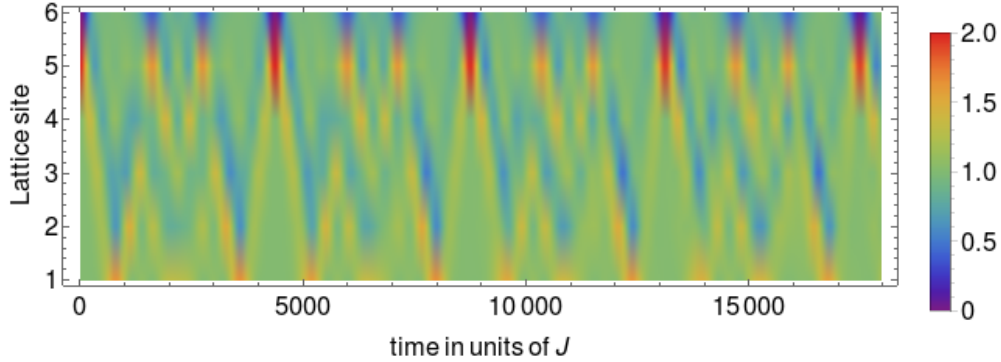


Figure 2.4: Time evolution of the population for the lattice sites of the chain. The color scale goes from blue for zero particles to red for two particles on a given lattice site. The initial state was $|111120\rangle$ and the value of the Stark force in our simulations was $F = 3U + \delta$.

physics from our model? Usually that can be done by a perturbative approach, and it is indeed the direction we will take here. In particular, we will be using the known Schrieffer-Wolff transformation [46, 47]. The explicit calculation of the second order correction using S-W transformation can be found in App. A and the construction of the effective model is done in Sec. 2.2.2.

What about interference? Well, naturally the wave function (WF) of the dipole acquires a phase as it evolves and propagates through the lattice. As it will be justified later, the dipole WF is build up by parts that travel with different velocities and as such they arrive at the edges at different moments in time. Therefore, as the evolution proceed there is an effect of self interference of matter waves that gives rise to the pattern observed in Fig. 2.4.

2.2.2 Effective model

In App. A we found the proper operator that accounts for the hopping of dipoles, it reads

$$O_{\text{SO}} = 2J^2 \left(\frac{1}{F-U} + \frac{1}{F} \right) (\hat{a}_{l+2}^\dagger \hat{a}_{l+1} \hat{a}_l^\dagger \hat{a}_{l+1} + \text{h.c.}), \quad (2.10)$$

where $\hat{a}_l$ ($\hat{a}_l^\dagger$) are bosonic annihilation (creation) operators. Following the form of the Schrieffer-Wolff transformation the effective model (see Eq. (A.5)) reads

$$H_{\text{eff}} = \frac{U}{2} \sum_l \hat{n}_l(\hat{n}_l - 1) + F \sum_l l \hat{n}_l + 2J^2 \left(\frac{1}{F-U} + \frac{1}{F} \right) \sum_l (\hat{a}_l^\dagger \hat{a}_{l+2}^\dagger \hat{a}_{l+1} \hat{a}_{l+1} + \text{h.c.}). \quad (2.11)$$

We have thus an explicit mechanism for the propagation of dipoles and the hopping of single particles is no longer part of the Hamiltonian as a natural consequence of the Schrieffer-Wolff transformation.

One interesting point about the Hamiltonian in Eq. (2.11) is that the center of mass is a conserved quantity (which can be easily proven). That is, $[H_{\text{eff}}, \sum_l l \hat{n}_l] = 0$. Therefore, if we go to the interaction picture in terms of the external Stark field we get

$$H_I = e^{-i\hat{A}t} H_{\text{eff}} e^{i\hat{A}t} - \hat{A}, \quad \text{with} \quad \hat{A} = F \sum_l l \hat{n}_l, \quad (2.12)$$

and thanks to the fact that the center of mass is a conserved quantity, the explicit form of the effective Hamiltonian in the interaction picture reads

$$H_I^{\text{eff}} = \frac{U}{2} \sum_l \hat{n}_l(\hat{n}_l - 1) + 2J^2 \left(\frac{1}{F - U} + \frac{1}{F} \right) \sum_l (\hat{a}_l^\dagger \hat{a}_{l+2}^\dagger \hat{a}_{l+1} \hat{a}_{l+1} + \text{h.c.}), \quad (2.13)$$

where this last expression is telling us that seeing from the excitations point of view the lattice is no longer tilted, and actually what the dipoles experience is a translationally invariant lattice.

2.2.3 From the single-band B-H model to Heisenberg XXZ-model

One of the main goals of this thesis is the study of spin chains by means of Bose-Hubbard like models. To that end we want to take advantage of the effective model accounting for the hopping of dipoles in Eq. (2.11) and connect it to the Heisenberg XXZ-chain.

First, we will work again with the definition of dipole operators that was given in Eq. (2.4). This definition allows us to rewrite the effective Hamiltonian as

$$H_d = (U - F) \sum_l \hat{d}_l^\dagger \hat{d}_l + 4J^2 \left(\frac{1}{F - U} + \frac{1}{F} \right) \sum_l (\hat{d}_{l+1}^\dagger \hat{d}_l + \text{h.c.}), \quad (2.14)$$

where the term accounting for the contact interaction has disappeared because now we are dealing with excitations and we do not care if such excitations are build up with two or more particles, we only care about the presence or absence of dipoles on a given lattice site. Therefore, the possibilities for the values of occupation number are now zero or one (see Eq. (2.6)). As stated in Sec. 2.2.2 seeing from the dipole point of view, the lattices is not tilted and we arrive to a translational invariant model.

The second step takes advantage of the already constructed mapping from dipoles to spins defined in Eq. (2.7) of Sec. 2.1.2, with the additional fact that such mapping defines the spin ladder operators as

$$\sigma_l^+ = 2d_l, \quad \text{and} \quad \sigma_l^- = 2d_l^\dagger. \quad (2.15)$$

By going through the mapping onto spin operators we arrive to the Hamiltonian

$$H_s = \frac{W}{4} \sum_l \sigma_{l+1}^z \sigma_l^z + 2J^2 \left(\frac{1}{F - U} + \frac{1}{F} \right) \sum_l (\sigma_{l+1}^x \sigma_l^x + \sigma_{l+1}^y \sigma_l^y) - \frac{1}{2} (W - (F - U)) \sum_l \sigma_l^z, \quad (2.16)$$

which is nothing but the Heisenberg XXZ-chain in presence of an external magnetic field as introduced in Chap. 1, but now all the model parameters are written in terms of the initial Bose-Hubbard parameters. We have the precise identification of the superexchange coupling $\tilde{J} = 2(\frac{2J^2}{F-U} + \frac{2J^2}{F})$, the magnetic field strength $h = \frac{1}{2}(W - (F - U))$, and the anisotropy parameter $\Delta = \frac{W}{4J}$. This identification of the XXZ-chain parameters with the Bose-Hubbard parameters instantly fixes a value to the ratio $\tilde{J}/h$ and Δ . Therefore, we can easily place our model in the phase diagram of the XXZ-chain (see Fig. 1.3). From the parameters we have used in the simulations we have $\tilde{J}/h \approx \tilde{J}$ since $h \approx 1$, and $\Delta \gg 1$. It implies that our XXZ-chain is deep inside the Néel phase. As a test of this we compute the time evolution of our system starting from a ferromagnet, *i.e.*, $|\uparrow\uparrow \dots \uparrow\rangle$, and find that the system does not evolve. Once we have placed

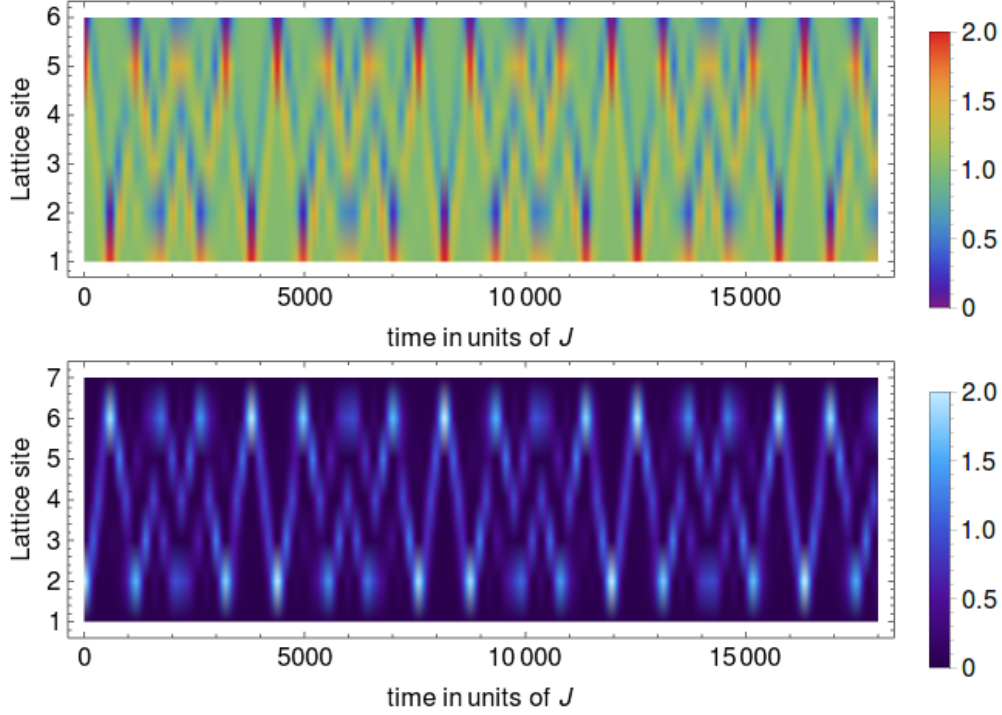


Figure 2.5: Top: Evolution for the population for the different lattice sites in the case of the effective Hamiltonian written in terms of boson creation (annihilation) operators in Eq. (2.11). The initial condition was $|111120\rangle$ and the rest of the parameters as in Fig. 2.4. Bottom: Evolution of the population for each of the different lattice sites with the effective XXZ-model in Eq. (2.16). The initial condition was $|\downarrow\downarrow\downarrow\downarrow\uparrow\downarrow\rangle$, the rest of parameters as in Fig. 2.4. In both cases we re-scale the time scale of the two effective models in order to compare them with the results obtained with the full model, since naturally those time scales do not coincide.

our model in the Néel phase (see Sec. 1.5 and Fig. 1.3) it is easy to see why we have propagation of dipole, by understanding this as propagation of a spin impurity after we have broken the necessary number of bonds starting from an antiferromagnetic ground state.

Now the question is whether or not this effective model, the one in Eq. (2.11) and the one in Eq. (2.16), reproduces the two main characteristics of the time evolution presented in Fig. 2.4. To answer that question we perform the respective time evolution with both effective Hamiltonians, starting with the proper initial condition. The results can be seen in Fig. 2.5, where the time scales of both plots were re-scaled in order to make clearer the comparison between the effective models and the original one.

In the following we will focus on the effective spin model. As we have seen in Sec. 1.5, in any of the two extremal phases (ferromagnetic and Néel) of the XXZ-chain we have possibilities of spin-waves. Our model is in the Néel phase and from the lower panel of Fig. 2.5 we see that indeed the propagation of the impurity occurs. However, as a consequence of the propagation, coherence triggers interference. But interference in the effective case appears later than in the full model. This is because we are moving a single particle and in order to interfere with itself after it bounces back on the edge it needs more time because the accumulation of phase in the wave function as it moves through the lattice takes more time (there is only one object traveling). The

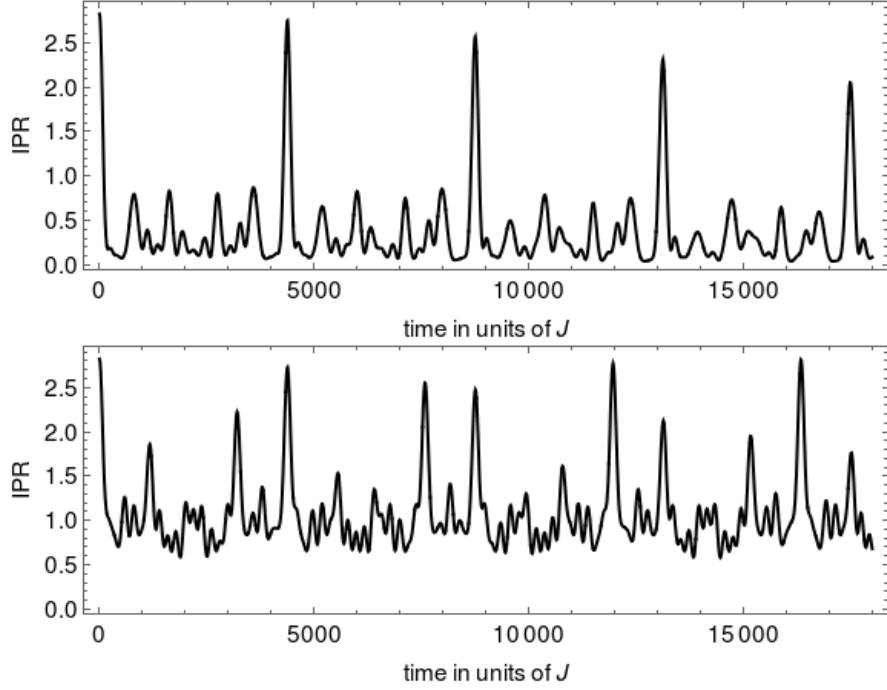


Figure 2.6: Top: IPR for the evolution of the doublon part of the dipole in the case of the Bose-Hubbard model. When contrasted with Fig. 2.4 we see that localization means peaks in the IPR plot and interference means regions of small amplitude. Bottom: IPR for the spin model, the evolution of which was presented in the lower panel of Fig. 2.5. We have re-scaled the time axis in the bottom panel such that the comparison between the full and effective-spin model is clearer.

same occurs in the case of the effective model written in bosonic operators. Though they act on individual particles, the effect of the operator accounting for the second order process is to move the dipole as a whole. Despite of that, the interference is there, and the pattern has the same structure. Even further it last the same amount of time. This will be studied in detail in the next section.

Among the different observables available to characterize our system, we compute the inverse-participation-ratio-like (IPR) functional. This allow us to have a measure of how localized or delocalized is the occupation distribution in Fig. 2.4 at some moment. This interplay between localization and delocalization is linked with the propagation of the dipole in the following way. When the dipole travels along the lattice it corresponds to a peak of localization and when the interference appears it corresponds to a region of delocalization. The IPR-like functional is defined as

$$IPR_{\text{BH}} = \int_0^L |P_{\text{B-H}}(x; t)|^2 dx, \quad (2.17)$$

$$IPR_{\text{s}} = \int_0^L |P_{\text{s}}(x; t)|^2 dx, \quad (2.18)$$

where P_i with $i = (\text{BH}, \text{s})$ are the probability distributions in the coordinate space that we define

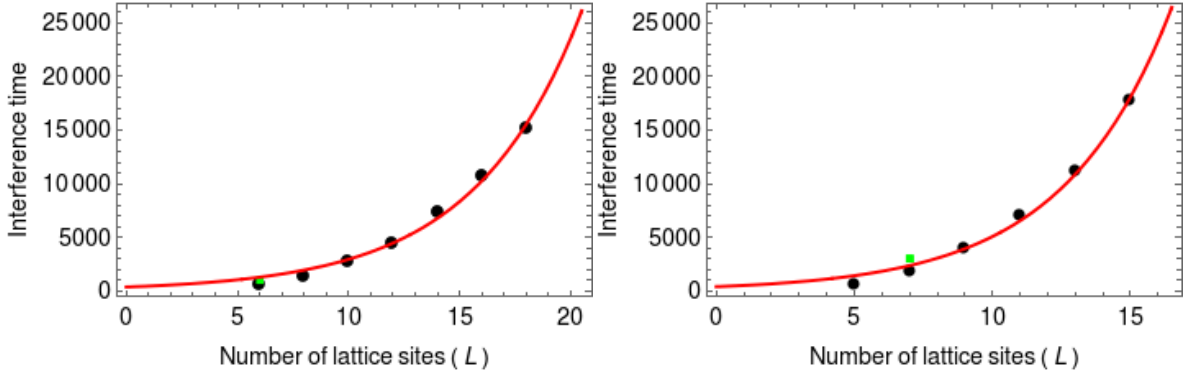


Figure 2.7: Left: Interference time as a function of the lattice length for B-H chains with even number of sites. The exponential fit is a good approximation to the behavior of the interference time as we scale the system size. Right: Time of interference for chains with odd number of lattice sites. Again, the exponential fit suits neatly to the behavior of the interference time as we scale the system. In both cases the cross marker represents the interference time within the full B-H model, for six and seven sites respectively. The green dots are the times within the effective XXZ-chain model and the continuous red line is the best exponential fit for the data.

as

$$P_{\text{BH}}(x; t) = \sum_{l=1}^L \frac{1}{2} \hat{n}_l (\hat{n}_l - 1) \delta(x - l) \quad \text{for bosons,} \quad (2.19)$$

$$P_{\text{s}}(x; t) = \sum_{l=1}^L \sigma_l^z \delta(x - l) \quad \text{for spins,} \quad (2.20)$$

with n_l the bosonic number operator, and σ_l^z the z -Pauli matrix. It is worth to notice that in the case of the B-H model we only track the localization of the doublon. Since the pair doublon-holon is a whole structure and behaves as it, it is enough to track one of its parts. In Fig. 2.6 we have plotted the IPR for the B-H model and the effective XXZ-chain model, respectively (in Fig. 2.6 the time scale of the bottom pannel was re-scaled to make clearer the comparition). In general, both, the interference phenomena and the interplay between localization and delocalization of the excitation in the successive periods of propagation are preserved. Furthermore, the effective model represents rather well these effects.

2.2.4 Interference in the effective model

The interference phenomena that can be related with the delocalization of the initial excitation along the lattice is without doubt an interesting phenomena. We take advantage of the good mapping of the B-H model into the spin chain to characterize that interference behavior. The reduced basis allows us to estimate the characteristic time of the delocalization, the interference time, faster than using the original model. The results are shown in Fig. 2.7 where we go up to $L = 18$, for which the basis scales linearly with the lattice length. We systematically compute the time evolution of the effective XXZ-chain for lattices the size of which ranged from six sites up to eighteen sites. One major feature that we found when doing this study is that the interference

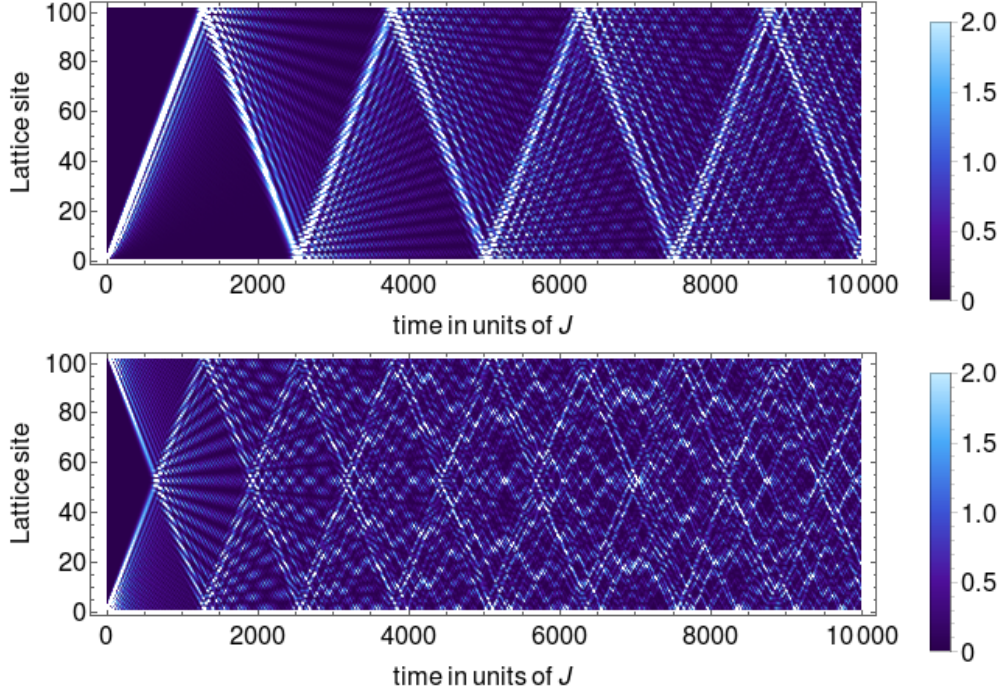


Figure 2.8: Top: Time evolution of the population for each lattice site computed with the effective XXZ-chain spin model for a lattice of $L = 100$ with rigid walls as boundary condition. Emergence of the typical interference pattern of a quantum carpet [45] as a consequence of the scaling of the lattice length. Bottom: Time evolution of the population for each lattice site computed with the effective XXZ-chain model for a lattice with $L = 100$ sites and periodic boundary conditions.

time is sensible to the parity of the number of lattice sites (see App. C). Therefore, lattices with even number of sites were studied apart of those with odd number of sites, the results can be seen in Fig. 2.7. The conclusion of the study is that in both cases, the interference time scales exponentially with the length of the lattice, but the interference time is larger in the case of an odd number of sites.

The reduction to the effective model allowed us to do something else. We are able to investigate the behavior of the interference for large lattices, say, $L = 100$ sites (with L the number of lattice sites). From Fig. 2.7 we can see that for these large lattices the interference time will be really large. However, at this sort of thermodynamic limit the differentiation between even and odd lattice lengths becomes irrelevant. And the system presents a unique long interference pattern. Such pattern can be interpreted as a quantum carpet [45], which is a phenomena known to appear due to the self interference of the wave function when confined in a box. Therefore, this interference-like behavior that appears for small lattices lengths is nothing more than the manifestation of a quantum carpet that emerges when we go to large lattices lengths (see Fig. 2.8). By going to the limit of large systems we find the right explanation we were looking for the interference pattern first depicted in Fig. 2.4. In this limit we can see that the dipole wave function consists of parts that travel with different velocities. Therefore, they arrive at slightly different times at the edge of the lattice and after bouncing back they start to interfere with each other. This phenomena happens always. However, in the case of small number of lattice sites the length of the lattice was not large

enough to make it evident. Additionally and as a mere curiosity we compute the time evolution of the system, for the same initial condition (an impurity in one of the edges), and the same number of sites $L = 100$ but now with periodic boundary conditions. The results can be seen in the lower panel of Fig. 2.8. There we see again the emergence of the quantum carpet as a consequence of the self interference process.

A question that arises is why in the case of periodic boundary conditions (PBC) the self interference appear? This is a natural question, given the fact that with PBC there are no edges in the lattice. The situation of PBC can be interpreted as placing the system in the surface of a cylinder, with time running in the direction of the axes and space wrapping the cylinder. In this scenario it does not matter where we place the single impurity since it sees a translationally invariant lattice. The WF always splits in parts that travel in both directions. That is, the WF goes around the cylinder clockwise and anticlockwise. Therefore, at some point these two parts are going to meet and there the interference appears. So, with PBC we have a different mechanism from that of bouncing back at the rigid walls by which the self interference can happen and hence the quantum carpet emerges.

Before closing this chapter let us give a short summary of what was discussed here. Mainly we deal with the many body problem of the single-band Bose-Hubbard Hamiltonian and how to effectively reduce it to a simple Hamiltonian for dipoles. We have shown that such effective reduction can be linked to spin models, namely, an antiferromagnetic Ising model and the XXZ-chain model. All this when we work with a scheme of energetically locked a Mott state in a tilted lattice and study both the appearance and dynamics of resonant excitations of this Mott state. These excitations are known as dipoles (pairs of doublon-holon in next neighboring sites). We focus our attention in an interference pattern that appears in the strong off-resonant regime of the B-H model. We studied it with the effective XXZ-chain model. We found that such interference pattern appears as a consequence of the self interference of the wave function for the dipole as it travels along the lattice. This is a consequence of the fact that such wave function is made up of components that travel with different velocities (see the different rays that travel along side each other in Fig. 2.8). Each of these components interferes with the others after they bounce back on the rigid edge of the lattice. Finally, we found that in the limit of long lattice lengths this interference has a beautiful interpretation in the emergence of a matter quantum carpet.

Chapter 3

Exploration of the doublon-mediated dynamics in the two-band Bose-Hubbard model

3.1 Motivation

In previous chapters we have worked with the single-band Bose-Hubbard model, and with it we have build quantum simulations of spin chains. That is a great way in which we can take advantage of the characteristic high degree of control featured in the ultracold matter. But it is not the only way. Actually the Bose-Hubbard model exhibits a lot of interesting physical phenomena. Though in many cases the study of it as itself turns out to be quite complex. However, this complexity can be translated to richness in a physical sense [30, 35, 36, 48]. Can we tackle the complexity of a Bose-Hubbard model in such a way that we can control the dynamical transition from one initial to target state(s)? To answer this, there exists different protocols that take advantage, for instance, on the properties of the characteristic quantum spectrum of the system under study [10, 12, 49], the interaction with the environment (an open quantum system), or more precisely techniques for optimal control [50, 51].

Here, aiming to get a clear answer to that question we propose a toy model based on a two-band Bose-Hubbard Hamiltonian where the only transport mechanism is a doublon-mediated inter-band coupling. We explore the manifold of accessible states. This exploration was done in two different ways. First, we shake in time the optical lattice with an external pulse (see Sec. 3.3). Second, we look for the existence of resonances allowed by the doublon-mediated inter-band coupling and we perform one-way parametric evolutions around the respective first order resonance (see Sec. 3.4).

3.2 Theoretical model

In Sec. 1.4 we discussed the explicit form of the Bose-Hubbard model. There, we stated that one can truncate the sum over the band index in order to have an approximation to the whole system.

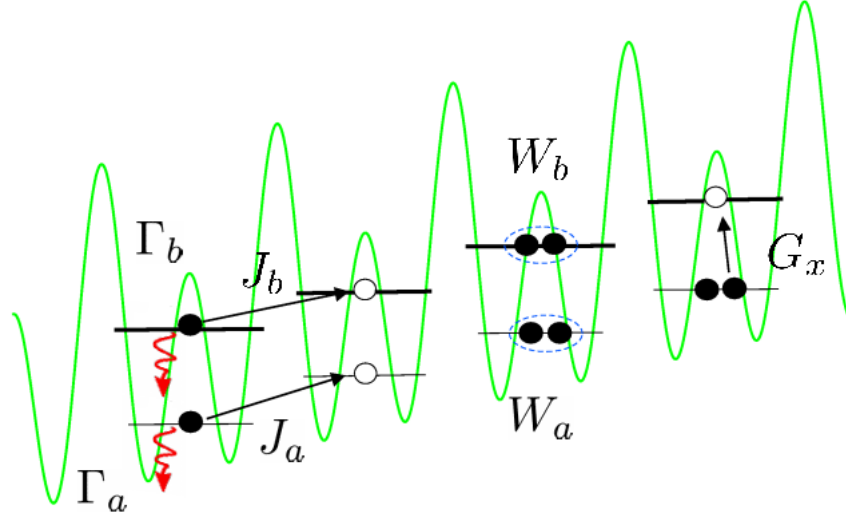


Figure 3.1: Schematic representation of the different processes that take place under the two-band Bose-Hubbard Hamiltonian in Eq. (3.1) with the doublon-mediated inter-band coupling.

One way to obtain the two-band Bose-Hubbard model is by truncating that sum up to $\alpha = 2$ in Eqs. (1.16)–(1.18) (see [36, 52]). Here, we have interest in a different two-band Bose-Hubbard model. The Hamiltonian that we work with through this chapter is

$$H = \sum_l \sum_{\beta=a,b} \left[-\frac{J_\beta}{2} (\beta_{l+1}^\dagger \beta_l + \text{h.c.}) + \frac{W_\beta}{2} n_l^\beta (n_l^\beta - 1) + 2\pi F l n_l^\beta - i\Gamma_\beta n_l^\beta \right] + \sum_l \Delta_g n_l^b + \sum_l G_x (b_l^\dagger a_l n_l^a (n_l^b - 1) + n_l^a (n_l^a - 1) a_l^\dagger b_l), \quad (3.1)$$

which is a model including the first two energy Bloch bands. The system is effectively open by introducing the respective decay rates ($\Gamma_{a,b}$) of each band [49]. A schematic representation of the process we consider in the Hamiltonian in Eq. (3.1) can be seen in Fig. 3.1. The interband coupling is realized via a term mediated by G_x that makes the interband transport possible only when there are doublons, *i.e.*, two particles in the same lattice site, in the lower band. This term can be introduced as a second order correction to the main Hamiltonian presented in [52]. This correction can be achieved using a Schrieffer-Wolff like transformation [47] (see App. A).

3.3 Shaking the lattice

It is known that driven systems offer a whole and rich new physics as is proven for example by the existence of the Floquet topological insulators and the appearance of magnetic like behavior in neutral atoms systems [9]. Here, instead of looking for new physics we want to do a dynamical exploration. That is, we look for dynamical stable states (or structures) which are robust against the coupling to an environment (a bosonic reservoir).

Table 3.1: Bose-Hubbard parameters.

V_0	S_0	Δ_g	J_a	J_b	W_a	W_b	G_x
11	3	0.108	0.006	0.006	0.034	0.034	0.03

Table 3.2: Fock basis for the 2/2 system.

i	1	2	3	4	5	6	7	8	9	10
state	$ 11; 00\rangle$	$ 10; 10\rangle$	$ 10; 01\rangle$	$ 01; 10\rangle$	$ 01; 01\rangle$	$ 20; 00\rangle$	$ 02; 00\rangle$	$ 00; 20\rangle$	$ 00; 02\rangle$	$ 00; 11\rangle$

To take advantage of the new term including inter-band transport via doublons we tilt the lattice, such that the doublon triggers interband transport. That is, the force at which the doublon can be destroyed to take at least one particle from the lower band to the upper band. This is done by the external force defined as

$$F = F_0 + F_A \sin^2(\omega_q t), \quad (3.2)$$

where $F_0 = \frac{W_a}{2\pi}$ is the value of the external force bringing close in energy a single-particle level with a two-particle level in the next neighboring site (towards the direction of the tilt), $F_A = \frac{\Delta_g - W_a}{2\pi}$ is the amplitude of the oscillation, and $\omega_q = \frac{\Delta_g - 2W_a}{2\pi}$ is the oscillation frequency. We may notice that the oscillation happens between the two-particle energy level and the single-particle first order resonance.

3.3.1 Results

We work with the smallest possible non trivial system, say two particles in two wells (2/2), where the filling factor is defined as N/L with N the number of particles and L the number of sites. The results presented in this section are obtained for that system and we expect to see a similar behavior when we move on to the larger system (4/4). Additionally, we have worked with the set of Bose-Hubbard parameters as specified in Table 3.1 in a way that we can guarantee $J_{a,b} \ll W_{a,b}$, with $\Gamma_{a,b}$ at least one order of magnitude smaller than $J_{a,b}$. These parameters were taken from App. 1 in [35]. For the numerical simulations we study the population inversion as our main observable, that is the difference between the population $M_b(t)$ of the upper band and the population $M_a(t)$ of the lower band,

$$M_b(t) - M_a(t) = \frac{1}{N} \left[\langle \psi(t) | \sum_l \hat{n}_l^b | \psi(t) \rangle - \langle \psi(t) | \sum_l \hat{n}_l^a | \psi(t) \rangle \right]. \quad (3.3)$$

We compute the time evolution looking for a stationary state. First, we study the main probability of appearance for each of the states in the Fock basis (the Fock basis was ordered as in Table 3.2) with the ratio Γ_b/Γ_a . The results are shown in Fig. 3.2. The value $\Gamma_b/\Gamma_a = 1$ splits the dynamics into two regimes. For $\Gamma_b/\Gamma_a > 1$ the probability remains in the initial state $|11; 00\rangle$, while for $\Gamma_b/\Gamma_a < 1$ there is a non-trivial evolution, for instance, in the case of $\Gamma_b/\Gamma_a \ll 1$ the

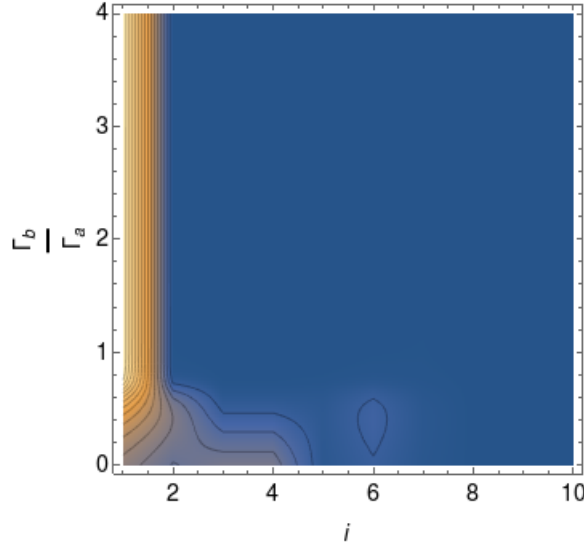


Figure 3.2: Average probability for each of the states in the Fock basis as a function of the ratio between the decay rates for all elements of the basis. We see that after a value $\Gamma_b/\Gamma_a = 1$ only the state $|11; 00\rangle$ is excited by the external force. The region of interest for us is $\Gamma_b/\Gamma_a \ll 1$.

states 3 and 4 get excited. We focus on the latter region. Although this division is valid only in the time scales and values of parameters at which we have worked here, it can be shown that for longer time scales there is a non trivial evolution for $\Gamma_b/\Gamma_a > 1$. Here, we are not interested in such long time scales.

With the ratio Γ_b/Γ_a fixed to the proper value, we turn off the modulation and compute the time evolution of our system. The results can be seen in Fig. 3.3, where it is evident that we reach a final state which is non stationary. It is a superposition of four states, and two of them are $|10; 01\rangle$ and $|01; 10\rangle$, the superposition of which is of interest due to the fact that it resembles a Bell's state $|10; 01\rangle \pm |01; 10\rangle$. But there is an undesirable contribution of other two states.

As a final test we turn on the shaking and performed the same computation as before, we look at the population inversion and the final state after the evolution. There is a stationary state and is given by the wanted superposition. From Fig. 3.4 is clear that the shaking cleans the final state giving us only the two desired states and in an equally weighted superposition. Hence we can conclude that in the $2/2$ system our scheme is successful.

Now we ask what would happen when we go to a larger system, do the superposition we just found survives? One can think that such superposition have to appear somewhere in the time evolution. To check that we work with a $4/4$ system. The first thing we need to guarantee is that the population inversion effectively approaches zero at some point in time and remains like that. That is, we end up with an equal number of particles in the lower an upper band. To check that we have computed the mean population inversion as a function of the ratio Γ_b/Γ_a , the results can be viewed in the right panel of Fig. 3.5.

As we can see the average population inversion as a function of Γ_b/Γ_a saturates at the value -1 for outside the region $\Gamma_b/\Gamma_a < 1$. That is, outside that region there is a small probability of finding a final state with equal occupation of both bands. However, inside $\Gamma_b/\Gamma_a < 1$ the population

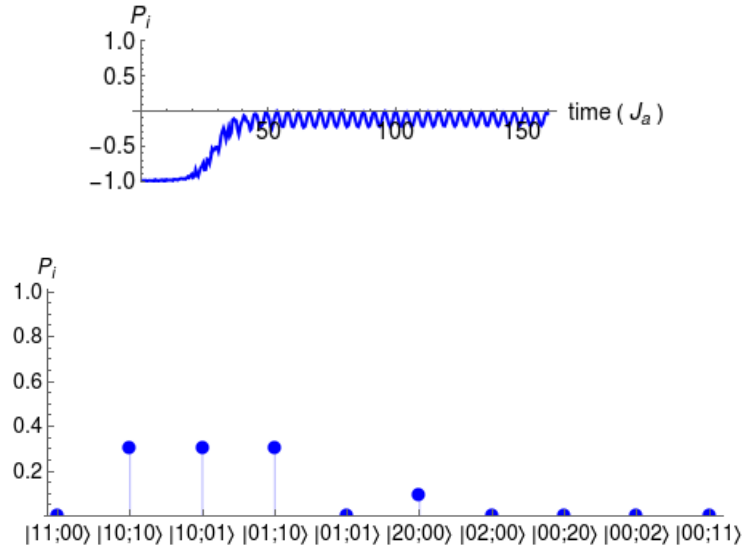


Figure 3.3: Top: population inversion as a function of time for the system without shaking. We see that even when the population inversion goes toward zero there is no stationary state. Bottom: final state found at the moment we stop the time evolution. From the behavior of the population inversion we see that there are oscillations between the states being excited (states 2, 3, 4, and 6 of Table 3.2).

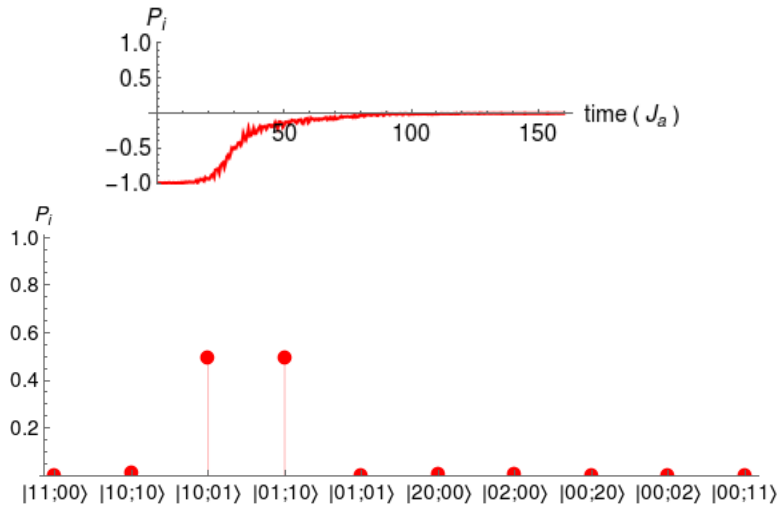


Figure 3.4: Top: population inversion as a function of time for the system with shaking. Now there is a saturation of the population inversion at zero, hence we have an stationary state. Bottom: final and stationary state found at the moment we stop the time evolution. This state is given by an equally weighted superposition between $|10;01\rangle$ and $|01;10\rangle$.

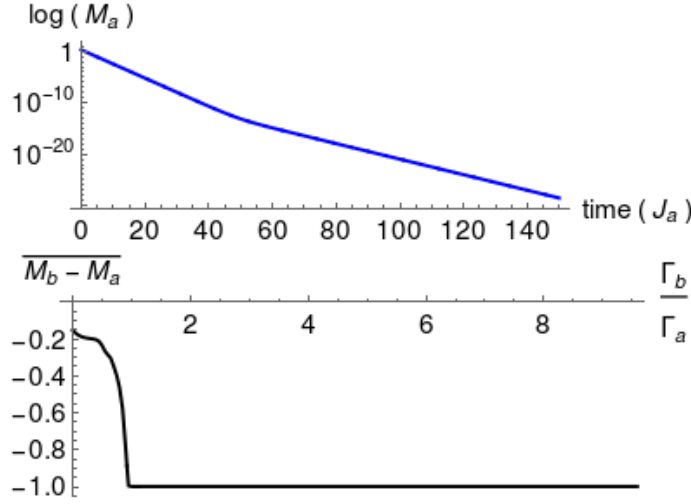


Figure 3.5: Top: behavior of the population in the lower band as a function of time without performing the renormalization after each evolution step. As expected from a dissipative dynamics, the population decays exponentially. Bottom: mean population inversion as a function of the ratio Γ_b/Γ_a for the 4/4 system. We can see that even in the region $\Gamma_b/\Gamma_a < 1$ that was the region of interest in the case of the 2/2 system, the population inversion never approaches zero. Therefore, the final state is not a state with equal number of particles in each band.

inversion remains smaller than one, which means that it is possible to have a final state with equal occupation of both bands. The population inversion never goes to zero due to fact that we are averaging it and there is always a contribution of some states with a varied occupation of both bands as we evolve towards the final state. However, in our numerical test we have not found the wanted superposition, though we find final states with equal occupation of the bands. We thus conclude that the shaking scheme works only in the case of the minimal system, but fails when we increase the number of lattice sites.

Comments regarding the dissipative dynamics.

One important clarification we shall do is about the dissipative dynamics we are implementing here. When we open the system we do not just add a decay rate to each band which makes those states metastable, we are allowing particles to scape from our system.

Thus every now and then we have to renormalize the probabilities of our evolution vector, in particular after each evolution step we performed the renormalization. Thanks to the fact that the evolution steps we had taken were always from zero to the respective time value at which we are evolving we did not alter the final result.

However, just to verify the correct behavior of the dissipative dynamics in our system we did a calculation of the population in the lower band as a function of time without performing the renormalization after each step. The results can be seen in the left panel of Fig. 3.5, and as expected from this kind of dynamics the population decays exponentially in time due to the escaping of particles.

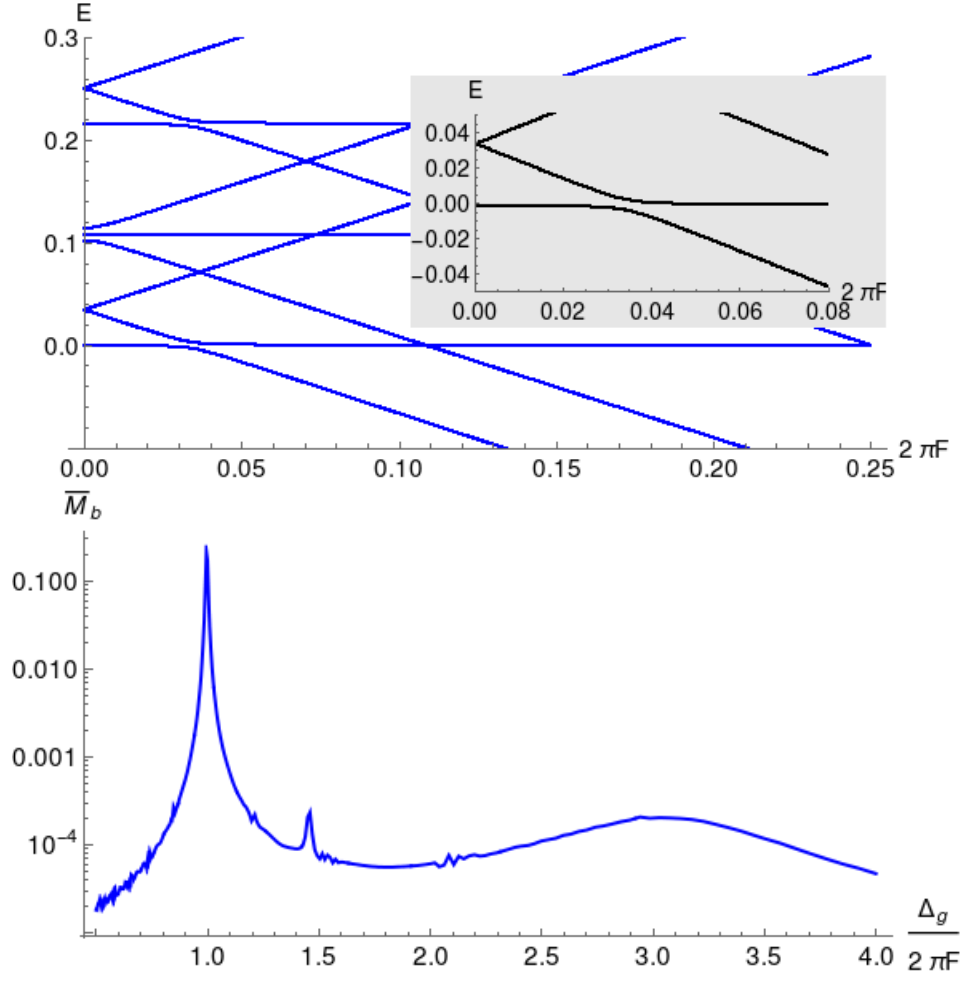


Figure 3.6: Top: energy spectrum of the Hamiltonian in Eq. (3.1) for the minimal system as a function of the force amplitude F . It is characterized by the presence of AC (see inset). Bottom: long time average occupation of the upper band as a function of the Stark force. We can see the resonant behavior in three points (with $\Delta_g = 0.108$).

3.4 Parametric evolution

As in the previous section we have strong interest to investigate what is the resulting dynamics of the Hamiltonian introduced in Eq. (3.1) when we vary the external Stark force. We have already presented the results in the minimal model and the expected results with the scaling of the system for a sinusoidal-like modulated Stark force. Here, we want to use a different approach, namely parametric evolution. By parametric evolution we mean a time evolution controlled by a single parameter which dictates the speed at which the evolution happens. In particular we have interest to implement such evolution to carry our initial state across an avoided crossing (AC). We understand AC as the phenomenon of repulsion between energy levels as a function of a control parameter.

The transit across the AC can be done by setting the external Stark force as a time dependent

parameter $F(t)$ and choosing the parameter governing the evolution as the sweeping rate α (see Eq. (3.4)). The goal of the present section is to look for such couplings between energy levels from different bands. Once we have found them, manifested as an AC, we evolve the initial Mott-like state parametrically across the AC looking for the different final states and finally comparing with the states that were found with the modulated external Stark force in Sec. 3.3. The present development was done mainly following Parra-Murillo (see Chap. 4 of [35]), specially the study of the different sweeping rates.

3.4.1 Methods and results

Since the AC is a manifestation of the coupling between two energy levels it is natural to link them with resonances. By resonance we understand the situation in which the external field is such that it brings to a degeneracy of the single-particle levels from different bands (see Fig. 2.1).

The first test we have to do is to check for the existence of resonances under the influence of the doublon-mediated inter-band coupling. Here we initially worked with the minimal model, say two wells with two particles (2/2), and rigid walls or open boundary conditions. We compute the energy spectrum of such system and the long time average occupation of the upper band as a function of the Stark force for the initial Fock state $|11; 00\rangle$ (similarly we compute such signal for other initial states, see App. B). Both results can be seen in Fig. 3.6.

In particular we observe the presence of AC in the energy spectrum and the respective resonant behavior at the same positions. We will focus our study around the region $\Delta_g/2\pi F \approx 1$ where we find the highest resonant response. Now we need to define the proper form of the external force to perform the navigation. Following Parra-Murillo (see chapter 4 of [35]) we will perform up to one sweep. We define the Stark force by

$$F = \alpha t + F_0, \quad \text{and} \quad t_\alpha = \frac{F_f - F_0}{\alpha}, \quad (3.4)$$

where F_0 and F_f are the initial and final values of the force such that we navigate the region around the first order resonance, which is the one we have interest in, and t_α determines the total time for the evolution. We shall notice that different values of α will provide different time steps. Therefore, α is a control parameter for the kind of dynamics we are implementing. The dynamics can be enclosed in three different regimes: adiabatic, diabatic (or sudden), and non-adiabatic [53]. In the following we have interest in the adiabatic regime with $\alpha/\delta(F_f - F_0) \ll 1$. By adiabatic we mean an evolution in which the system remains in an eigenvalue of the instantaneous Hamiltonian. In this regime, as we show later, we find a major appearance of different states as final ones without contribution of the initial state.

Now we only need to find the proper value of α and get the desired adiabatic evolution. In order to do that we build a mesh of α values and compute the time evolution of an initial state $|11; 00\rangle$ and check for the states participating in the dynamics for different α values. We present the results of that study in Fig. 3.7. We can recognize there three different regimes, each one associated with a different kind of dynamics. Although there is an ambiguity when we want to define the boundaries of each regime, we have found that for our study, the adiabatic regime ranges between (0, 0.1), the non-adiabatic regime between (0.1, 0.2), and the diabatic regime between (0.2, 1) in units of $\frac{\alpha}{\delta(F_f - F_0)}$.

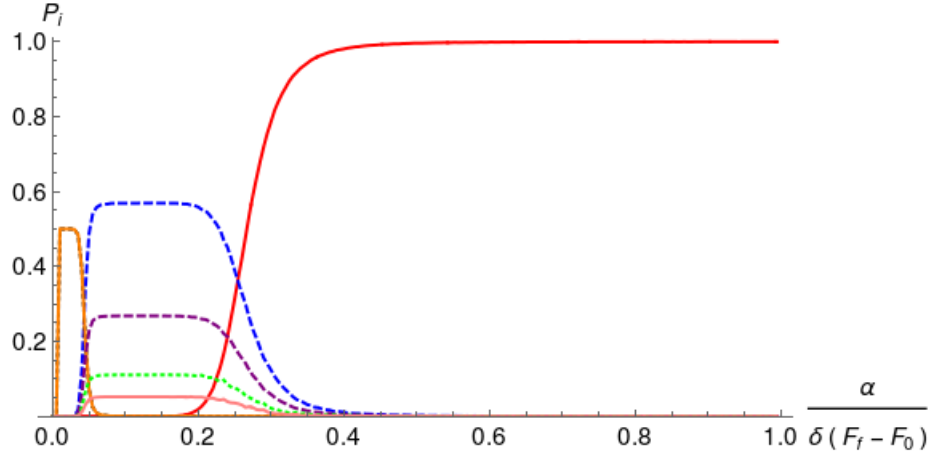


Figure 3.7: Probability of participation (P_i) for the states that take part in the dynamics as function of the sweeping rate α . We can clearly observe the three different regimes of dynamics governed each one by a different set of α values. We have, for small $\alpha \rightarrow |10; 01\rangle$ (black) and $|01; 10\rangle$ (orange) in an equally weighted superposition, for intermediate $\alpha \rightarrow |10; 10\rangle$ (blue), $|01; 01\rangle$ (purple), $|20; 00\rangle$ (green), and $|02; 00\rangle$ (pink), for large $\alpha \rightarrow |11; 00\rangle$ the initial state in red. Here, α represents the sweeping rate, F_f and F_0 are the final and initial values of the Stark force between which the evolution takes place, and δ is a characteristic parameter that measures the width of the AC.

For small α values we lost the information of the initial state and gain some new and interesting states as consequence of the adiabatic evolution. For example, an equally weighted superposition between the two alternating states, given by $\frac{1}{\sqrt{2}}(|10; 01\rangle + |01; 10\rangle)$, where the color code is $|10; 01\rangle$ in black and $|01; 10\rangle$ in orange. On the other hand, for intermediate values of α we find a four-state superposition given by $|10; 10\rangle$ (blue), $|01; 01\rangle$ (purple), $|20; 00\rangle$ (green), and $|02; 00\rangle$ (pink). As a consequence of the non-adiabatic dynamics the navigation process is not complete and we end up with an intermediate state as our final state. Finally, for large α values we find the diabatic regime, where we navigate the spectrum fast enough and the system is not able to couple to other states ending up in the same initial state $|11; 00\rangle$ in red.

From the results presented in Fig. 3.7 we will focus our attention in the first region, the adiabatic region, since it is there where we find a successful navigation process. From our numerical computation we were able to obtain a given α within that region and perform the time evolution of our system. The results can be seen in Fig. 3.8. At this point we should notice that, besides the exploration of the doublon induced dynamics, we have found that such dynamics can sustain an interesting superposition as the one of Sec. 3.3 which resembles an entangled Bell-like state for the minimal system in the model defined by the Hamiltonian introduced in Eq. (3.1).

Before closing this section we will deliver some comments regarding the dynamics of a larger system (4/4), and once there, we should check if it is possible to find some interesting superpositions as the one we just found for the minimal (2/2) system. For the 4/4 system we followed a similar procedure than that of the 2/2 system. First we check if in the energy spectrum there were regions with AC at which we can perform spectral navigation. To that inquiry we found an affirmative response (results can be seen in App. B). Then we compute the time evolution of a given initial state $|1111; 0000\rangle$ for each of the α values in the proper mesh. In Fig. 3.9 we present the above mentioned results.

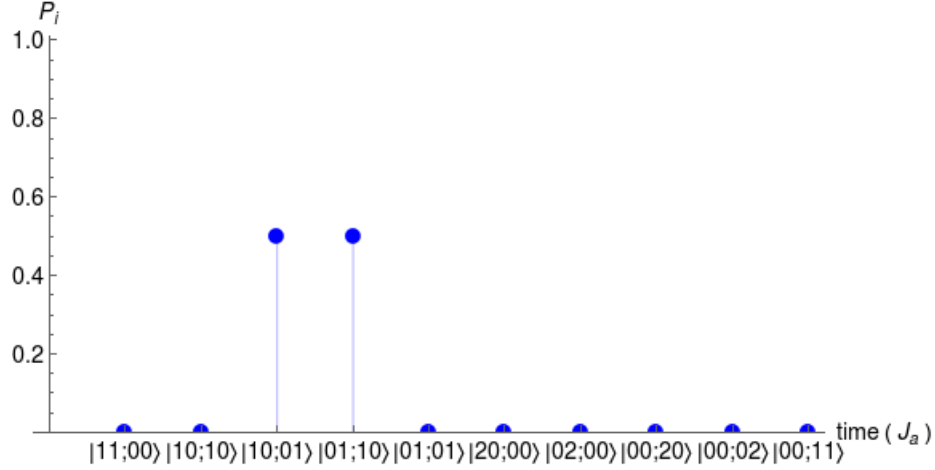


Figure 3.8: Final state after the evolution for a value of α with the region of adiabatic dynamics. The state is given by an equally weighted superposition between $|10; 01\rangle$ and $|01; 10\rangle$. The value of α that we used in the calculation was $\alpha = 1.33 \times 10^{-6}$.

Table 3.3: Dynamical states for the initial condition $|1111; 0000\rangle$. We tabulate the maximum probability P_i (on the left of each column) of finding the i -th state (on the right of each column) in the final state.

Diabatic region		Non-adiabatic region		Adiabatic region	
$P_{21} = 0.9994$	$ 1111; 0000\rangle$	$P_{49} = 0.1252$	$ 1011; 1000\rangle$	$P_{242} = 0.7638$	$ 1000; 0210\rangle$
		$P_{67} = 0.1254$	$ 1101; 0100\rangle$	$P_{251} = 0.2224$	$ 0001; 0120\rangle$
		$P_{81} = 0.1251$	$ 1110; 0010\rangle$		
		$P_{149} = 0.2754$	$ 1010; 1010\rangle$		
		$P_{160} = 0.1298$	$ 0110; 0110\rangle$		
		$P_{229} = 0.1300$	$ 0100; 0300\rangle$		
		$P_{236} = 0.2683$	$ 1000; 1110\rangle$		
		$P_{240} = 0.1804$	$ 0010; 0210\rangle$		
		$P_{249} = 0.2350$	$ 0100; 0120\rangle$		

From Fig. 3.9 we can see that the diabatic region is governed by the initial state, meaning that we go through the AC too fast and the system does not have time to coupled to another state. In addition, the non-adiabatic region has a high population of different states. Finally, the adiabatic region, the one at which we have found a successful navigation process, is mainly governed by two states, $|1000; 0210\rangle$ and $|0001; 0120\rangle$, with a higher contribution of the first one.

In Table 3.3 we find the respective states, with their respective maximum participation probability labeled by their position in the Fock basis, for each one of the three dynamical regions, with the proper color code to make the association easier. We may notice that the states sharing the same color label appear as an equally weighted superposition.

In general terms the global results are not too far from those obtained in the 2/2 system. However, we were not able to find an equally weighted superposition of alternating states. In fact the adiabatic region favors the appearance of states with a population of three particles in the upper

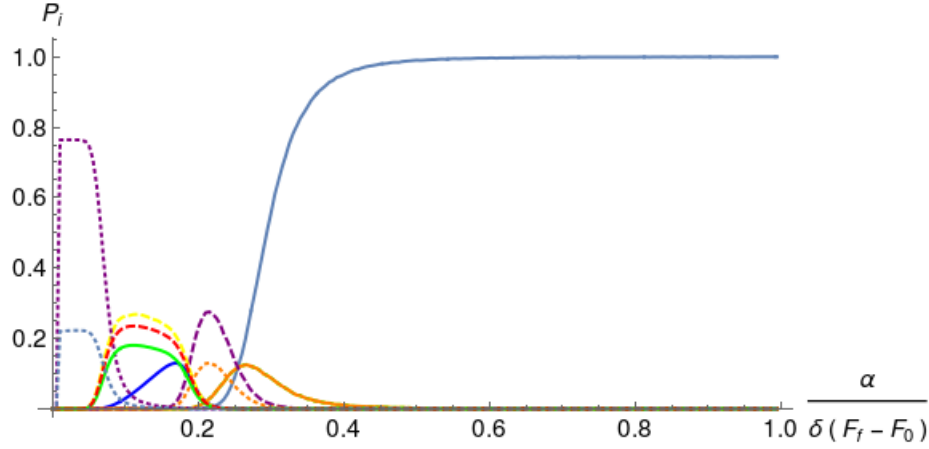


Figure 3.9: Different states participating in the navigation process for the initial state $|1111; 0000\rangle$. There are three different dynamical regions, adiabatic, non-adiabatic and adiabatic, just as in the case of the 2/2 system. However, the interplay between the states starts to be more complex due to the large number of states involved on the evolution.

band. We do find some states with equal population of both bands, but they were not alternating states and were inside the non-adiabatic regime of α values, as for example $|0110; 0110\rangle$.

We performed the same calculation for other two initial conditions, say $|0202; 0000\rangle$ and $|2020; 0000\rangle$, since they are easily accessible states from the state $|1111; 0000\rangle$ through the first order resonance between a single-particle level and a two-particle level, both states in the first band (see [39, 40]). These results can be seen in App. B. Also, when we take a look at the coupling obtained in Eq. (A.15) of App. A we see that the Schrieffer-Wolff transformation introduces an inter-site coupling rather than an intra-site coupling as the one considered for the calculations of this section. Due to that we repeated the same set of calculations for a Hamiltonian with such a coupling (see further details in App. B).

Last but not least, let us give a brief summary. We have devoted this chapter to the study of the dynamical consequences of the inclusion of a doublon-mediated interband coupling to the two-band Bose-Hubbard model. The time evolution was done in two different ways. First, by shaking the lattice, and second by searching for the presence of AC in the energy spectrum and performing parametric evolution in order to go through them. For both cases the external Stark force was a time-dependent parameter $F(t)$ over which we have control. The study had two stages. The first one was developed on the minimal system, *i.e.*, two particles in two wells (2/2). The second one referred to the investigation of the robustness of the final states against the scaling of the lattice length. The main conclusion is that, the doublon-mediated interband coupling allows us to target some interesting states but such states are not robust against the scaling of the system. Finally, a broader set of results can be found in App. B.

Chapter 4

Conclusion and outlook

Throughout this thesis we did two things. First, we use a well defined quantum simulator based on a Heissenberg chain to characterize second order processes in the single-band Bose-Hubbard model far from the known single and many-body resonances. This simulation was based on a previously explored simulation of the antiferromagnetic Ising chain [7]. The quantum simulation of this chain takes advantage of the fact that once we energetically lock the Mott insulator state on a tilted lattice, a strong tilt couples the Mott state to a certain manifold by resonant transitions. These transitions are given by movement of particles between next neighboring sites when the energy level of a single particle and two particles are degenerated. Finally, we can define pseudo-spins based on this transitions to make the link between the two models. Later we found the existence of second order processes that are not explicitly considered within the single-band B-H model. These processes consist on the propagation of the holon-doublon quasiparticle along the lattice. We compute the explicit form of the proper operator accounting for this process using a Schrieffer-Wolff transformation. The link between the B-H model and the Heissenberg XXZ-model is obtained by the same pseudo-spin mapping as in the simulation of the antiferromagnetic Ising chain. With this identification we found that the propagation of the holon-doublon quasiparticle can be interpreted as a spin-wave in the XXZ-chain.

Second, we present a variation of the open two-band B-H model that couples the bands by means of a doublon-mediated inter-band coupling. These coupling has its justification in the fact that when the Stark field induced resonant enhance tunneling in the first band, the leading process is the creation of doublons in that band. We explored the dynamics of the system finding a complete set of the allowed states. First, for the minimal system the main result was that among the accessible states there is one that resembles a Bell state. Later, when exploring the dynamics of larger systems we did not find such a state, from which we conclude that such a state is not robust against the scaling of the system, at least no under the two approaches of the dynamics studied in this thesis.

There are open questions in both cases. In the quantum simulation we dealt with, it is necessary a deeper study of the second order processes in the single-band B-H model in order to propose an experimental scheme that could look for them and to get a better understanding of their interpretation as spin waves. In the case of quantum control presented in Chap. 3, it is necessary to do additional studies of the consequences of the doublon-mediated inter-band coupling and the proper mechanism by means of which it appears in the two-band B-H Hamiltonian.

Additionally, there is a need of finding the right protocol that allows us to have a better control over the dissipation such that the obtained Bell-like state in the minimal system survives the scaling of the system.

Appendix A

On the Schrieffer-Wolff transformation

Unitary transformations are among the more useful resources theoretical physics count with to build a better interpretation of some initially tricky problem. The possibility of re-writing a problem in a more friendly and handy way has shown to be of great advantage. Sometimes they unveil deep connections between physical systems that one initially could have thought as totally uncorrelated. For instance, this is the case of the Ising model in a transverse field and the one dimensional p -wave superconductor connected through the Jordan-Wigner transformation (see Chap. 5 of [54]), or the connection between the single-impurity Anderson model and the Kondo model proved in 1966 by Schrieffer and Wolff [46] using the unitary transformation named after them. The latter transformation constitutes the topic of this brief appendix. For some rigorous review of the Schrieffer-Wolff transformation (SWT) we recommend [55].

A.1 General remarks

The SWT is an unitary transformation that allows us to effectively isolate low energy physical phenomena of a system under study. In this sense, it provides us with an effective representation of our problem that in many examples has been proven to be in excellent agreement with the physics and information we get from the full system [46, 56, 57].

There are scenarios in which some physical systems manifest second or higher order processes that occur as consequence of first order processes like hopping or tunneling being virtual ones. One can think of a one dimensional lattice system described by a Hamiltonian that allows hopping of particles only between next neighboring sites. This system might, nevertheless, exhibit a regime which features long range hoppings. Such processes can be understood as composed by next neighboring hoppings that virtually occur as intermediate steps. In this situation one's interest is to write a Hamiltonian which accounts for those second order hoppings. The SWT accomplishes precisely this: it allows one to get rid of the parts of the Hamiltonian that account for the first order process and introduces the proper operator for the second order process (and higher orders if necessary) which is built as products of first order process operators.

As a starting point let us think of a Hamiltonian that can be written as

$$H = H_0 + V, \tag{A.1}$$

where H_0 is a Hamiltonian for which the eigenvalues are known and V stands for a perturbative term. The first step consists in a canonical transformation of the form

$$H_{\text{eff}} = e^S H e^{-S}, \quad (\text{A.2})$$

where the operator S is called the generator and it has to be found in a way that no linear terms appear in the Hamiltonian H_{eff} . Using the Baker-Campbell-Hausdorff formula, the transformed Hamiltonian can be written as the expansion

$$H_{\text{eff}} = \sum_{m=0}^{\infty} \frac{1}{m!} [S, H]_m = H + [S, H] + \frac{1}{2} [S, [S, H]] + \frac{1}{6} [S, [S, [S, H]]] + \dots \quad (\text{A.3})$$

By imposing that $V = -[S, H_0]$ we can achieve the required Hamiltonian without the linear terms. Including the expression for V in the series expansion in Eq. (A.3) in an iterative way, one gets

$$H_{\text{eff}} = H_0 + \frac{1}{2} [S, V] + \frac{1}{3} [S, [S, V]] + \frac{1}{8} [S, [S, [S, V]]] + \dots, \quad (\text{A.4})$$

where we have already included higher order terms. Since we are interested only in the description of second order processes, we may truncated the expansion up to that order. It will thus look like

$$H_{\text{eff}} = H_0 + \frac{1}{2} [S, V]. \quad (\text{A.5})$$

At this point it remains to introduce the Hamiltonian of the specific problem we are studying and compute the respective generator. However, this is in general not an easy task. It is easier to compute the specific matrix elements, that is, we use the eigenstates of H_0 to write

$$\langle i | H_{\text{eff}} | j \rangle = \epsilon_{i,j} \delta_{i,j} + \frac{1}{2} (\langle i | S V | j \rangle - \langle i | V S | j \rangle). \quad (\text{A.6})$$

The matrix elements of SV and VS can be further evaluated by introducing the identity sum $\sum_k |k\rangle \langle k| = 1$. Eq. (A.6) can be thus written as

$$\langle i | H_{\text{eff}} | j \rangle = \epsilon_{i,j} \delta_{i,j} + \frac{1}{2} \sum_k (\langle i | S | k \rangle \langle k | V | j \rangle - \langle i | V | k \rangle \langle k | S | j \rangle). \quad (\text{A.7})$$

Using $V = -[S, H_0]$ it follows

$$\langle i | V | j \rangle = -(\langle i | S H_0 | j \rangle - \langle i | H_0 S | j \rangle) = (\epsilon_j - \epsilon_i) \langle i | S | j \rangle, \quad (\text{A.8})$$

where we have exploited the fact of $|i\rangle$ and $|j\rangle$ being eigenstates of H_0 . Eq. (A.8) implies

$$\langle i | S | j \rangle = \frac{\langle i | V | j \rangle}{\epsilon_i - \epsilon_j}. \quad (\text{A.9})$$

Plugging this into Eq. (A.7) we find

$$[H_{\text{eff}}]_{i,j} = \epsilon_{i,j} \delta_{i,j} + \frac{1}{2} \sum_k \left(\frac{1}{\epsilon_i - \epsilon_k} - \frac{1}{\epsilon_k - \epsilon_j} \right) \langle i | V | k \rangle \langle k | V | j \rangle, \quad (\text{A.10})$$

where the complete set of states $|k\rangle$ that we introduced in Eq. (A.7) turns out to be all intermediate or virtual states that allows for the transition from state $|i\rangle$ to state $|j\rangle$. The identification of these intermediate states is an easier task than the full calculation of the generator S . In the next sections we apply the Schrieffer-Wolff transformation as presented here to the Bose-Hubbard Hamiltonians we study in Chaps. 2 and 3.

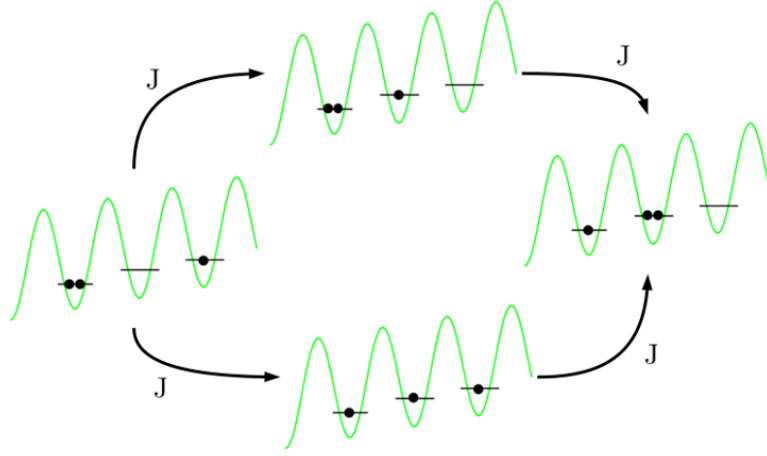


Figure A.1: Schematic representation of the second order processes corresponding to the hopping of a dipole between successive sites. This time the intermediate states corresponds to the dipole vacuum (Mott state), and a state where the initial dipole has been separated and its individual constituents are in different sites separated by at least one well.

A.1.1 Application of the SWT to the single-band Bose-Hubbard model

We are interested in second order processes in the single-band Bose-Hubbard model. These processes can be represented as successive hoppings of particles, as for example the one depicted in Fig. A.1. In particular we want to explore the possibility to build an effective model in which the hopping of dipoles as defined in Sec. 2.1.2 is allowed. Such a model will require a second order process in the creation/annihilation operators for bosons. Therefore, as presented in Sec. A.1 the Schrieffer-Wolff transformation turns out to be the perfect mechanism to do it.

First, we need to set the source and target states of the process. They are the Fock states $|i\rangle = |201\rangle$ and $|j\rangle = |120\rangle$, respectively. Here, we are working on a $3/3$ system because it is the minimal system that can have the process we want to describe, though for a B-H system to have dipoles it is enough if we have a $2/2$ system. But for the dipole to be allowed to hop we need at least one more site. Second, we notice that within the possibilities of the single-band model the only way to connect the source and target states is by hopping processes of single particles. Thus There are two intermediate virtual states given by $|k\rangle = |111\rangle$ and $|k\rangle = |210\rangle$ (see Fig. A.1).

We need now to identify the respective energies of the states $|201\rangle$, $|120\rangle$, $|111\rangle$, and $|210\rangle$. Once we have that it is easy to compute the expression in Eq. (A.10) by taking into account that V is the hopping operator given by

$$V = -J \sum_l (a_{l+1}^\dagger a_l + \text{h.c.}). \quad (\text{A.11})$$

It follows that the operator that accounts for the process in Fig. A.1 is

$$O_{\text{SO}} = 2J^2 \left(\frac{1}{F-U} + \frac{1}{F} \right) (a_{l+2}^\dagger a_{l+1} a_l^\dagger a_{l+1} + \text{h.c.}), \quad (\text{A.12})$$

where the coefficients $\frac{2J^2}{F-U}$ and $\frac{2J^2}{F}$ were obtained computing the expression in Eq. (A.10). Interestingly each of the two possible virtual process depicted in Fig. A.1 are represented by combinations of the same creation (annihilation) operators acting on different sites that turn out to be equivalent ones. To see that, let us describe what is happening on each channel of Fig. A.1. If we label the sites by l , $l+1$, and $l+2$, then we are creating two particles in site $l+1$ and annihilating one particle in each site l and $l+2$. The two successive hoppings in top and bottom channels are represented by $a_{l+1}^\dagger a_l a_{l+1}^\dagger a_{l+2}$ and $a_{l+1}^\dagger a_{l+2} a_{l+1}^\dagger a_l$, respectively. These two operators are equivalent ones due to the commutation relations for bosonic operators.

A.1.2 Application of the SWT to the two-band Bose-Hubbard model

As described in Sec. A.1, we need to identify the intermediate states that are part of the full transit we want to perform. First, the initial and target states of our transit are the Fock states $|i\rangle = |11; 00\rangle$ and $|j\rangle = |10; 10\rangle$. This final state was chosen based on the results obtained in Sec. 3.3 where we could observe that once we are in such a state the dissipation leads us to the desired superposition.

It is enough for our study to work with a system of two particles in two wells (2/2). In that case, as we saw in Chap. 3 the Fock space of our problem has only 10 elements. It turns out that from all the possible eight intermediate states there is only one such state that will allow us to complete the desired transit. We are talking about $|k\rangle = |20; 00\rangle$ and the second order processes behind this transit consist of a hopping and a successive action of the inter-band coupling as depicted in Fig. A.2.

The Hamiltonian of our problem is given by

$$H = H_{B-H}^a + H_{B-H}^b + 2\pi F C_0 \sum_l (a_l^\dagger b_l + b_l^\dagger a_l), \quad (\text{A.13})$$

where $H_{B-H}^{a,b}$ stands for the single-band Bose-Hubbard Hamiltonian for each of the Bloch bands, and the extra term is the well known dipole coupling. In order to apply the Schrieffer-Wolff transformation we define V as,

$$V = J_a \sum_l (a_{l+1}^\dagger a_l + \text{h.c.}) + 2\pi F C_0 \sum_l (a_l^\dagger b_l + \text{h.c.}), \quad (\text{A.14})$$

the hopping in the lower band and the inter-band coupling. Once we have settled that we can easily compute the value in Eq. (A.10). Thus, the operator that accounts for the processes in Fig. A.2 is

$$\begin{aligned} O_{\text{SO}} &= \left(\frac{1}{2\pi F - W_a/2} - \frac{1}{W_a/2 - \Delta_g} \right) (2\pi F C_0 J_a) (b_l^\dagger a_l a_l^\dagger a_{l+1} + \text{h.c.}) \\ &= U_{\text{SO}} (b_l^\dagger a_{l+1} + \text{h.c.}) + U_{\text{SO}} (b_l^\dagger a_{l+1} + \text{h.c.}) n_l^a, \end{aligned} \quad (\text{A.15})$$

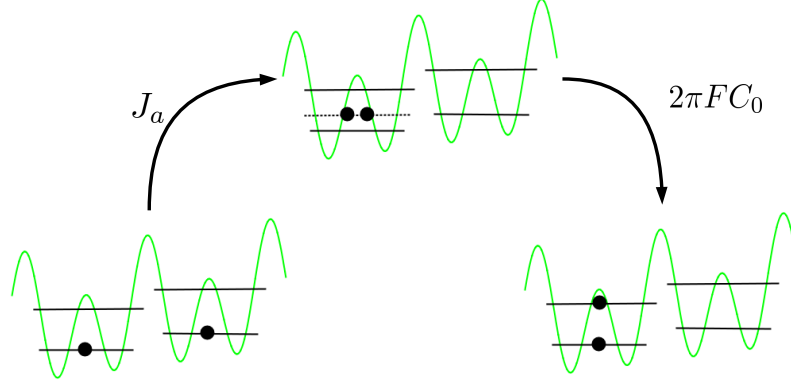


Figure A.2: Schematic representation of the second order processes that take place in our system. We start with a state $|11; 00\rangle$, then a hopping carry us to the intermediate state $|20; 00\rangle$, and finally the inter-band coupling makes us end in the desired state $|10; 10\rangle$.

where we have included the hermitian conjugate to guarantee conservation of energy, and $U_{\text{SO}} = \left(\frac{1}{2\pi F - W_a/2} - \frac{1}{W_a/2 - \Delta_g} \right)$. The parameter we have defined as U_{SO} is the respective form in terms of the Bose-Hubbard parameters for the value G_x introduced along with the Hamiltonian we have presented in Chap. 3.

Appendix B

Miscellaneous results regarding the parametric evolution

We have splitted this section in two main parts. First, results with the intra-site coupling (Sec. B.1), and second, results with the inter-site coupling (Sec. B.2). Why two different kind of couplings? The answer is simple, there are two different ways of introducing an inter-band coupling in the two-band Bose-Hubbard Hamiltonian. This coupling can connect the two bands by means of energy levels in the same site, just like the one we present in Chap. 3. Also, the coupling can connect the bands by means of energy levels in next neighboring sites. The last coupling is not an intuitive one, but we have to consider it since it is the one that the Schrieffer-Wolff transformation gives us (see Eq. (A.15)).

Along this appendix we preserve the same color code for figures and tables when labeling curves and states, respectively, for each pair of figure-table that stands for the results of the evolution with the same initial state. In addition, we have included in the tables the maximum probability of participation for the states that take part in the dynamics. We shall notice that such probabilities does not happen for the same value of α for all the states.

B.1 Results with the intra-site coupling

As stated at the end of Sec. 3.4 we have worked the dynamical evolution of our system for each of the α values in the proper mesh for two other different initial conditions. First we use $|2020; 0000\rangle$. The results for this initial condition can be seen in top panel of Fig. B.1. One interesting aspect of the results is the behavior of the states that get excited in the diabatic regime. Even when we are doing a fast sweep the system seems to have enough time to coupled some states to the initial one, and this coupling introduces oscillations among the participating states.

We have found that not even in the adiabatic regime the system is able to end in a superposition of states with alternating site population like $|1010; 0101\rangle$ and $|0101; 1010\rangle$, and the only one with equal population of both bands $|1010; 1010\rangle$ is being mixed in the diabatic regime. In top panel of Table B.1 we present the corresponding states with their respective maximum participation probability labeled by their position in the Fock basis. These probabilities are shown in top panel

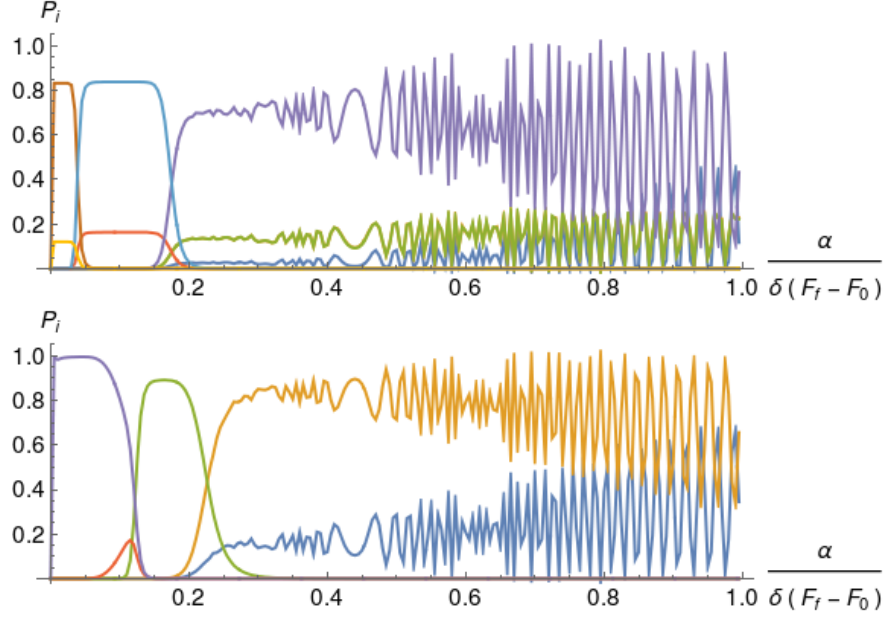


Figure B.1: Top: states participating in the navigation process for the initial state $|2020; 0000\rangle$. Bottom: states participating in the navigation process for the initial state $|0202; 0000\rangle$. In both cases there are three different dynamical regimes, adiabatic, non-adiabatic, and diabatic just as for the $2/2$ system.

Table B.1: Dynamical states for the initial condition $|2020; 0000\rangle$ (top) and $|0202; 0000\rangle$ (bottom). We tabulate the probability P_i (on the left of each column) of finding the i -th state (on the right of each column) in the final state for the diabatic, non-adiabatic and adiabatic regimes.

Diabatic regime		Non-adiabatic regime		Adiabatic regime	
$P_{10} = 0.4375$	$ 2020; 0000\rangle$	$P_{148} = 0.1630$	$ 0200; 1010\rangle$	$P_{233} = 0.8308$	$ 0100; 2010\rangle$
$P_{43} = 0.2519$	$ 1020; 1000\rangle$	$P_{237} = 0.8370$	$ 0100; 1110\rangle$	$P_{245} = 0.1201$	$ 0100; 1020\rangle$
$P_{80} = 0.2518$	$ 2010; 0010\rangle$				
$P_{149} = 0.9986$	$ 1010; 1010\rangle$				
Diabatic regime		Non-adiabatic regime		Adiabatic regime	
$P_{28} = 0.6621$	$ 0202; 0000\rangle$	$P_{73} = 0.9993$	$ 0102; 0100\rangle$	$P_{251} = 0.9948$	$ 0001; 0120\rangle$
		$P_{165} = 0.8911$	$ 0002; 0110\rangle$		
		$P_{242} = 0.1719$	$ 0010; 0210\rangle$		

of Fig. B.1 using the same color code of the previous table. States sharing the same color appear as equally weighted superpositions.

Then we use the state $|0202; 0000\rangle$ as initial condition. Here, the states that are excited as a consequence of the navigation present, in all the three regimes, a similar behavior of those of the $|2020; 0000\rangle$ initial condition (see Fig. B.1 (top)). In bottom panel of Table B.1 we present the respective states with their respective maximum participation probability labeled by their position in the Fock basis. We did not find in this case any equally weighted superposition of any kind. The only state with equal population of both bands $|0002; 0110\rangle$ participating in the dynamics is in the non-adiabatic regime being part of a superposition.

B.2 Results with the inter-site coupling

In App. A we found that the second order process we were after, appears as a correction to the Hamiltonian as a higher order term in the creation/annihilation operators for both Bloch bands. The two single particle energy levels in different bands that are being connected by this term are from next neighboring sites, hence, we talk of an inter-site coupling.

B.2.1 Results for the 2/2 system

Following the procedure depicted in Sec. 3.4 we performed the same steps and calculations for the 2/2 system, but now with a Hamiltonian which has an inter-site coupling rather than an intra-site coupling.

First, we look at the long time average population of the second band as a function of the Stark force (see left panel of Fig. B.2). We found signatures of resonant behavior around three different points, and it is of special interest for our study the one corresponding to the first order resonance, featuring the largest resonant response.

Then, we settled up our force functions to perform parametric evolution around this first order resonance. We compute the time evolution of our system with the initial condition of $|11; 00\rangle$ and investigate the states that got excited for different α values. The results can be seen in the right panel of Fig. B.2. We found that in the adiabatic and non-adiabatic regimes the only state that is excited by the time evolution is $|01; 10\rangle$, and for the diabatic regime we end up in the state $|11; 00\rangle$.

B.2.2 Results for the 4/4 system

Similarly to the previous section on the 2/2 system, here we focus our attention on the adiabatic regime of the 4/4 system and define our Stark force such that we evolve around the first order resonance. We compute the time evolution of our system for different α values. This calculation was done for three different initial conditions given by $|1111; 000\rangle$, $|2020; 0000\rangle$, and $|0202; 0000\rangle$.

First, for $|1111; 000\rangle$ there are only five states that take part in the evolution (see Fig. B.3 and Table B.2). Now there are no equally weighted superpositions in any of the three dynamical regimes. There is only one state with equal population of the bands, located inside the non-adiabatic regime, given by $|0011; 1100\rangle$.

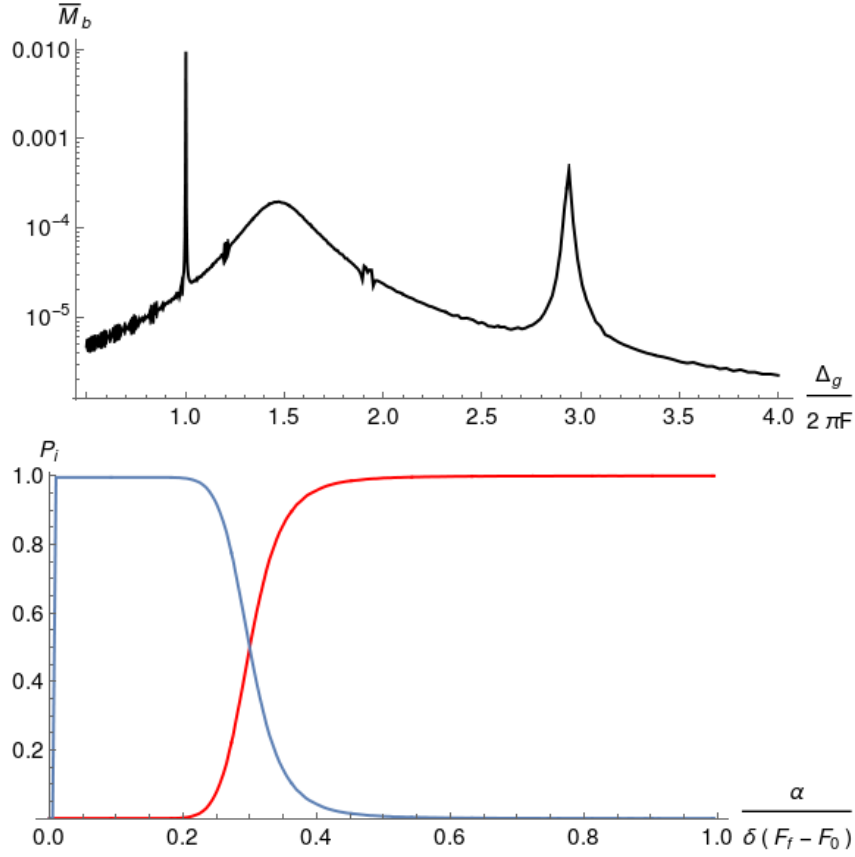


Figure B.2: Top: long time average of the population in the second band as a function of the external force tilting the system. We observe clear signatures of resonant behavior around three specific values of $\frac{\Delta_g}{2\pi F} = \{1, 1.5, 3\}$. We have interest in the first one, being this the respective value of the first order resonance. Bottom: different states participating in the time evolution for different values of α . There is only one state $|01; 10\rangle$ that is excited in both the adiabatic and non-adiabatic regime, and only one in the diabatic regime $|11; 00\rangle$.

Second, for the $|2020; 0000\rangle$ there are only four different states participating in the dynamics, see Fig. B.4 and Table B.3. Now in the diabatic regime we have presence of the initial state $|2020; 0000\rangle$ and an additional state $|2010; 0100\rangle$. Thus even when we go fast through the AC the system has enough time to couple the initial state to some other state. However, as we go deep in the diabatic regime we recover the normal behavior that is expected for this regime, ending completely in the initial state. Interestingly the adiabatic regime and the non-adiabatic regime have presence of the same two states, $|0100; 2100\rangle$ and $|0010; 1200\rangle$.

Third, for the initial condition $|0202; 0000\rangle$ there are only four dynamical states, see Fig. B.5 and Table B.4. There is one state in the adiabatic regime, $|0010; 1200\rangle$. There is one state in the non-adiabatic regime given by $|0002; 1100\rangle$. And the diabatic regime has two states. Initially there is a sub-regime within the diabatic one where the state $|0102; 1000\rangle$ dominates the dynamics, and later, deep in the diabatic regime, there is a sub-regime where the initial state $|1111; 0000\rangle$ dominates the dynamics.

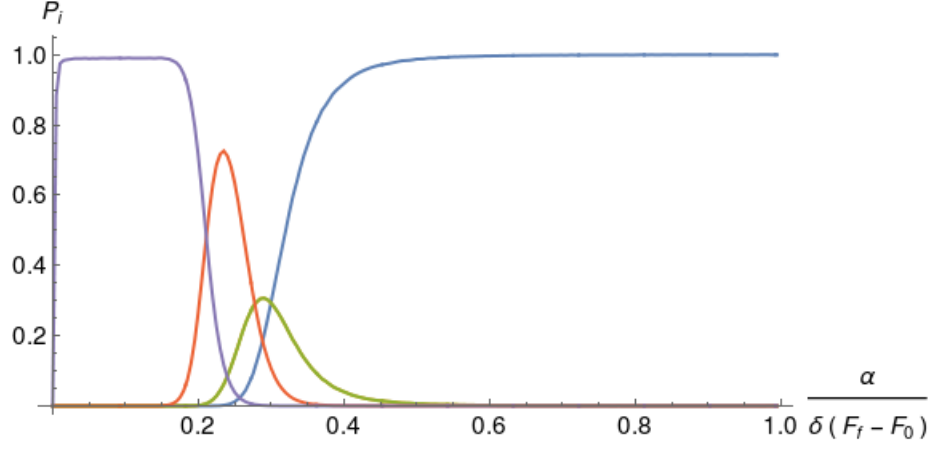


Figure B.3: Different states participating in the navigation process for the initial state $|1111; 0000\rangle$. There are three different dynamical regimes, adiabatic, non-adiabatic, and adiabatic just as for the $2/2$ system.

Table B.2: Dynamical states for the initial condition $|1111; 0000\rangle$ with Inter-site coupling. We tabulate the maximum probability P_i (on the left of each column) of finding the i -th state (on the right of each column) in the final state for the diabatic, non-adiabatic and adiabatic regimes.

Diabatic regime	Non-adiabatic regime	Adiabatic regime
$P_{21} = 0.9995$ $ 1111; 0000\rangle$	$P_{50} = 0.3071$ $ 0111; 1000\rangle$ $P_{69} = 0.3069$ $ 1011; 0100\rangle$ $P_{134} = 0.7257$ $ 0011; 1100\rangle$	$P_{226} = 0.9902$ $ 0010; 1200\rangle$

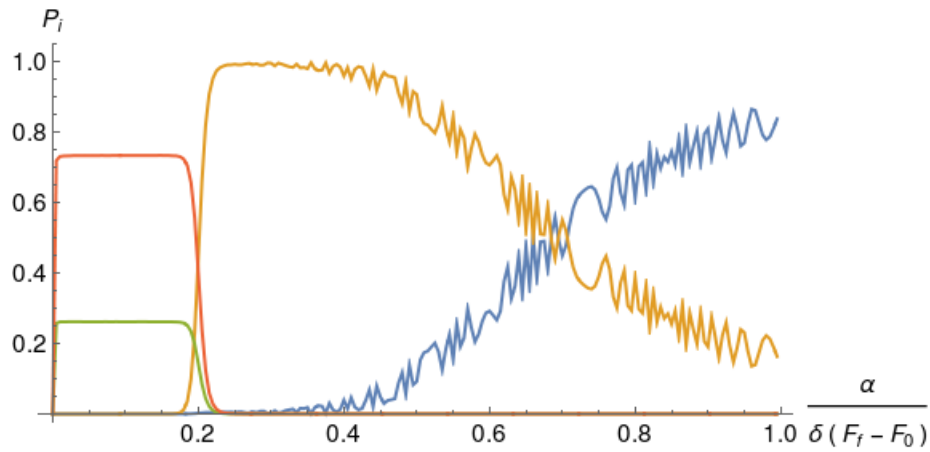


Figure B.4: Different states participating in the parametric evolution for the initial state $|2020; 0000\rangle$. There are three different dynamical regimes, adiabatic, non-adiabatic, and diabatic.

Table B.3: Dynamical states for the initial condition $|2020; 0000\rangle$ with inter-site coupling. We tabulate the maximum probability P_i (on the left of each column) of finding the i -th state (on the right of each column) in the final state for the diabatic, non-adiabatic and adiabatic regimes.

Diabatic regime		Non-adiabatic regime		Adiabatic regime	
$P_{10} = 0.8639$	$ 2020; 0000\rangle$	$P_{221} = 0.2613$	$ 0100; 2100\rangle$	$P_{221} = 0.2613$	$ 0100; 2100\rangle$
$P_{60} = 0.9959$	$ 2010; 0100\rangle$	$P_{226} = 0.7329$	$ 0010; 1200\rangle$	$P_{226} = 0.7329$	$ 0010; 1200\rangle$

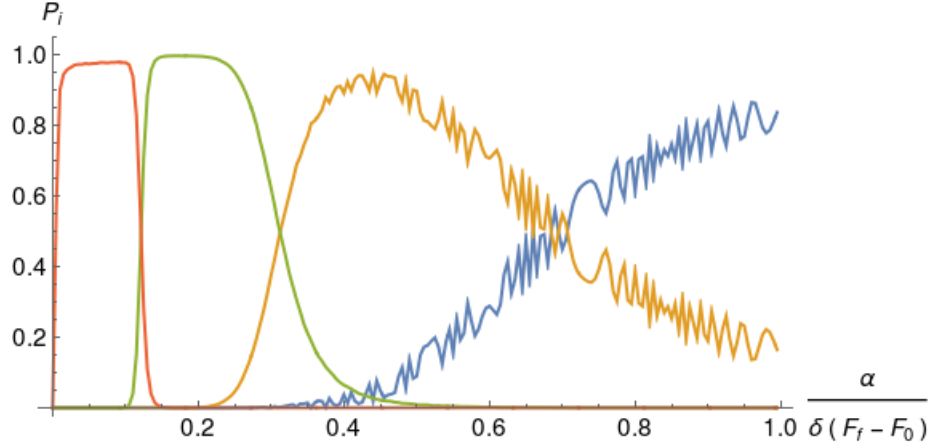


Figure B.5: Different states participating in the parametric evolution for the initial state $|0202; 0000\rangle$. There are three different dynamical regimes, adiabatic, non-adiabatic, and diabatic.

Table B.4: Dynamical states for the initial condition $|0202; 0000\rangle$ with inter-site coupling. We tabulate the maximum probability P_i (on the left of each column) of finding the i -th state (on the right of each column) in the final state for the diabatic, non-adiabatic and adiabatic regimes.

Diabatic regime		Non-adiabatic regime		Adiabatic regime	
$P_{28} = 0.8627$	$ 0202; 0000\rangle$	$P_{135} = 0.9943$	$ 0002; 1100\rangle$	$P_{226} = 0.9767$	$ 0010; 1200\rangle$
$P_{53} = 0.9444$	$ 0102; 1000\rangle$				

Appendix C

Interference time and a dipole in the middle of the lattice

This brief appendix is devoted to two issues. We expand on the results presented in Sec. 2.2.4 about the length of the interference patterns when we increase the size of the system. We also present a different example of the time evolution and behavior a dipole can have when it is placed in a different position than the edge of the chain.

C.1 Interference time

In Sec. 2.2.4 we presented the main result for the interference time which exhibits an exponential behavior with the size of the system. This conclusion was drawn with the help of the effective model, and we could see that the results in the whole model and the effective one match pretty well.

However, there is still a question for which we have not given an answer yet. Why did we have to study the case of even lattice size apart from those of odd size? From Fig. 2.7 it is clear that interference in odd sized systems last longer than in even sized systems. Such a differentiation can be attributed to the process by means of which the initial excitation (the dipole) delocalizes on the lattice space and later reconstruct its initial configuration. This can be seen in the IPR-like functional as defined in Sec. 2.2.3 which is plotted in Fig. C.1 (red curves). More precisely, we observe a series of decreasing peaks at short times characterizing the delocalization process of the wave packet, followed by a region of interference. For even number of sites the relocation occurs after this region of interference. For odd number of sites the situation is different. After the first region of interference the wave packet behavior alternates partial revivals of the initial configuration with interference. Only at large times the initial condition is recovered.

In left part of Fig. C.1 we present two examples of the time evolution of B-H systems with 8 and 12 sites, respectively. We see the appearance of the interference and how it clearly increases as we scale the number of lattice sites. The interference time we are reporting was taken to be the time between the peak of the IPR at zero and the highest value to the IPR following the previous one. In right panels of Fig. C.1 we present the same study but for systems with odd size: 9 and

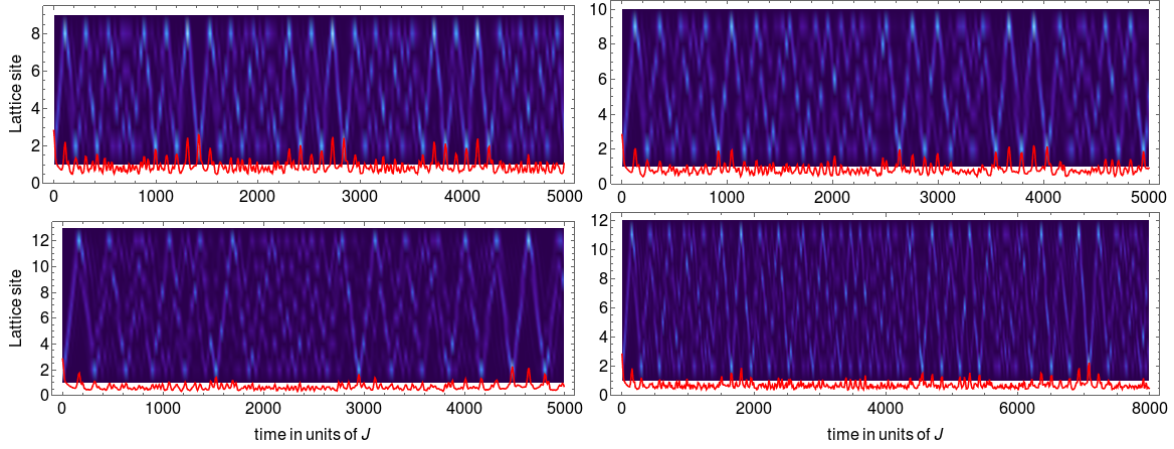


Figure C.1: Time evolution of the population in each lattice site within the effective XXZ-chain model representing a B-H system of eight (top-left), twelve (bottom-left), nine (top-right) and eleven (bottom-right) sites. For even number of sites the reconstruction of the wave packet occurs after the first interference process, while for odd number of sites there is a large region of interference and partial revivals before the initial wave packet is recovered.

11 sites, respectively.

Although the differentiation between odd sized and even sized systems is necessary from the point of view of the interference time. The neat result here is that this differentiation is only a finite size effect. We saw the evidence supporting this in last part of Sec. 2.2.4.

C.2 A dipole in the middle of the lattice

In Sec. 1.5 we present how it is possible to connect the single-band Bose-Hubbard model with the Heisenberg XXZ-model by means of tilting the lattice and a proper second order tunneling process. This connection allowed us to interpret the propagation of one single dipole as the propagation of a single spin impurity, in other words as a spin-wave.

So far the results we have presented were for a dipole placed in one edge of the lattice. In general one can think of other configurations. We consider here the special case when the dipole is placed in the middle of the lattice. That is, we choose as initial condition the Fock state $|112011\rangle$. For the sake of shortness we only present the results of its time evolution. We do not include extensive studies of the interference and other parts of the analysis we did in Chap. 2 because they are essentially very similar to the results already presented there.

What would be the evolution of our system with such initial condition? Since we are working in a tilted lattice where the translational invariance has been broken one might think that there is a natural direction for the propagation of excitations. In Fig. C.2 we present the results of the time evolution for the initial condition $|112011\rangle$ for both the full B-H model and the effective model.

The major result that can be seen in Fig. C.2 is that our initial assumption about the time evolution was wrong. That is remarkable, because even though we are in a system where the translational invariance has been broken, excitations, dipoles in our case, undergo a translational

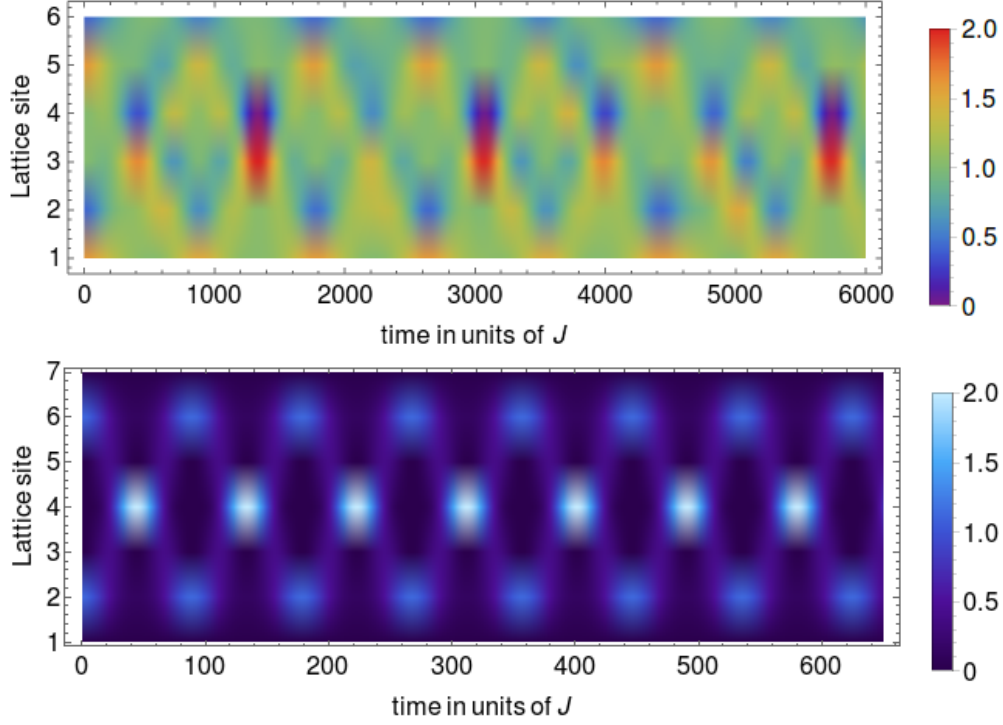


Figure C.2: Top: time evolution of the population for the different lattice sites in the Bose-Hubbard model with initial condition $|112011\rangle$. Blue refers to a vacancy or a holon while red means double population or doublon. Bottom: time evolution of the population of the lattice sites in the case of the effective model for the same initial condition as in the upper part.

invariant lattice and therefore there is no preferred direction of propagation. Also, the dipole propagates as a whole entity and does not split in its individual components, holon propagating in one direction and doublon propagating in the opposite one. Finally, the lower panel of Fig. C.2 we can see that the effective model is a neat representation of the dynamics in the whole B-H system.

Bibliography

- [1] C. C. Bradley, C. A. Sackett, and R. G. Hulet. *Bose-Einstein Condensation of Lithium: Observation of Limited Condensate Number*. *Physical Review Letters* **78**(6), 985–989 (1997). DOI: [10.1103/PhysRevLett.78.985](https://doi.org/10.1103/PhysRevLett.78.985).
- [2] K. Davis, M. Mewes, M. Andrews, N. van Druten, D. Durfee, D. Kurn, and W. Ketterle. *Bose-Einstein Condensation in a Gas of Sodium Atoms*. *Physical Review Letters* **75**(22), 3969–3973 (1995). DOI: [10.1103/PhysRevLett.75.3969](https://doi.org/10.1103/PhysRevLett.75.3969).
- [3] M H Anderson, J R Ensher, M R Matthews, C E Wieman, and E A Cornell. *Observation of bose-einstein condensation in a dilute atomic vapor*. *Science (New York, N.Y.)* **269**(5221), 198–201 (1995). DOI: [10.1126/science.269.5221.198](https://doi.org/10.1126/science.269.5221.198).
- [4] Markus Greiner, Olaf Mandel, Tilman Esslinger, Theodor W Hänsch, and Immanuel Bloch. *Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms*. *Nature* **415**(6867), 39–44 (2002). DOI: [10.1038/415039a](https://doi.org/10.1038/415039a).
- [5] Immanuel Bloch, Jean Dalibard, and Wilhelm Zwerger. *Many-body physics with ultracold gases*. *Reviews of Modern Physics* **80**(3), 885–964 (2008). DOI: [10.1103/RevModPhys.80.885](https://doi.org/10.1103/RevModPhys.80.885).
- [6] Immanuel Bloch, Jean Dalibard, and Sylvain Nascimbène. *Quantum simulations with ultracold quantum gases*. *Nature Physics* **8**(4), 267–276 (2012). DOI: [10.1038/nphys2259](https://doi.org/10.1038/nphys2259).
- [7] Jonathan Simon, Waseem S Bakr, Ruichao Ma, M Eric Tai, Philipp M Preiss, and Markus Greiner. *Quantum simulation of antiferromagnetic spin chains in an optical lattice*. *Nature* **472**(7343), 307–12 (2011). DOI: [10.1038/nature09994](https://doi.org/10.1038/nature09994).
- [8] M. Aidelsburger, M. Atala, M. Lohse, J. T. Barreiro, B. Paredes, and I. Bloch. *Realization of the Hofstadter Hamiltonian with Ultracold Atoms in Optical Lattices*. *Physical Review Letters* **111**(18), 185301 (2013). DOI: [10.1103/PhysRevLett.111.185301](https://doi.org/10.1103/PhysRevLett.111.185301).
- [9] J Struck, C Ölschläger, R Le Targat, P Soltan-Panahi, A Eckardt, M Lewenstein, P Windpassinger, and K Sengstock. *Quantum simulation of frustrated classical magnetism in triangular optical lattices*. *Science (New York, N.Y.)* **333**(6045), 996–9 (2011). DOI: [10.1126/science.1207239](https://doi.org/10.1126/science.1207239).
- [10] Carlos A. Parra-Murillo, Javier Madroñero, and Sandro Wimberger. *Quantum diffusion and thermalization at resonant tunneling*. *Physical Review A* **89**(5), 053610 (2014). DOI: [10.1103/PhysRevA.89.053610](https://doi.org/10.1103/PhysRevA.89.053610).

- [11] Michael Lubasch, Florian Mintert, and Sandro Wimberger. *Dynamical enhancement of spatial entanglement in massive particles*. *Physical Review A* **84**(6), 063615 (2011). DOI: [10.1103/PhysRevA.84.063615](https://doi.org/10.1103/PhysRevA.84.063615).
- [12] C. Sias, H. Lignier, Y. Singh, A. Zenesini, D. Ciampini, O. Morsch, and E. Arimondo. *Observation of Photon-Assisted Tunneling in Optical Lattices*. *Physical Review Letters* **100**(4), 040404 (2008). DOI: [10.1103/PhysRevLett.100.040404](https://doi.org/10.1103/PhysRevLett.100.040404).
- [13] C. Sias, A. Zenesini, H. Lignier, S. Wimberger, D. Ciampini, O. Morsch, and E. Arimondo. *Resonantly Enhanced Tunneling of Bose-Einstein Condensates in Periodic Potentials*. *Physical Review Letters* **98**(12), 120403 (2007). DOI: [10.1103/PhysRevLett.98.120403](https://doi.org/10.1103/PhysRevLett.98.120403).
- [14] Andreas Trabesinger. *Quantum simulation*. *Nature Physics* **8**(4), 263–263 (2012). DOI: [10.1038/nphys2258](https://doi.org/10.1038/nphys2258).
- [15] R. Blatt and C. F. Roos. *Quantum simulations with trapped ions*. *Nature Physics* **8**(4), 277–284 (2012). DOI: [10.1038/nphys2252](https://doi.org/10.1038/nphys2252).
- [16] Alán Aspuru-Guzik and Philip Walther. *Photonic quantum simulators*. *Nature Physics* **8**(4), 285–291 (2012). DOI: [10.1038/nphys2253](https://doi.org/10.1038/nphys2253).
- [17] Andrew A. Houck, Hakan E. Türeci, and Jens Koch. *On-chip quantum simulation with superconducting circuits*. *Nature Physics* **8**(4), 292–299 (2012). DOI: [10.1038/nphys2251](https://doi.org/10.1038/nphys2251).
- [18] T.W. Hänsch and A.L. Schawlow. *Cooling of gases by laser radiation*. *Optics Communications* **13**(1), 68–69 (1975). DOI: [10.1016/0030-4018\(75\)90159-5](https://doi.org/10.1016/0030-4018(75)90159-5).
- [19] P. D. Lett, W. D. Phillips, S. L. Rolston, C. E. Tanner, R. N. Watts, and C. I. Westbrook. *Optical molasses*. *Journal of the Optical Society of America B* **6**(11), 2084 (1989). DOI: [10.1364/JOSAB.6.002084](https://doi.org/10.1364/JOSAB.6.002084).
- [20] Harold J. Metcalf and Peter van der Straten. *Laser Cooling and Trapping*, volume 9. Springer Science & Business Media (2001).
- [21] Wolfgang Ketterle and N.J. Van Druten. *Evaporative Cooling of Trapped Atoms*. *Advances In Atomic, Molecular, and Optical Physics* **37**, 181–236 (1996). DOI: [10.1016/S1049-250X\(08\)60101-9](https://doi.org/10.1016/S1049-250X(08)60101-9).
- [22] C. J. Pethick and H. Smith. *Bose-Einstein Condensation in Dilute Gases*. Cambridge University Press (2002).
- [23] S. Bose. *Plancks Gesetz und Lichtquantenhypothesen*. *Zeitschrift für physik* **26**, 178 (1924).
- [24] Claude Cohen-Tannoudji, Jacques Dupont-Roc, and Gilbert Grynberg. *Photons and Atoms: Introduction to Quantum Electrodynamics*. Wiley (1997).
- [25] Roberto B. Diener, Georgios A. Georgakis, Jianxin Zhong, Mark Raizen, and Qian Niu. *Transition between extended and localized states in a one-dimensional incommensurate optical lattice*. *Physical Review A* **64**(3), 033416 (2001). DOI: [10.1103/PhysRevA.64.033416](https://doi.org/10.1103/PhysRevA.64.033416).

- [26] M Glück, Andrey R. Kolovsky, and Hans Jürgen Korsch. *Wannier–Stark resonances in optical and semiconductor superlattices*. *Physics Reports* **366**(3), 103–182 (2002). DOI: [10.1016/S0370-1573\(02\)00142-4](https://doi.org/10.1016/S0370-1573(02)00142-4).
- [27] Andrey Kolovsky and Andreas Buchleitner. *Floquet-Bloch operator for the Bose-Hubbard model with static field*. *Physical Review E* **68**(5), 056213 (2003). DOI: [10.1103/PhysRevE.68.056213](https://doi.org/10.1103/PhysRevE.68.056213).
- [28] C. Zener. *A Theory of the Electrical Breakdown of Solid Dielectrics*. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **145**(855), 523–529 (1934). DOI: [10.1098/rspa.1934.0116](https://doi.org/10.1098/rspa.1934.0116).
- [29] A. Zenesini, H. Lignier, G. Tayebirad, J. Radogostowicz, D. Ciampini, R. Mannella, S. Wimberger, O. Morsch, and E. Arimondo. *Time-Resolved Measurement of Landau-Zener Tunneling in Periodic Potentials*. *Physical Review Letters* **103**(9), 090403 (2009). DOI: [10.1103/PhysRevLett.103.090403](https://doi.org/10.1103/PhysRevLett.103.090403).
- [30] Andrea Tomadin. *Quantum Chaos with Ultra Cold Atoms in Optical Lattices*. Master’s thesis, University of Pisa (2006).
- [31] A. Fetter and J. Walecka. *Quantum Theory of Many-Particle Systems*. McGraw-Hill, New York (1971).
- [32] M. Olshanii. *Atomic Scattering in the Presence of an External Confinement and a Gas of Impenetrable Bosons*. *Physical Review Letters* **81**(5), 938–941 (1998). DOI: [10.1103/PhysRevLett.81.938](https://doi.org/10.1103/PhysRevLett.81.938).
- [33] Neil W. Ashcroft and N. David Mermin. *Solid State Physics*. Holt, Rinehart and Winston (1976).
- [34] W. Kohn. *Construction of Wannier Functions and Applications to Energy Bands*. *Physical Review B* **7**(10), 4388–4398 (1973). DOI: [10.1103/PhysRevB.7.4388](https://doi.org/10.1103/PhysRevB.7.4388).
- [35] Carlos A. Parra-Murillo. *Many-Body Dynamics of Ultra Cold Atoms in Optical Lattices*. Ph.d. thesis, Heidelberg University (2013).
- [36] Patrick Plötz. *Complex Dynamics of Ultra Cold Atoms*. Ph.d. thesis, Heidelberg University (2010).
- [37] Hans-Jürgen Mikeska and Alexei K. Kolezhuk. *One-dimensional magnetism*. In Ulrich Schollwöck, Johannes Richter, Damian J. J. Farnell, and Raymod F. Bishop, editors, *Quantum Magnetism*, volume 645 of *Lecture Notes in Physics*, pages 1–88. Springer Berlin Heidelberg, Berlin, Heidelberg (2004).
- [38] A. Langari. *Phase diagram of the antiferromagnetic XXZ model in the presence of an external magnetic field*. *Physical Review B* **58**(21), 14467–14475 (1998). DOI: [10.1103/PhysRevB.58.14467](https://doi.org/10.1103/PhysRevB.58.14467).
- [39] Subir Sachdev, K. Sengupta, and S. Girvin. *Mott insulators in strong electric fields*. *Physical Review B* **66**(7), 075128 (2002). DOI: [10.1103/PhysRevB.66.075128](https://doi.org/10.1103/PhysRevB.66.075128).

- [40] Andrey Kolovsky. *Bloch oscillations in the Mott-insulator regime*. *Physical Review A* **70**(1), 015604 (2004). DOI: [10.1103/PhysRevA.70.015604](https://doi.org/10.1103/PhysRevA.70.015604).
- [41] Ian B Spielman. *Atomic physics: A route to quantum magnetism*. *Nature* **472**(7343), 301–2 (2011). DOI: [10.1038/nature10101](https://doi.org/10.1038/nature10101).
- [42] A. A. Ovchinnikov, D. V. Dmitriev, V. Ya. Krivnov, and V. O. Cheranovskii. *Antiferromagnetic Ising chain in a mixed transverse and longitudinal magnetic field*. *Physical Review B* **68**(21), 214406 (2003). DOI: [10.1103/PhysRevB.68.214406](https://doi.org/10.1103/PhysRevB.68.214406).
- [43] Subir Sachdev. *Quantum Phase Transitions*. Cambridge University Press, 2nd edition (2011).
- [44] F. Meinert, M. J. Mark, E. Kirilov, K. Lauber, P. Weinmann, A. J. Daley, and H.-C. Nägerl. *Quantum Quench in an Atomic One-Dimensional Ising Chain*. *Physical Review Letters* **111**(5), 053003 (2013). DOI: [10.1103/PhysRevLett.111.053003](https://doi.org/10.1103/PhysRevLett.111.053003).
- [45] Michael V Berry, I Marzoli, and W Schleich. *Quantum carpets, carpets of light*. *Physics World* **June 2001** (2001).
- [46] J. Schrieffer and P. Wolff. *Relation between the Anderson and Kondo Hamiltonians*. *Physical Review* **149**(2), 491–492 (1966). DOI: [10.1103/PhysRev.149.491](https://doi.org/10.1103/PhysRev.149.491).
- [47] Raymond Chan and Miklós Gulácsi. *The exact Schrieffer–Wolff transformation*. *Philosophical Magazine* **84**(12), 1265–1279 (2004). DOI: [10.1080/14786430310001653107](https://doi.org/10.1080/14786430310001653107).
- [48] Andrea Tomadin, Riccardo Mannella, and Sandro Wimberger. *Many-Body Interband Tunneling as a Witness of Complex Dynamics in the Bose-Hubbard Model*. *Physical Review Letters* **98**(13), 130402 (2007). DOI: [10.1103/PhysRevLett.98.130402](https://doi.org/10.1103/PhysRevLett.98.130402).
- [49] Andrea Tomadin, Riccardo Mannella, and Sandro Wimberger. *Many-body Landau-Zener tunneling in the Bose-Hubbard model*. *Physical Review A* **77**(1), 013606 (2008). DOI: [10.1103/PhysRevA.77.013606](https://doi.org/10.1103/PhysRevA.77.013606).
- [50] Alessandro Zenesini, Hans Lignier, Donatella Ciampini, Oliver Morsch, and Ennio Arimondo. *Coherent Control of Dressed Matter Waves*. *Physical Review Letters* **102**(10), 100403 (2009). DOI: [10.1103/PhysRevLett.102.100403](https://doi.org/10.1103/PhysRevLett.102.100403).
- [51] H. Lignier, C. Sias, D. Ciampini, Y. Singh, A. Zenesini, O. Morsch, and E. Arimondo. *Dynamical Control of Matter-Wave Tunneling in Periodic Potentials*. *Physical Review Letters* **99**(22), 220403 (2007). DOI: [10.1103/PhysRevLett.99.220403](https://doi.org/10.1103/PhysRevLett.99.220403).
- [52] Carlos A. Parra-Murillo, Javier Madroñero, and Sandro Wimberger. *Two-band Bose-Hubbard model for many-body resonant tunneling in the Wannier-Stark system*. *Physical Review A* **88**(3), 032119 (2013). DOI: [10.1103/PhysRevA.88.032119](https://doi.org/10.1103/PhysRevA.88.032119).
- [53] Mark G. Bason, Matthieu Viteau, Nicola Malossi, Paul Huillery, Ennio Arimondo, Donatella Ciampini, Rosario Fazio, Vittorio Giovannetti, Riccardo Mannella, and Oliver Morsch. *High-fidelity quantum driving*. *Nature Physics* **8**(2), 147–152 (2011). DOI: [10.1038/nphys2170](https://doi.org/10.1038/nphys2170).

- [54] Shen Shun-Qing. *Topological Insulators - Dirac Equation in Condensed Matters*. Springer-Verlag Berlin Heidelberg, 1st edition (2012).
- [55] Sergey Bravyi, David P. DiVincenzo, and Daniel Loss. *Schrieffer–Wolff transformation for quantum many-body systems*. *Annals of Physics* **326**(10), 2793–2826 (2011). DOI: [10.1016/j.aop.2011.06.004](https://doi.org/10.1016/j.aop.2011.06.004).
- [56] M. Dalmonte, E. Ercolessi, M. Mattioli, F. Ortolani, and D. Vodola. *Magnetic properties of commensurate Bose-Bose mixtures in one-dimensional optical lattices*. *The European Physical Journal Special Topics* **217**(1), 13–27 (2013). DOI: [10.1140/epjst/e2013-01750-2](https://doi.org/10.1140/epjst/e2013-01750-2).
- [57] T. Barthel, C. Kasztelan, I. P. McCulloch, and U. Schollwöck. *Magnetism, coherent many-particle dynamics, and relaxation with ultracold bosons in optical superlattices*. *Physical Review A* **79**(5), 053627 (2009). DOI: [10.1103/PhysRevA.79.053627](https://doi.org/10.1103/PhysRevA.79.053627).



UNIVERSIDAD DEL VALLE
FACULTAD DE CIENCIAS NATURALES Y EXACTAS
ACTA DE EVALUACION DE TRABAJO DE GRADO
PROGRAMA ACADEMICO DE FISICA

JURADO CONFORMADO POR:

1. DOCTORA KAREM RODRIGUEZ
2. DOCTOR JAVIER MADROÑERO.

El día 29 de Octubre de 2015 a las 9:00AM, se llevó a cabo la SUSTENTACION del TRABAJO DE GRADO titulado **"Estados planetarios en sistemas atómicos de dos electrones"**. Presentado por la estudiante ISABEL GUZMÁN NARANJO código: 0838134, bajo la dirección del Profesor: JAVIER MADROÑERO.

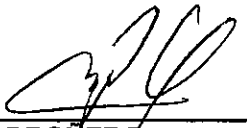
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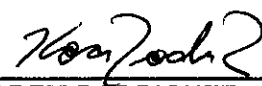
- ☒ APROBADO.
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☐ RECOMENDACIÓN DE DISTINCION DE LAUREADO.
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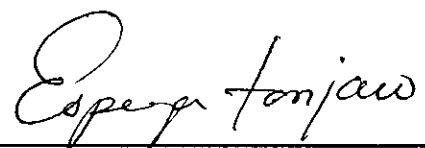
Se recomienda modificaciones: SI () NO ☒.

OBSERVACIONES

No se presentan observaciones adicionales


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Trabajo de grado
(Proyecto de investigación)
Departamento de Física
Facultad de Ciencias Naturales y Exactas
Universidad del Valle



Planetary States in Two-electron Atomic Systems

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Abstract

Complexity is found in physics even in “small” and simple systems such as the helium atom. This system represents the paradigm of the three body Coulomb problem which is non-integrable due to the interelectronic interaction. This interaction is the origin of its high complexity and electronic correlations. The non-integrability manifest itself classically in the mixed phase space of the helium atom, which is formed of small regular regions inside a chaotic sea. Of special interest is the stable region that corresponds to the frozen planet configuration (FPC). It is large enough to support the quantum states called *frozen planet states* (FPS). They are doubly excited states and under periodic driving they might transform into non-dispersive wave packets. Those wave packets are quantum objects that propagate along the classical trajectories of the system *without* dispersion.

The major interest for the study of these objects arises from their many possible applications in the quantum control and quantum information fields. However, any experimental evidence has not been obtained yet not even of the existence of the FPS. In this work we will be focus in deepen the understanding of the above mentioned states and to study the mechanisms to obtain them. In particular, the characterization of both decay channels: the radiative decay and the photoionization decay and the atomic transitions from those states through few photons will be studied.

Resumen

La complejidad se encuentra en la física atómica incluso en sistemas “pequeños” y aparentemente simples como el átomo de helio. Este sistema es el paradigma del problema de Coulomb de tres cuerpos, caracterizado por ser no integrable debido a la interacción interelectrónica, que a su vez es el origen de la alta complejidad y de correlaciones electrónicas. La no integrabilidad se manifiesta clásicamente en el carácter mixto del espacio de fase del átomo de helio, formado por pequeñas regiones regulares inmersas en un mar caótico. En especial, es interesante la región asociada a la configuración estable de planeta congelado. Dichas regiones son suficientemente grandes como para soportar estados del análogo cuántico. Por ejemplo, encontramos los *estados de planeta congelado* que son estados doble y altamente excitados y que bajo la acción de un forzamiento externo periódico pueden transformarse en paquetes de onda no dispersivos. Estos paquetes son objetos cuánticos que se propagan a lo largo de trayectorias clásicas del sistema *sin* dispersión.

El mayor interés por el estudio de estos objetos viene de sus posibles aplicaciones en las áreas de control cuántico e información cuántica. Sin embargo, aún no se ha obtenido ninguna evidencia experimental ni siquiera de la existencia de los estados de planeta congelado. Aquí nos centraremos en ampliar el conocimiento sobre dichos estados y en estudiar mecanismos para su obtención. En particular, se estudiarán los canales de decaimiento radiativo y de fotoionización y las transiciones atómicas desde estos estados mediadas por pocos fotones.

1 Introduction

The three body problem -as in the helium atom- has kept the interest for decades and even today there are still phenomena that remain unexplained. The high degree of complexity is due to the interelectronic interaction. This leads to the non integrability of the system, which produces in the classical description chaotic dynamics and also the complex ionization spectrum of the atom [1–3]. The non integrability of the unperturbed atom entails the partial destruction of good quantum numbers to describe the system. This characteristic is the origin of surprising effects such as the autoionizing doubly excited states [4]; resonance overlap that leads to fluctuations in the atomic spectrum [5]; highly correlated states [1, 6, 7], in which highly asymmetrical, but very stable configurations of frozen planet are found in the doubly excited atom [1, 6].

The energy spectrum of helium is composed of series of states converging to the single ionization thresholds, where one electron is ionized from the atom (see figure 1). Above the single ionization thresholds there are the continua of those free electrons. Below the first ionization threshold the states are bound with one electron in its ground state and the other in an excited state while doubly excited states are found above this threshold. Due to the interelectronic interaction, most of the doubly excited states [8, 9] are not bound states but resonances, that is, states that can decay by autoionization into the continua of lower series of states.

From the classical point of view the helium atom exhibits mixed regular and chaotic dynamics, that is, only for special initial conditions the motion of the two electrons is stable. A particular stable configuration is the frozen planet configuration (FPC) where the nucleus and the two electrons are collinear and the electrons are located on the same side of the nucleus. The stability is a consequence of the fast oscillations of the inner electron bouncing on the nucleus which generate a weakly attractive adiabatic potential for the outer electron [10]. The FPC is a paradigm of the relation between the classical system and its quantum counterpart. This can be understood using semiclassical arguments. For Coulomb type potentials the energy regime close to zero is a semiclassical regime, where the classical dynamics mimics the quantum dynamics [11, 12]. In case of helium, this corresponds to the regime of highly doubly excited states. Therefore, if the regular region of the FPC is large enough¹ it can support quantum states which are called frozen planet states (FPS). FPS are thus localized along the classical trajectories of the FPC.

FPS are a particular type of planetary states, that is, states with highly asymmetrical electronic excitations. FPS were predicted more than two decades ago [6], but they still await for the experimental observation. This fact is due to the negligible dipole coupling between the ground state of helium and FPS, that is, the transition probability between these two states is close to zero when the atom interacts with a photon with energy equal to the energy difference between the initial and final states [2, 3]. Nevertheless, evidence for the existence of planetary states has been already found [13]. Therefore, one process to obtain an atom in a FPS requires a multiphoton excitation and for that reason is important to investigate the coupling between singly excited states and doubly excited states, FPS in particular. Additionally, the decay channels, that are the possible processes in which the atom can decay to lower energy states, carry important information about the stability of both the intermediate states and FPS. Among these processes, the photoionization and the radiative decay are relevant. The first decay mechanism is due to the electron-electron interaction and produces the spontaneous ionization of one electron in an excited state. The second mechanism arises from the interaction between the atom and the electromagnetic field,

¹That is, the classical action of periodic orbits of the FPC is larger than $\hbar$.

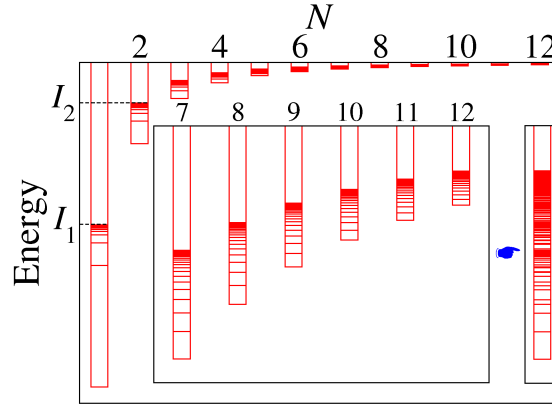


Figure 1: Sketch of helium spectrum. The states are organized in Ridgberg series converging to the ionization thresholds I_N , where N is the principal quantum number of the inner electron, and all series converge to the double ionization threshold at $E = 0$. The states below I_1 are bound. The states above I_1 are coupled to the continua of lower series and are thus resonances than can undergo autoionization processes.

where the atom emits a photon when the transition of an electron from an excited state to a lower energy state occurs.

The last mechanism has been recently thoroughly studied theoretically [14–17] and experimentally [17–19]. It has been found that for special series of doubly excited states below the second ionization threshold the fluorescence is the principal mechanism above photoionization. In consequence, the complete characterization of FPS and the description of the transitions to these states should be done in order to look for intermediate states that can mediate in a multiphoton process between the helium ground state and FPS.

In this work we are going to study the coupling between excited bound states and FPS. Going beyond the second ionization threshold in a realistic 3D approach is challenging. Therefore, in a first approach we are going to restrict to a planar model where both electrons and the nucleus is restricted to a plane, which has been proved to provide a good qualitative and even quantitative description of helium [20].

The structure of this work is the following: after this brief introduction we provide in chapter 2 the theoretical background to describe the quantum dynamics of the planar helium atom. Here we present an appropriate representation of the stationary Schrödinger equation in terms of harmonic oscillators in order to give a proper treatment to the singularities of the hamiltonian. We also introduce the complex rotation method, which combined with the above representation provides the energies and autoionization rates of the doubly excited states of the atom. Furthermore, this approach allows us to calculate useful observables, such as the photoionization cross section, the spontaneous emission and the probability density. The numerical diagonalization of the resulting generalized eigenvalue problem is achieved with the help of the Lanczos algorithm.

Chapter 3 starts with a brief description of the most important known aspects of the FPC and FPS. Then, the coupling of FPS with bound states is analysed using the theoretical tools described in chapter 2. We conclude this chapter with a brief discussion on a possible way to experimentally prepare FPS.

We conclude this document in chapter 4 with a brief summary of our work and an outlook for

possible further stability analysis of FPS, the extension of the present analysis to the real 3D helium atom and the possibility of formation of non dispersive wave packets when considering the driven system.

Finally, we have also included appendix [A](#) which contains some technical details about the spontaneous emission for excited states in the 2D helium atom and the channel theory in sections [A.1](#) and [A.2](#), and further results of the coupling between bound states and FPS in section [A.3](#).

2 The Planar Model for the Helium Atom

In this chapter we describe the most important aspects of our planar model. We start by introducing an appropriate set of coordinates which allows us to represent the SSE in terms of four coupled harmonic oscillators. The description of autoionizing states is achieved with the help of the complex rotation method. Within this approach we can calculate observables such as projections in configuration space of the probability density of resonances, the photionization cross section from bound states into the regime of doubly excited states and rates of spontaneous emission of resonances.

2.1 Justification of Helium Planar Model

The dynamics of the three body Coulomb problem can be described in a simplified manner by the Schrödinger equation taking a fixed nucleus at the origin and neglecting the relativistic corrections. For the description and subsequent identification of doubly excited states and the transitions from bound states to FPS through few photons we need a proper representation of the stationary Schrödinger equation (SSE). For that, we start with the hamiltonian of a two electron atom, which is given in atomic units (a.u) ²

$$H = \frac{p_1^2}{2} + \frac{p_2^2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \quad (1)$$

where Z is the atomic number, r_i is the distance from the nucleus to each electron, p_i is the corresponding momentum, and r_{12} is the distance between the two electrons. In the present work we are going to be restricted to a planar model of the atom, i.e. we confine both electrons and the nucleus to a plane. It has been shown that the planar model reproduces qualitatively and even quantitatively well the dynamics of highly excited states of helium [21–23]. The reason for this is twofold: on the one hand, the semiclassical limit of the Coulomb interaction lies in the high energy regime $E \rightarrow 0$, that is in the range of highly excited states [11]. On the other hand, the scaling properties of the classical dynamics of helium ensure that the total angular momentum scales as $|E|^{\frac{1}{2}}$ [12]. Consequently, for $E \rightarrow 0$ the scaled total angular momentum is close to zero and the classical dynamics is planar [24].

2.2 Coordinate Representation

The most difficult aspect to handle in the SSE is the singularities r_i and r_{12} , however, they can be regularized with three coordinate transformations.

First Transformation

First a parabolic transformation is performed which changes from $\{x_1, y_1, x_2, y_2\}$ to $\{\mu_1, \nu_1, \mu_2, \nu_2\}$

$$\begin{aligned} x_1 &= \frac{1}{2} (\mu_1^2 - \nu_1^2), & x_2 &= \frac{1}{2} (\mu_2^2 - \nu_2^2), \quad \text{for } i = 1, 2, \\ y_1 &= \mu_1 \nu_1, & y_2 &= \mu_2 \nu_2. \end{aligned}$$

²We use all over this document atomic units unless it is stated otherwise.

The expression for r_i and for the kinetic term are given by

$$r_i = \frac{1}{2} (\mu_i^2 + \nu_i^2), \quad \nabla_i^2 = \frac{1}{\mu_i^2 + \nu_i^2} \left(\frac{\partial^2}{\partial \mu_i^2} + \frac{\partial^2}{\partial \nu_i^2} \right),$$

however, the interaction term r_{12} is still given in terms of a square root.

Second Transformation

The second transformation is a rotation of $\theta = 45^\circ$ and it changes from $\{\mu_1, \nu_1, \mu_2, \nu_2\}$ to $\{\mu_p, \nu_p, \mu_m, \nu_m\}$

$$\begin{aligned} \mu_p &= \frac{1}{\sqrt{2}} (\mu_1^2 + \mu_2^2), & \mu_m &= \frac{1}{\sqrt{2}} (\mu_1^2 - \mu_2^2), \\ \nu_p &= \frac{1}{\sqrt{2}} (\nu_1^2 + \nu_2^2), & \nu_m &= \frac{1}{\sqrt{2}} (\nu_1^2 - \nu_2^2). \end{aligned}$$

Third Transformation

The last transformation is another parabolic transformation that changes from $\{\mu_p, \nu_p, \mu_m, \nu_m\}$ to $\{x_p, y_p, x_m, y_m\}$

$$\begin{aligned} \mu_p &= \frac{1}{2} (x_p^2 - y_p^2), & \mu_m &= \frac{1}{2} (x_m^2 - y_m^2), \\ \nu_p &= x_p y_p, & \nu_m &= x_m y_m, \end{aligned}$$

with this transformation now r_i and r_{12} are polynomial expressions of the new set of coordinates and are given by

$$\begin{aligned} 16r_1 &= ((x_p - y_m)^2 + (x_m + y_p)^2)((x_p + y_m)^2 + (x_m - y_p)^2), \\ 16r_2 &= ((x_p - x_m)^2 + (y_p - y_m)^2)((x_p + x_m)^2 + (y_p + y_m)^2), \\ 4r_{12} &= (x_p^2 + y_p^2)(x_m^2 + y_m^2). \end{aligned}$$

Then, the regularized Schrödinger equation is obtained multiplying the SSE by the Jacobian of the three transformations

$$\begin{aligned} B &= 16r_1 r_2 r_{12}, \\ \left(-\frac{1}{2}T + V \right) |\psi\rangle &= EB |\psi\rangle, \end{aligned}$$

where the polynomial expressions of the kinetic and potential energy are

$$\begin{aligned} T &= 16r_1 r_2 r_{12} (\nabla_1^2 + \nabla_2^2), \\ V &= 16(Zr_2 r_{12} + Zr_1 r_{12} + \gamma r_1 r_2). \end{aligned}$$

2.3 Harmonic Oscillator Representation

As both the kinetic and potential terms are polynomial expressions in the new set of coordinates and in their derivatives is natural to introduce creation and annihilation operators

$$\begin{aligned} a_{x_p} &= \frac{1}{\sqrt{2}} \left(x_p + i \frac{\partial}{\partial x_p} \right), & a_{x_m} &= \frac{1}{\sqrt{2}} \left(x_m + i \frac{\partial}{\partial x_p} \right), \\ a_{y_p} &= \frac{1}{\sqrt{2}} \left(y_p + i \frac{\partial}{\partial y_p} \right), & a_{y_m} &= \frac{1}{\sqrt{2}} \left(y_m + i \frac{\partial}{\partial y_m} \right). \end{aligned}$$

Moreover, as it is possible to obtain the expression for the coordinates and derivatives in terms of these operators then, both the kinetic and potential terms are also polynomial expressions of the ladder operators. Further simplifications can be made if circular operators are introduced

$$\begin{aligned} a_1 &= \frac{1}{\sqrt{2}} (a_{x_p} - i a_{y_p}), & a_3 &= \frac{1}{\sqrt{2}} (a_{x_m} - i a_{y_m}), \\ a_2 &= \frac{1}{\sqrt{2}} (a_{x_p} + i a_{y_p}), & a_4 &= \frac{1}{\sqrt{2}} (a_{x_m} + i a_{y_m}). \end{aligned}$$

The new set of coordinates in terms of the circular operators are given by

$$\begin{aligned} x_p &= \frac{1}{2} (a_1 + a_2 + a_1^\dagger + a_2^\dagger), \\ y_p &= \frac{1}{2} (a_1 - a_2 - a_1^\dagger + a_2^\dagger), \\ x_m &= \frac{1}{2} (a_3 + a_4 + a_3^\dagger + a_4^\dagger), \\ y_m &= \frac{1}{2} (a_3 - a_4 - a_3^\dagger + a_4^\dagger). \end{aligned}$$

For example, the angular momentum L_z in terms of circular operators reads

$$L_z = \frac{1}{4} (a_1^\dagger a_1 - a_2^\dagger a_2 - a_3^\dagger a_3 - a_4^\dagger a_4).$$

Circular operators obey the same commutation relations as ladder operators

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0, \quad [a_i, a_j^\dagger] = \delta_{ij}.$$

Thus, a basis set of Fock states, which is a complete basis of the Hilbert space of wave functions, can be used and to each pair of circular operators a harmonic oscillator is associated.

$$|\psi\rangle = |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle \otimes |n_4\rangle \equiv |n_1, n_2, n_3, n_4\rangle.$$

However, when the parabolic transformations are performed unphysical symmetries are introduced because the parabolic transformation $(x, y) \rightarrow (\mu, \nu)$ is a double mapping of the Cartesian plane into the plane of the new coordinates. Then, the physical wave function must satisfy the parity condition $\psi(\mu, \nu) = \psi(-\mu, -\nu)$, which is taken into account by a proper symmetrization of the Fock basis.

The symmetrization of the basis can be done analysing the permutation of the indices of the circular operators of the Fock states S_{3412} (that is $(1, 2, 3, 4) \mapsto (3, 4, 1, 2)$) to show that the states $|n_1, n_2, n_3, n_4\rangle$ and $|n_3, n_4, n_1, n_2\rangle$ represent the same physical state. From the three coordinate

transformation it can be shown that the permutation corresponds to the transformation of the new set of coordinates

$$S_{3412} \begin{pmatrix} x_p \\ y_p \\ x_m \\ y_m \end{pmatrix} = \begin{pmatrix} x_m \\ y_m \\ x_p \\ y_p \end{pmatrix} \leftrightarrow \begin{pmatrix} \mu_m \\ \nu_m \\ \mu_p \\ \nu_p \end{pmatrix} \leftrightarrow \begin{pmatrix} \mu_1 \\ \mu_2 \\ \nu_1 \\ \nu_2 \end{pmatrix} \leftrightarrow \begin{pmatrix} x_1 \\ y_1 \\ x_2 \\ y_2 \end{pmatrix} .$$

This shows that this permutation leaves invariant the Cartesian coordinates (x_1, y_1, x_2, y_2) . Then S_{3412} is the identity in the space of cartesian coordinates. However $S_{3412} |n_1, n_2, n_3, n_4\rangle = |n_3, n_4, n_2, n_1\rangle$ the action of S_{3412} on the basis $|n_1, n_2, n_3, n_4\rangle$ is not the identity. Therefore, the elements of the basis must be symmetrized as

$$|n_1, n_2, n_3, n_4\rangle^+ = |n_1, n_2, n_3, n_4\rangle + |n_3, n_4, n_1, n_2\rangle .$$

In addition, an invariance group of the Hamiltonian (1) contains the reflections Π_x and Π_y with respect to the x and y axis, and the particle exchange operator P_{12} [8, 21]. Since L_z^2 commutes with the hamiltonian (1) and with these simmetry operations, a good set of quantum numbers is constituted by the absolute value $|l|$ of the angular momentum L_z , the exchange symmetry P_{12} quantum number (singlet and triplet states) and the symmetry Π_x quantum number $\epsilon_x = \pm 1$. Since the efect of Π_x on a basis element is given by

$$\Pi_x |n_1 n_2 n_3 n_4\rangle = |n_2 n_1 n_4 n_3\rangle ,$$

it can be shown that the appropriate symmetrized basis addapted for Π_x , L_z^2 and P_{12} is [8, 21]

$$|n_1 n_2 n_3 n_4\rangle^{+\epsilon_x} = |n_1 n_2 n_3 n_4\rangle^+ + \epsilon_x |n_2 n_1 n_4 n_3\rangle^+$$

with $\epsilon_x = \pm 1$.

In order to calculate the matrix elements of the hamiltonian, the action of the circular operators on a state is needed

$$a |n\rangle = \sqrt{n} |n-1\rangle , \quad a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle ,$$

then, the non-zero matrix elements of the hamiltonian $\langle n'_1 n'_2 n'_3 n'_4 | H | n_1 n_2 n_3 n_4 \rangle \neq 0$ have analytical expressions that can be easily calculated. The SSE takes the form of the generalized eigenvalue problem (EVP)

$$\mathcal{A} |\psi\rangle = E B |\psi\rangle . \quad (2)$$

2.4 Helium Spectrum

The understanding of the complex helium spectrum is essential before the SSE is solved. In order to give a brief description we consider the full hamiltonian of the system in a compact way

$$H = \left(\frac{\mathbf{p}_1^2}{2} + \frac{Z}{r_1} \right) + \left(\frac{\mathbf{p}_2^2}{2} + \frac{Z}{r_2} \right) + \frac{\gamma}{r_{12}} .$$

If the electron-electron interaction in H is neglected ($\gamma = 0$), then, the sum of two hydrogenic hamiltonians is obtained

$$H = H_1 + H_2 ,$$

with a well known spectrum organized in Rydberg series whose energy is given by ³

$$E = -\frac{2}{(N_1 - 1/2)^2} - \frac{2}{(N_2 - 1/2)^2},$$

for each integer quantum number N_i of both electrons. These series converge to single ionization thresholds I_N and all of them converge to the double ionization threshold at zero energy. If now the interaction is turned on ($\gamma = 1$) the single ionization thresholds $I_N = -\frac{2}{(N-1/2)^2}$ are expected to remain at the same energy position, because if one electron is ionized the separation between the two electrons tends to infinity and the interaction term $1/r_{12}$ is negligible. Also, above I_1 most states are coupled to the continuum of lower series and therefore, they are no longer bound states but resonances, that can decay into those continua.

2.5 Complex Rotation-Dilation Method

To extract the resonant states and their decay rates we use complex rotation and dilation. Here we present only the most important results of the method because the complete description and understanding of it is far beyond the scope of this work. The rotation method is based on the analytic continuation of the Green's function into the complex plane. The green's function for a time-independent Hamiltonian is

$$G(E) = \frac{1}{E - H}.$$

The complex poles of G correspond to the energies $\text{Re}(E_i)$ and decay rates $-2 \text{Im}(E_i)$ of the resonant states. However, the Green's function is not calculated, instead the coordinates of the complex plane are rotated an angle $0 < \theta < \pi/4$ and a dilation is also introduced. The rotation-dilation operator is defined as

$$D_\alpha(\theta) = e^{\beta \frac{\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}}{2}}, \quad (3)$$

where β has been defined in general as a complex number

$$\beta = \theta + i \log \alpha.$$

The action of the operator $D_\alpha(\theta)$ on a state $|\phi\rangle$ is

$$D_\alpha(\theta)\phi(\mathbf{r}) = e^{i \log \alpha + \theta} \phi(e^{i \log \alpha + \theta} \mathbf{r}).$$

The corresponding *transformed hamiltonian* is given by

$$H_\alpha(\theta) = D_\alpha(\theta) H D_\alpha^{-1}(\theta), \quad (4)$$

where $D_\alpha(\theta)$ generates the transformations

$$\mathbf{r} \rightarrow \mathbf{r} \alpha e^{i\theta}, \quad \mathbf{p} \rightarrow \mathbf{p} \frac{e^{-i\theta}}{\alpha},$$

Therefore, the rotated-dilated hamiltonian reads

$$H_\alpha(\theta) = \frac{e^{-2i\theta}}{\alpha^2} \left(\frac{\mathbf{p}_1^2 + \mathbf{p}_2^2}{2} \right) + \frac{e^{-i\theta}}{\alpha} \left(\frac{1}{r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_1} \right).$$

³The eigenvalues of planar hydrogen are $E_N = -\frac{1}{2(N-\frac{1}{2})^2}$

The operator $\frac{\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}}{2}$ is hermitian. Therefore, from (3) it follows that a dilation ($\theta = 0$) is a unitary transformation while a rotation or a dilation-rotation is not. Consequently, the dilated-rotated hamiltonian $H_\alpha(\theta)$ is non hermitian. However, the spectrum of the rotated hamiltonian is related to the spectrum of the original one and has the following properties [25–28]

- (a) The eigenvectors $|\psi_{E_{i\theta}}\rangle$ of $H_\alpha(\theta)$ form a complete basis set of Hilbert space.
- (b) The bound spectrum of $H_\alpha(\theta)$ is invariant under complex rotation.
- (c) There are θ -independent eigenvalues of $H_\alpha(\theta)$ located in the lower half of the complex plane, which correspond to the resonances of the hamiltonian. The real part is the real energy E of the resonance and the imaginary part is related with the autoionization rate $-\Gamma/2$.
- (d) The continuum states are located on parallel half lines that are rotated an angle -2θ around the single ionization thresholds I_N .

Since the dilation is an unitary transformation it leaves invariant the eigenvalues of the hamiltonian. However, due to the truncation of the basis in the numerical implementation there is a dependence of the results on the dilation parameter. Therefore, this parameter can be used as a variational parameter for optimization of the numerical results [8].

2.6 Wave Function Representation

To analyse the localization properties of FPS the expression for the probability density of the wave functions is needed in terms of the eigenvalues of the rotated hamiltonian and it was taken from [8]. If we have an energy state $|\varphi\rangle$ then the electronic probability density in configuration space reads

$$|\varphi_E(\mathbf{r})|^2 = \langle \mathbf{r} | \varphi_E \rangle \langle \varphi_E | \mathbf{r} \rangle = \frac{1}{\pi} \text{Im} \sum_j \frac{\langle \mathbf{r} | R(-\theta) | \varphi_{j\theta} \rangle^2}{E_{j\theta} - E} \approx \frac{1}{\pi |\text{Im} E_{j\theta}|} \text{Re} \langle \mathbf{r} | R(-\theta) | \varphi_{j\theta} \rangle^2,$$

where the approximation is called the single pole approximation and it is achieved by taking into account only a well isolated resonance $|E_{j\theta}\rangle$ with $E_{j\theta} \approx E$ and $|E_{j\theta} - E_{i\theta}| \gg |E_{j\theta} - E|$, $\forall i \neq j$ that gives the main contribution to the sum.

2.7 Photoionization Cross Section

The Fermi golden rule, which gives the probability for the electronic transition between two states of an atom when it interacts with an external field, applied to the photoionization process leads to the expression for the cross section [29]. The photoionization process is a two step process: first, an atom is excited into a resonance state by absorption of a photon from an external electromagnetic field. Second, the autoionization of this doubly excited state decays produces an ion and a free electron. The autoionization process is due to the interelectronic interaction. The photoionization cross section reads

$$\sigma(\omega_0) = 4\pi^2 \omega_0 \sum_j |\langle \phi_{jE} | D(\hat{\mathbf{e}}_0) | \phi_g \rangle|^2,$$

where $|\phi_g\rangle$ is the bound initial atomic state with energy E_g , ω_0 is the transition energy, $|\phi_{jE}\rangle$ is the energy normalized continuum eigenstate with energy $E = E_g + \omega_0$, D is the dipole operator and $\hat{\mathbf{e}}_0$ is the polarization vector of the incident photon beam.

To introduce the complex rotation method the projection operator of a resonant eigenstate $|\varphi_E\rangle$ is expressed in the base of the rotated states [30, 31]

$$|\varphi_E\rangle\langle\varphi_E| = \frac{1}{2\pi i} \sum_i \left(\frac{R(-\theta) |\varphi_{i\theta}\rangle \langle\varphi_{i\theta}| R(\theta)}{E_{i\theta} - E} - \frac{R(-\theta) |\overline{\varphi_{i\theta}}\rangle \langle\varphi_{i\theta}| R(\theta)}{i\theta - E} \right).$$

Using the complex rotation method the expression for the photoionization cross section (PCS) reads [24]

$$\sigma(\omega_0) = 4\pi\alpha\omega_0 \text{Im} \sum_i \frac{|\langle\varphi_{i\theta}| R(\theta) DB |\phi_g\rangle|^2}{E_{i\theta} - E_g - \omega_0}, \quad (5)$$

where $|\varphi_{i\theta}\rangle$ is the resonant state with complex energy $E_{i\theta} = E_i - i\Gamma/2$, $D = \hat{e}_0 \cdot \mathbf{r} = x_1 + x_2$ in 2D with the incident photon beam linearly polarized in the x direction.

2.8 Spontaneous Emission

In the spontaneous emission, a photon is emitted when the atom in an excited state undergoes a transition to a lower energy state, due to the interaction with the vacuum electromagnetic field. The spontaneous emission of an atom in an excited state can be obtained from the Fermi Golden rule applied to the 2D system. We use the expression for the radiative decay in 3D (see appendix A.1 and A.2 for details). This can be justified using semiclassical arguments: The helium atom in a high energy regime $E \rightarrow 0$, which corresponds to the semiclassical regime, behaves like a 2D object in space [11]. Therefore, in order to calculate the radiative decay of a doubly excited state in helium, the position vector $\mathbf{r}$ for the electrons has to be expressed as a 2D vector in the Fermi Golden rule. However, the density of photon states is the same as in the 3D case. Also, as there are no restrictions to the direction or polarization of the emitted photon, the integration is performed over all directions and different polarizations. After the integration the expression for the partial decay rate of a state $|\phi_n\rangle$ is obtained [29]

$$\gamma_{n \rightarrow f} = \sum_{\lambda} \left(\frac{4\omega_{\lambda}^3 \alpha^3}{2} \right) |\hat{\pi}_{\lambda}^* \cdot \langle\phi_f| \mathbf{r} |\phi_n\rangle|^2,$$

where $\hat{\pi}_{\lambda}^*$ is the polarization vector, $|\phi_n\rangle$ and $|\phi_f\rangle$ are the initial and final states, and ω_{λ} is the energy difference between them. If the contributions to all states with energies $E_f < E_n$ are added the total spontaneous emission of the state ϕ_n is obtained

$$\gamma_n = \frac{4\omega^3 \alpha^3}{3} \sum_f (\langle\phi_f| x_1 + x_2 |\phi_n\rangle^2 + \langle\phi_f| y_1 + y_2 |\phi_n\rangle^2).$$

If the initial state is a resonance $|\varphi_{n\theta}\rangle$ in the frame of complex rotation, the total decay rate is [32]

$$\gamma = \frac{4\alpha^3}{3} \sum_f (\text{Re}(E_n) - E_f)^3 \text{Re}(\langle\varphi_{f\theta}|(x_1 + x_2)B|\varphi_{n\theta}\rangle^2 + \langle\varphi_{f\theta}|(y_1 + y_2)B|\varphi_{n\theta}\rangle^2),$$

where E_f is real because only bound states are considered in the sum. Only the real part of the dipole transition elements is taken into account (see appendix A.2 for details) since it is equal to the dipole coupling between the initial state and the bound part of the wave function.

2.9 Numerical Implementation

In order to calculate numerically the coupling between the bound states and the FPS first of all the diagonalization of the EVP (2) is required. For this, we use the code used in [24], which allows us to obtain the eigenvalues and eigenvectors of the planar helium that are needed to calculate the photoionization cross section (5). We have implemented in this code a subroutine to calculate the dipole matrix elements $\langle \varphi_{i\theta} | R(\theta) DB | \phi_g \rangle$ in the representation described above, which includes the jacobian B of the four coordinate transformations.

For the diagonalization of the generalized EVP (2) a Lanczos algorithm is used, which allows one to calculate the largest eigenvalues of an eigenvalue problem. Here, the most basic aspects of the method are briefly described. The details of the original method can be found in [33] and further details about the subroutine we use can be found in [34–36]. In our generalized EVP the involved matrices $\mathcal{A}$ and B are complex symmetric, banded, sparse and rather large. However, we are not interested in all the eigenvalues of the system but those within a energy range centred around a given energy E_0 . To achieve this, the generalized eigenvalue problem (2) can be modified to an EVP by multiplication from the left with $\mathcal{A}^{-1}$

$$\mathcal{A}^{-1} B |\psi\rangle = \frac{1}{E} |\psi\rangle.$$

Using the Lanczos algorithm we obtain the largest eigenvalues (i.e. $E \approx 0$). But before using this algorithm the matrix $\mathcal{A}$ is shifted by E_s to obtain the set of eigenvalues near the energy value E_s , i.e.

$$\mathcal{A} \rightarrow \mathcal{A} - E_s B.$$

The generalized eigenvalue problem is changed to

$$(\mathcal{A} - E_s B)^{-1} B |\psi\rangle = \frac{1}{E - E_s} |\psi\rangle.$$

The largest eigenvalues ($E \approx E_s$) are obtained for a given shift parameter E_s and also the corresponding eigenvectors.

3 Frozen Planet States and their Coupling to Bound States

We start this chapter providing a summary of the most important known aspects of the FPC and the FPS in section 3.1 and 3.2, respectively. Then, in section 3.3, we analyse the couplings of these states with bound states (BS), with the machinery described in the previous chapter. This will be done in order to shed some light for the experimental realization of FPS.

The nomenclature used here for BS is ${}_L\mathcal{B}_i$ where L is the total angular momentum and i is the number of the bound state, with $i = 1$ to 6. The BS considered in this work are presented in the table 1 with the color code established for each state. The nomenclature for FPS is similar ${}_L\mathcal{F}_k^N$ where N is the ionization threshold at which FPS of the series converge and k is an ascending number used to identify FPS in the series they belong to.

Table 1: Bound states ${}_L\mathcal{B}_i$, energy E , color code.

${}_L\mathcal{B}_i$	E (a.u)	Color code
${}_1\mathcal{B}_1$	-8.211542	Magenta
${}_1\mathcal{B}_2$	-8.077637	Cyan
${}_1\mathcal{B}_3$	-8.039947	Purple
${}_1\mathcal{B}_4$	-8.024280	Orange
${}_1\mathcal{B}_5$	-8.01630	Blue
${}_1\mathcal{B}_6$	-8.0117	Green

3.1 Classical Frozen Planet Configuration

In the FPC the two electrons are localized at the same side of the nucleus in a highly asymmetrical collinear configuration, as is shown in figure 2(a). Although it may seem unstable, it has been shown in classical studies [37–39] that the FPC is very stable indeed. The inner electron moves in highly eccentric orbits colliding with the nucleus and the outer electron experiences a time-independent weakly attractive potential, which is shown in figure 2(b), due to the rapid motion of the inner electron. The outer electron is thus localized around an equilibrium position far away from the nucleus characterized by slow oscillations. This potential is obtained when the rapid motion of the inner electron is averaged [10] in its characteristic time scale [39] and from it, the equilibrium distance of the outer electron can be determined.

The classical dynamics of the FPC is regular as can be seen in the Poincarè surface of section (figure 2(c)) [37, 39]. Each point of this surface represents the position x_1 and momentum p_1 of the outer electron when the inner electron collides with the nucleus. The volume occupied by the stability region of the FPC is large enough to support eigenstates of the quantum hamiltonian, which are localized along the classical frozen planet orbits. These states are characterized by a long life-time as their classical counterpart and they can be identified in 2D helium [8].

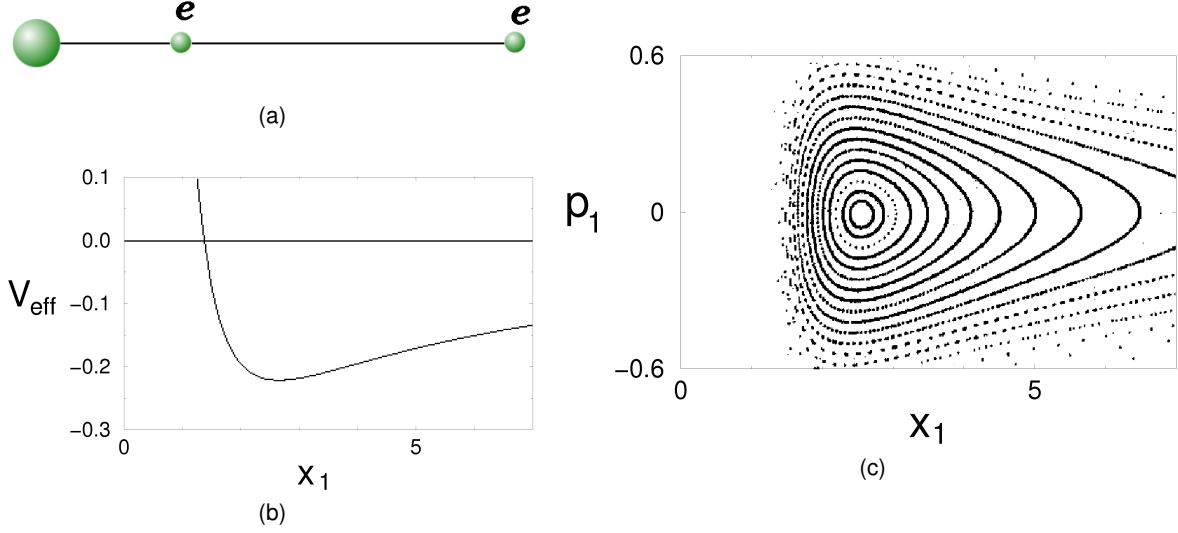


Figure 2: (a) Frozen planet configuration with both electrons at the same side of the nucleus in an asymmetrical configuration. (b) Effective time-independent weakly attractive potential [10] experienced by the outer electron and generated by the rapid motion of the inner electron near the nucleus. (c) Poincaré surface of section [39], where each point of this surface represents the position x_1 and momentum p_1 of the outer electron when the inner electron collides with the nucleus [10].

3.2 Frozen Planet States

When the generalized EVP (2) with the rotated hamiltonian is solved the energies and photoionization rates are obtained. The complex spectra of the hamiltonian converging to the ionization thresholds I_4 and I_5 are shown in figures 3(a) and 4(a), respectively. In those figures we can identify FPS, which are localized close to the real energy axis (red circles), having large life-times and being organized in series converging to each ionization threshold. These states should have the smallest photoionization decay rates Γ due to the large stability of the classical frozen planet configuration, compared to other resonances. The classical FPC was shown to be collinear in section 3.1. Therefore, the expectation value of $\langle \cos \theta_{12} \rangle$ for these states has to be close to 1. In figures 3(b) and 4(b) the expectation value $\langle \cos \theta_{12} \rangle$ of the resonances converging to I_4 and I_5 are shown, where the resonances highlighted in figures 3(a) and 4(a) have the values $\langle \cos \theta_{12} \rangle$ close to 1. For the FPS below I_4 $\langle \cos \theta_{12} \rangle \approx 0.78$ and below I_5 , $\langle \cos \theta_{12} \rangle \approx 0.84$ and as we go to more excited FPS this value goes closer to 1, i.e θ_{12} is closer to 0.

Figure 5(a) shows the projection of the wave function on the plane $\theta_{12} = 0$ of ${}_0\mathcal{F}_2^4$. It can be seen that the position of the electrons at maximum probability density are significantly different: the inner electron is very close to the nucleus at $r_2 \approx 8$, while the outer electron is localized far away at $r_1 \approx 57$. In figure 5(b) two plots are joined together: in the left plot, we have the projection of the probability density of the same FPS into the inner electron coordinates (x_2, y_2) , fixing the outer electron coordinates at the maximum probability density obtained in figure 5(a); and in the right plot, we do the same but with the outer electron, fixing the inner electron coordinates at the maximum probability density. We can observe in a clearer way that the position of the maxima of both electron are farther apart. This electronic configuration was expected from the classical

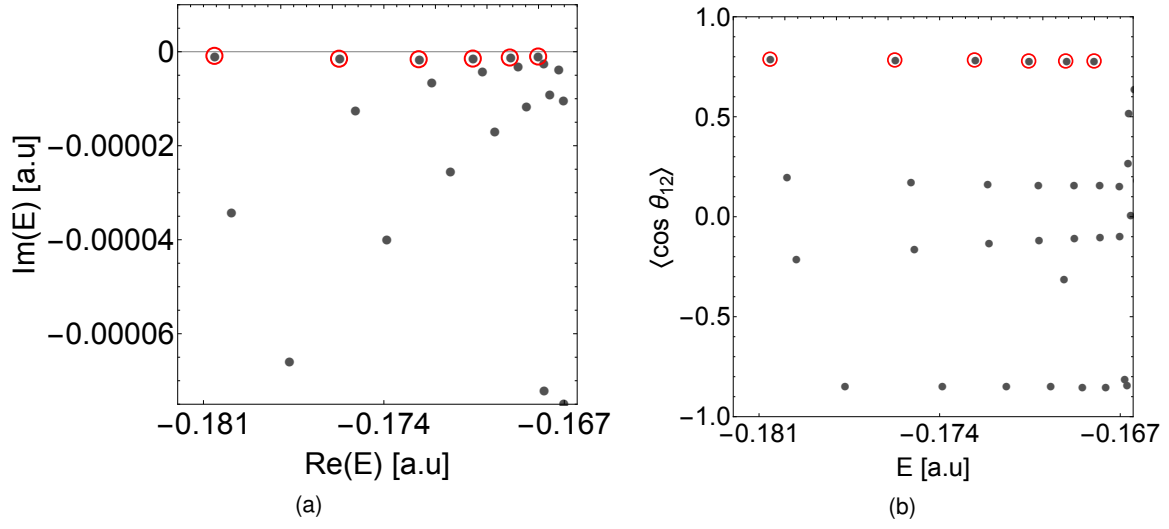


Figure 3: (a) Singlet spectrum of the rotated hamiltonian below the 4th ionization threshold, where FPS (red circles) show large life-times. (b) Expectation value $\langle \cos \theta_{12} \rangle$ for the states converging to I_4 , where FPS (red circles) have a value $\langle \cos \theta_{12} \rangle$ close to 1.

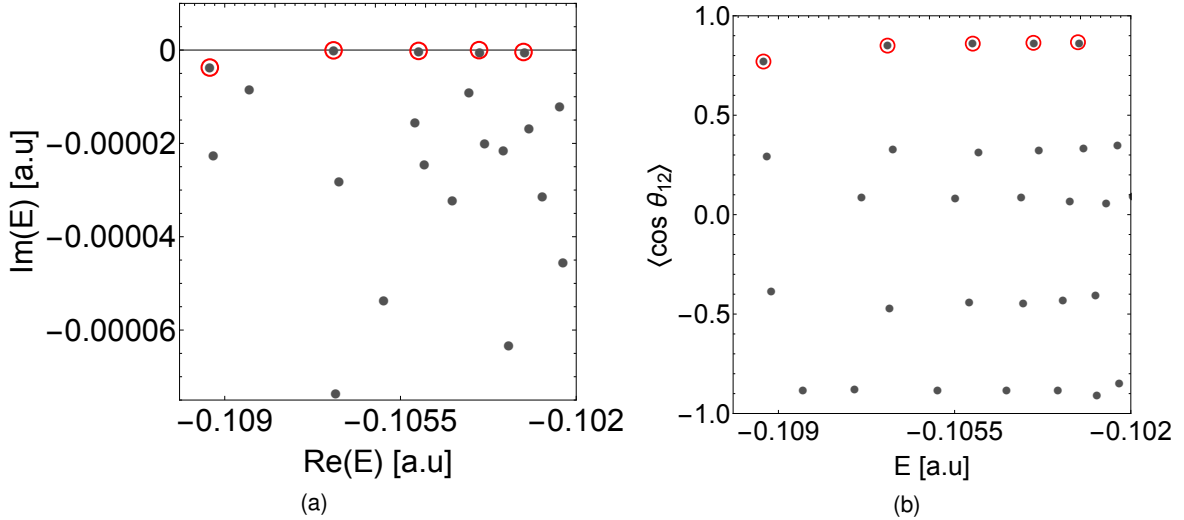


Figure 4: (a) Singlet spectrum of the rotated hamiltonian below the 5th ionization threshold, where FPS (red circles) show large life-times. (b) Expectation value $\langle \cos \theta_{12} \rangle$ for the states converging to I_5 , where FPS (red circles) have a value of $\langle \cos \theta_{12} \rangle$ close to 1.

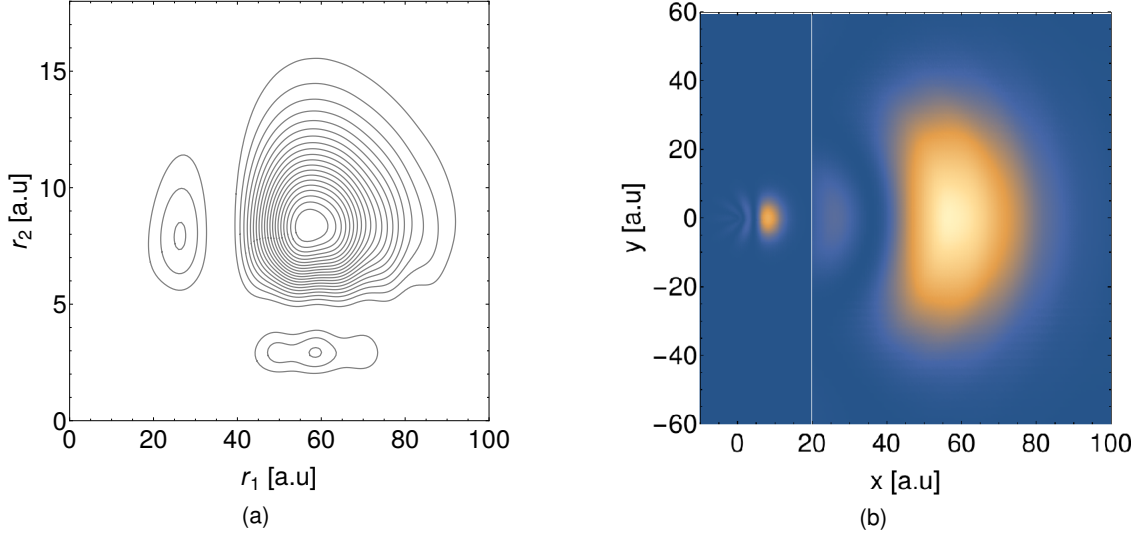


Figure 5: (a) Probability density of ${}_0\mathcal{F}_2^4$ projected into the plane $\cos \theta_{12} = 0$. (b) Probability density of ${}_0\mathcal{F}_2^4$ projected into the inner electron coordinates (left part of the graph), keeping fixed the outer electron coordinates at $(57, 0)$, and probability density projected into the outer electron coordinates (right part of the graph), keeping fixed the inner electron coordinates at $(8, 0)$. The positions of the electrons at the maximum probability density are farther apart, being the inner electron close to the nucleus and the outer electron far away from it.

Table 2: FPS ${}_L\mathcal{F}_k^N$ below I_4 and I_5 , energy E , $-\Gamma/2$ and expectation value of $\langle \cos \theta_{12} \rangle$.

${}_L\mathcal{F}_k^N$	E (a.u)	$-\Gamma/2$ (a.u)	$\langle \cos \theta_{12} \rangle$
${}_0\mathcal{F}_1^4$	-0.180560506	-0.00000087	0.787
${}_0\mathcal{F}_2^4$	-0.175570510	-0.00000148	0.785
${}_0\mathcal{F}_3^4$	-0.172615384	-0.00000159	0.782
${}_0\mathcal{F}_4^4$	-0.170535542	-0.00000132	0.781
${}_0\mathcal{F}_1^5$	-0.109297550	-0.00000374	0.772
${}_0\mathcal{F}_2^5$	-0.106832792	-0.00000006	0.856
${}_0\mathcal{F}_3^5$	-0.105139479	-0.00000017	0.869

description of the three-body Coulomb problem discussed in section 3.1. We can also see the remain of the classical motion of the inner electron close to the nucleus as small orbits at the left of the position of the maximum probability density of this electron.

A more thorough study of the stability properties of FPS requires an insight into the radiative decay rates. The formalism has been already described in section 2.8 and appendix A.1 and A.2. The numerical implementation is in ongoing work.

3.3 Photoionization Cross Section of FPS

To study the coupling between BS with $L = 1$ and FPS with $L = 0$, we focus our analysis on FPS converging to I_4 and I_5 . These FPS are trivially not coupled to the the ground state of planar helium ${}_0\mathcal{G}$ due to the selection rules of the dipole operator. It is worth to mention that ${}_0\mathcal{G}$ is neither coupled to any $L = 1$ FPS (${}_1\mathcal{F}_k^N$) [23]. Therefore, to populate $L = 0$ or $L = 1$ FPS from the

ground state it is necessary at least a two-photon transition. Here we explore the possibility of populating $L = 0$ FPS ${}_0\mathcal{F}_k^N$ by a two-photon excitation process using as intermediate states the BS ${}_1\mathcal{B}_i$.

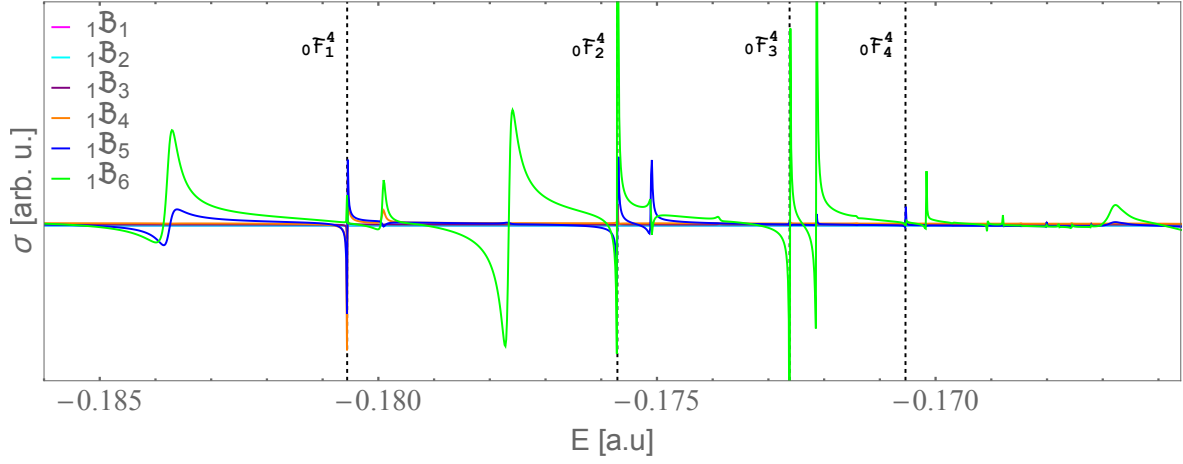


Figure 6: PCS from the initial states ${}_1\mathcal{B}_i$ $i = 1$ to 6 to the final states between I_3 and I_4 . The FPS ${}_0\mathcal{F}_i^4$ (dashed lines) converge also to the ionization threshold.

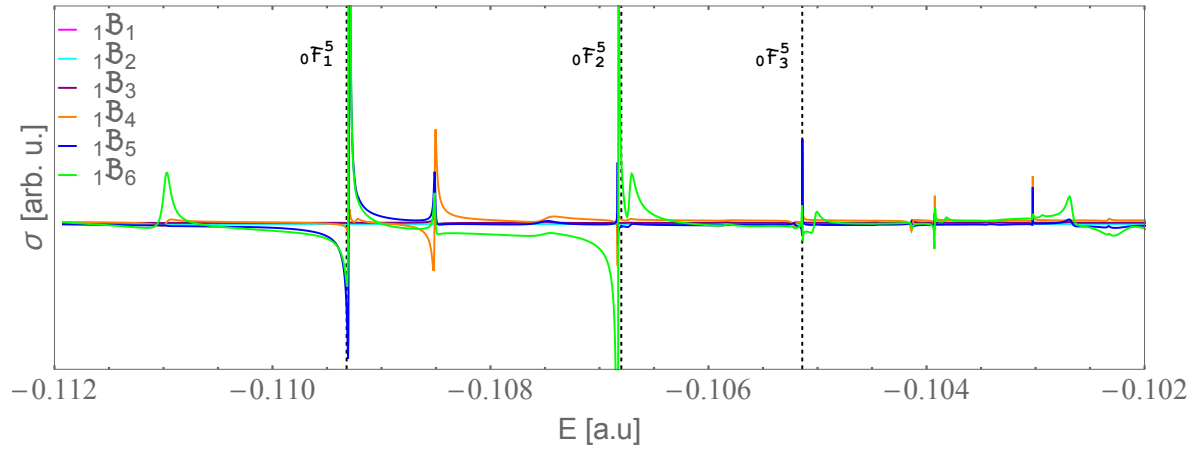


Figure 7: PCS from the initial states ${}_1\mathcal{B}_i$ $i = 1$ to 6 to the final states between I_4 and I_5 . The FPS ${}_0\mathcal{F}_i^5$ (dashed lines) converge also to the ionization threshold.

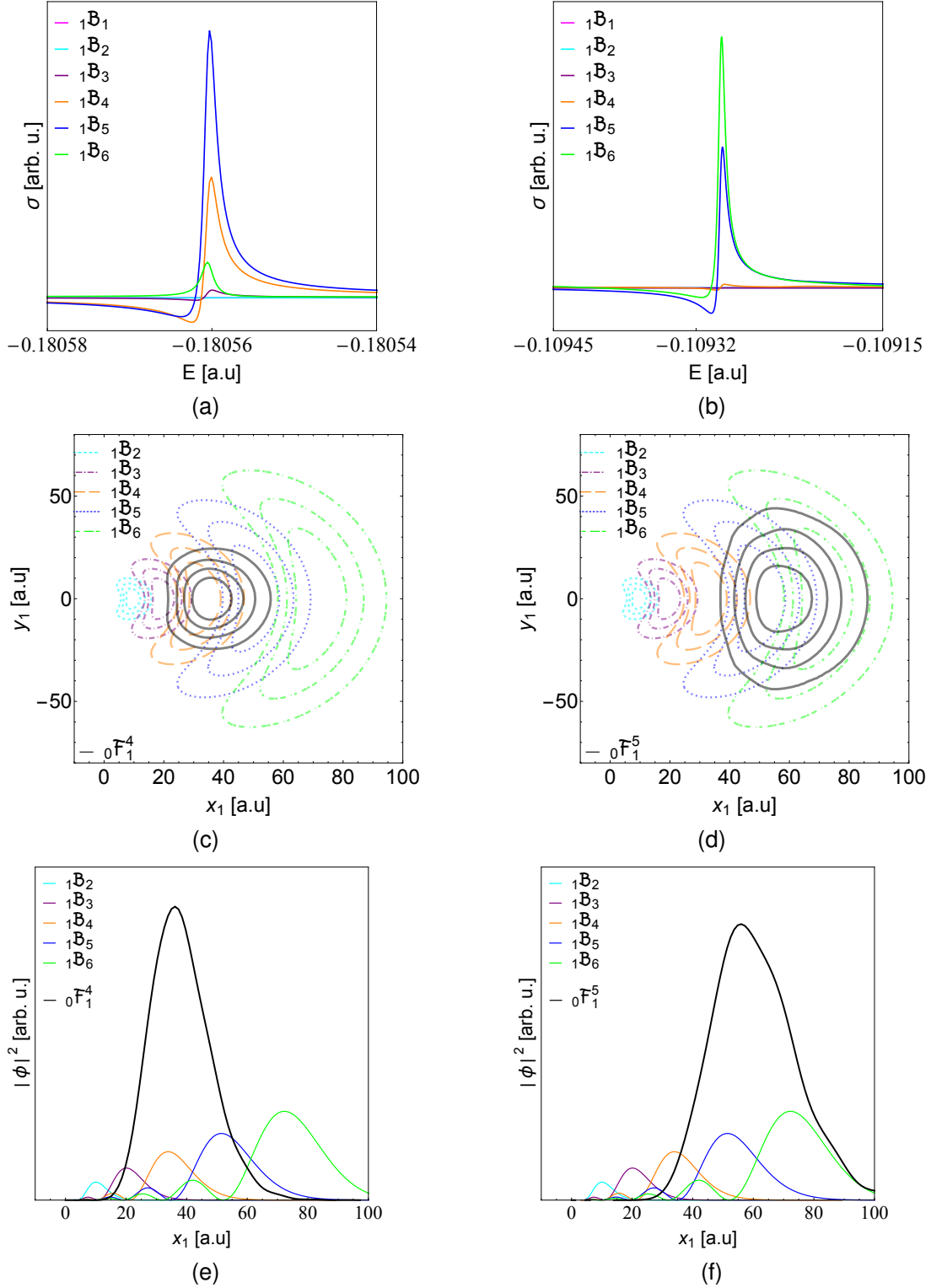


Figure 8: (a) and (b) PCS near the energies of ${}_0\mathcal{F}_1^4$ and (b) ${}_0\mathcal{F}_1^5$, respectively. (c) and (d) contour plot of the electronic density $|\phi|^2$ into the configuration subspace of the BS ${}_1\mathcal{B}_i$ $i = 2$ to 6 and ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_1^5$, respectively. The projection correspond to the probability distribution for the outer electron, keeping the inner electron coordinates fixed at the maximum of the probability density, (0.2, 0) for BS, (8.1, 0) for ${}_0\mathcal{F}_1^4$ and (15, 0) for ${}_0\mathcal{F}_1^5$. (e) and (f) $|\phi|^2$ of BS and ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_1^5$, respectively, as a function of the outer electron coordinate x_1 , keeping $y_1 = 0$ fixed and the inner electron coordinates fixed at the maximum of the electronic density.

The energies and decay rates of ${}_0\mathcal{F}_k^4$ and ${}_0\mathcal{F}_k^5$ are listed in table 2. In figures 6 and 7 the total photoionization cross sections (see section 2.7) are shown with BS ${}_1\mathcal{B}_i$ with $i = 1$ to 6 as initial states and taking all the doubly excited states converging to the 4th and 5th ionization thresholds. The soft background generated by the contribution from the continua of lower series is not taken into account here leaving only the fluctuating part of (5). The amplitude of the cross section depends on the initial state and the height of the peaks is an indicator of the coupling strength between the initial and final states. Here, we are not interested in the absolute values of the PCS. We are rather interested in the relative heights of the peaks associated to FPS in the PCS from different bound states. For this reason we are not concerned about the absolute units of the PCS. Instead, we use arbitrary units (arb. u.) along this work for PCS. FPS are characterised by small decay rates (see table 2) and therefore, when they are coupled to the initial BS they exhibit very narrow profiles. The positions of FPS are marked by dashed lines in both graphs. In figures 6 and 7 we observe that for one final state the strength of the coupling varies with the initial BS. In the following we perform a more thorough analysis in order to gain insight into the understanding of the difference in the electronic transitions between FPS and those BS.

The PCS near the energies of ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_1^5$ are presented in figures 8(a) and (b), respectively. For ${}_0\mathcal{F}_1^4$ the strongest coupling is from ${}_1\mathcal{B}_5$, but also there are important contributions from ${}_1\mathcal{B}_4$ and ${}_1\mathcal{B}_6$. For ${}_0\mathcal{F}_1^5$ the strongest coupling is from ${}_1\mathcal{B}_6$, being the second contribution from ${}_1\mathcal{B}_5$. In order to explain these differences in the coupling strengths we analyse the projections of the corresponding wave functions in configuration space. This will help us to understand the coupling between these states through the oscillator strength $\langle \phi_i | R(-\theta) B(x_1 + x_2) | \phi_f \rangle$, which actually will be non-zero when the initial and final states overlap. For that purpose it is important to notice that each of the three series of states, ${}_1\mathcal{B}_i$, ${}_0\mathcal{F}_k^4$ and ${}_0\mathcal{F}_k^5$, respectively converge to the same ionization threshold, that is, ${}_1\mathcal{B}_i$ converge to I_1 , ${}_0\mathcal{F}_k^4$ to I_4 and ${}_0\mathcal{F}_k^5$ to I_5 . Therefore, all states that belong to one of these series share the same excitation of the inner electron, which implies that the electrons occupy the same region of the configuration space. For this reason as the inner electron from the bound states does not provide information about the different coupling strengths we only consider the projections of the outer electron in the x_1 - y_1 plane.

In figure 8(c) we show these projections for ${}_0\mathcal{F}_1^4$ and the BS ${}_1\mathcal{B}_i$, $i = 1 \dots 6$, while figure 8(d) compares the projections of ${}_0\mathcal{F}_1^5$ and the same BS. The position of the inner electron is fixed at the coordinates corresponding to the maximum of the probability density at (0.2, 0) for ${}_1\mathcal{B}_i$, at (8.1, 0) for ${}_0\mathcal{F}_1^4$ and at (15, 0) for ${}_0\mathcal{F}_1^5$. We see that the overlap between BS and FPS is large for the same states where the coupling is also large. However, a larger overlap does not imply a larger coupling in the PCS because, according to the expression for the oscillator strengths, it is more important the product of the initial and final state functions. For example, ${}_0\mathcal{F}_1^4$ has the largest overlap with ${}_1\mathcal{B}_4$, however, it exhibits a stronger coupling to ${}_1\mathcal{B}_5$ and yet the overlap of the latter is smaller. This can be understood comparing the maxima of the probability densities.

Figure 8(e) compares the transversal sections of the probability densities of ${}_0\mathcal{F}_1^4$ and the BS. These sections are obtained from the projections of 8(c) for $y_1 = 0$.⁴ We observe that in figure 8(e) ${}_1\mathcal{B}_5$ has a larger probability density than ${}_1\mathcal{B}_4$ and in x direction there is full overlap with ${}_0\mathcal{F}_1^4$. This explains why it exhibits a larger coupling in the PCS. The same analysis is even clearer for ${}_0\mathcal{F}_1^5$ in figure 8(f), where the largest peak of ${}_0\mathcal{F}_1^5$ is localized around the largest peak of ${}_1\mathcal{B}_5$ and ${}_1\mathcal{B}_6$. As the maximum of the probability density of the latter is the largest of these BS, the coupling to ${}_0\mathcal{F}_1^5$

⁴The largest peak of the FPS probability density maximum is typically smaller than the maxima for BS. Therefore, in order to get a better insight in figures 8(e) and 8(f) the FPS densities have been rescaled and as the absolute value of the peaks is not important for the analysis, arbitrary units are used for this projection.

Table 3: FPS ${}_L\mathcal{F}_k^N$ below I_4 and I_5 and BS ${}_L\mathcal{B}_i$ strongly coupled to each FPS (arranged in decreasing coupling strength).

${}_L\mathcal{F}_k^N$	${}_L\mathcal{B}_i$
${}_0\mathcal{F}_1^4$	${}_1\mathcal{B}_5$ ${}_1\mathcal{B}_4$ ${}_1\mathcal{B}_6$
${}_0\mathcal{F}_2^4$	${}_1\mathcal{B}_6$
${}_0\mathcal{F}_3^4$	${}_1\mathcal{B}_6$
${}_0\mathcal{F}_4^4$	${}_1\mathcal{B}_5$
${}_0\mathcal{F}_1^5$	${}_1\mathcal{B}_6$ ${}_1\mathcal{B}_5$
${}_0\mathcal{F}_2^5$	${}_1\mathcal{B}_6$
${}_0\mathcal{F}_3^5$	${}_1\mathcal{B}_6$ ${}_1\mathcal{B}_5$ ${}_1\mathcal{B}_4$

is stronger which is consistent with figure 8(b).

It is worth to mention again that the ground state of helium is not coupled to any FPS [23]. A single photon transition is not enough to populate FPS from the ground state. For that reason the analysis presented in this section is the first step to populate those states. Our study shows that a two photon transition from the ground state mediated by single excited states ${}_1\mathcal{B}_i$ might excite the atom into FPS. In appendix A.3 we extend the analysis described in this section for ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_1^5$ to further FPS ${}_0\mathcal{F}_k^4$ and ${}_0\mathcal{F}_k^5$. Summarizing these results, in table 3, we present the BS which exhibit the largest couplings with those FPS.

We expect the results found within the planar model are valid to some extend for the real system. We emphasize that the planar model reproduce qualitatively and even quantitatively well the dynamics of helium in highly excited states [11, 12, 21–24] as the BS and FPS we have considered in the present analysis. Therefore, the analysis presented here can also be applied to the real system. This requires to take into account the following aspects. (i) FPS have been already identified in 3D theoretical studies [6] and it has been found some non-conclusive experimental evidence for their existence [13]. Quantitatively, the energies and the decay rates of FPS are different from the 2D results presented in this work [22]. In any case these states are characterised by small autoionization rates and $\langle \cos \theta_{12} \rangle \approx 1$, that is, they are associated to the collinear classical configuration. (ii) After characterizing FPS in the 3D system, the photoionization cross section can be calculated using again different BS as initial states. From the planar analysis we have presented we are certain that there are 3D BS coupled to FPS. For this it should be enough the overlap of the respective wave function projections of the outer electron. This must be the case, since it is always possible to find BS and FPS with similar excitations of the outer electron. We do not know, of course, which are the coupled states beforehand. (iii) The stability analysis has to be made for every FPS for the 3D helium atom, considering both the photoionization and the radiative decay rates. Although there is not evidence yet of the relevance of the fluorescence for FPS, it has been shown in theoretical [14–16] and experimental studies [17–19] for the $(-1, 0)_n^0$ series⁵ of 3D helium below the second ionization threshold, that the radiative decay channel dominates over the autoionization channel.

Finally, from the above discussion and the results presented in this section we can estimate the wavelengths for the expected transitions needed in a real experiment to populate FPS. Figure 9 depicts the two-photon scheme from the ground state to FPS using BS as intermediate states of the real system. The bound states, though unknown, are located close to the first ionization at $I_1 =$

⁵These doubly excited states are labelled using the $(K, T)_n^A$ classification scheme [40].

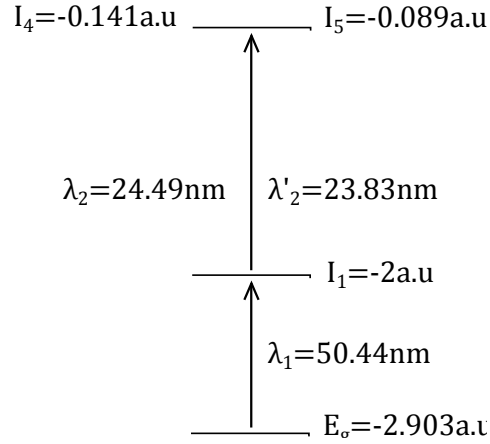


Figure 9: Two-photon transition scheme from the ground state to FPS below I_4 and I_5 , using BS as intermediate states, for 3D helium. The wavelength of the first transition, between ground state $E_0 = -2.903 \text{ a.u.}$ and BS $E_{\text{BS}} = -2 \text{ a.u.}$ is $\lambda_1 = 50.44 \text{ nm}$ and for the second transition $\lambda_2 = 24.49 \text{ nm}$ and for FPS below I_4 and $\lambda'_2 = 23.83 \text{ nm}$ for FPS below I_5 . All photons involved in these electronic transitions are in the far-ultraviolet region (200 nm, 10 nm).

-2 a.u. The energies of 3D FPS ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_1^5$ are -0.141064 a.u. and -0.089570 a.u. , respectively [7], which are located very close to the ionization thresholds I_4 and I_5 . The approximate wavelength of the photon required for each transition is presented there. From the ground state to the BS the photon should have a wavelength of $\lambda_1 = 50.44 \text{ nm}$. The second photon has wavelengths of $\lambda_2 = 24.49 \text{ nm}$ and $\lambda'_2 = 23.83 \text{ nm}$ for the transitions between BS and ${}_0\mathcal{F}_k^4$ and ${}_0\mathcal{F}_k^5$, respectively. All the photons involved in these electronic transitions are in the far-ultraviolet region (200 nm, 10 nm). The experimental realization of these FPS requires an exact photon energy to excite the right couplings. The lasers for generation of ultraviolet radiation can be already found with different sources [41], though the required spectral precision is still far from being achieved.

4 Summary and Perspective

4.1 Summary

In the present work, we give a brief description of the spectrum of planar helium and we focus our attention in the study of frozen planet states in order to analyse the coupling to bound states. For that purpose we use a well established approach which combines a representation in parabolic coordinates with the complex rotation method. The choice of parabolic coordinates leads to an exact representation in creation and annihilation of four coupled harmonic oscillators. The matrix elements of the resulting generalized eigenvalue problem have simple analytic expressions which can be numerically exactly calculated. The complex rotation method allows us to identify the resonance states of the atom providing their energies and autoionization decay rates. Furthermore, within this approach we provide a theoretical description of radiative decay rates.

After the description of frozen planet states we study their dipole coupling with bound states. This is achieved by calculating both the photoionization cross section, starting from different initial bound states, and the projections of the probability density wave function into different planes. On the one hand the photoionization cross sections allows us to identify bound states which are strongly coupled to frozen planet states. On the other hand the projections on the configuration space of the outer electron provide information about the overlap between these states and, thus, it helps us to explain the different coupling strengths: We found that the coupling between bound states and frozen planet states is stronger whenever the overlap between the initial and final wave functions is large and the largest peaks of the wave functions are located in the same region of configuration space, that is, the outer electrons of the frozen planet state and the bound state are located around the same positions. These observations open a door in the direction of preparation of the so far unobserved frozen planets states using a two photon transition from the ground state mediated by single excited states. Furthermore, the frequencies required for the electronic transitions to obtain the FPS can be estimated, being in the far ultraviolet region. Although for this energy range different types of lasers can be found, the spectroscopic precision has not been achieved yet.

4.2 Outlook

Fluorescence is the dominant decay channel for special series of series of doubly excited states [14–19]. However, the relevance of the radiative decay rate of frozen planet states is not yet understood. In the present work we have developed the theoretical background for the study of the radiative decay rate for 2D helium. The numerical implementation will help us to understand the role of the radiative decay in frozen planet states and to gain more insight into their possible experimental preparation.

Qualitatively, we expect the coupling of states in the real atom and in the planar system exhibit similar properties. Nevertheless, the quantitative description of these couplings requires an accurate treatment of the 3D helium atom.

Finally, the effect of an external driving on frozen planet states is the creation of non-dispersive wave packets. Though important advances have been achieved in the understanding of the nature and properties of these objects, we still are far from their experimental realization.

A Appendices

A.1 Spontaneous Emission

In this section, the main results of the radiative process of an atom are summarized from [29] in section A.1 and section A.1.1. Then it is applied to two systems: the 3D helium atom and planar helium, where some considerations will have to be made in order to justify the interaction between a 2D object and a 3D external field.

In order to calculate the partial decay rate of a state the Fermi Golden Rule is used, which is given by the expression [29]

$$P_{i \rightarrow f} = \left(\frac{4\pi^4}{\hbar L^3} \right) \frac{(E_f - E_i)^2}{\omega_\lambda} |(\hat{\pi}_\lambda \cdot \mathbf{r}_{fi})F_{fi}^{\text{abs}} + (\hat{\pi}_\lambda^* \cdot \mathbf{r}_{fi})F_{fi}^{\text{em}}|^2 \rho_l d\Omega,$$

where E_i and E_f are the energies of the initial and final state, respectively and $\omega_\lambda = \frac{E_f - E_i}{\hbar}$ is the energy difference between the states. For the spontaneous emission process the absorption and emission coefficients are $F_{fi}^{\text{abs}} = 0$ and $F_{fi}^{\text{em}} = 1$, respectively and the occupation number for each mode are $n_\lambda = 0$, for every mode λ of the initial state of the field, $n'_\lambda = 1$, for every mode λ of the final state of the field. Finally the photon density in 3D is given by

$$\rho_l d\Omega = \left(\frac{L}{2\pi} \right)^3 \frac{(\hbar\omega_\lambda)^2}{(\hbar c)^3} d\Omega.$$

Substituting the last expressions in the transition probability between the initial and final states we obtain the following expression for one possible polarization λ

$$P_{i \rightarrow f} = \frac{1}{2\pi\hbar} \left(\frac{\omega_\lambda^3 e^2}{c^3} \right) |\hat{\pi}_\lambda^* \cdot \langle \phi_f | \mathbf{r} | \phi_i \rangle|^2 d\Omega.$$

A.1.1 3D Helium Atom

To obtain the total decay rate of the state $|\phi_i\rangle$ the contributions from the two possible polarization directions, and from the different possible directions of the emitted photon have to be taken into account. The position vector written in the vector basis $\{\hat{\pi}_1, \hat{\pi}_2, \hat{k}\}$, with $\mathbf{k}_\lambda$ the wave vector, is given by

$$\begin{aligned} \mathbf{r}_{fi} &= (\hat{\pi}_1 \cdot \mathbf{r}_{fi})\hat{\pi}_1 + (\hat{\pi}_2 \cdot \mathbf{r}_{fi})\hat{\pi}_2 + (\hat{k} \cdot \mathbf{r}_{fi})\hat{k} \\ &= r_{fi} \sin \theta \sin \phi \hat{\pi}_1 + r_{fi} \sin \theta \cos \phi \hat{\pi}_2 + r_{fi} \cos \theta \hat{k}. \end{aligned}$$

The magnitude of the projection of the position vector on the plane $\hat{\pi}_1$ - $\hat{\pi}_2$ is

$$\begin{aligned} |\hat{\pi}_1 \cdot \mathbf{r}_{fi}|^2 + |\hat{\pi}_2 \cdot \mathbf{r}_{fi}|^2 &= r_{fi}^2 \sin^2 \theta [\cos^2 \phi \|\hat{\pi}_1\|^2 + \sin^2 \phi \|\hat{\pi}_2\|^2] \\ &= r_{fi}^2 \sin^2 \theta. \end{aligned}$$

The probability per unit time $P_{i \rightarrow f}^{\text{se}}$ for the atomic transition from ϕ_i to ϕ_f plus the emission of a photon of arbitrary polarization is given by

$$\begin{aligned} P_{i \rightarrow f}^{\text{se}} = \int P_{i \rightarrow f} d\Omega &= \frac{\omega_\lambda^3 e^2}{2\pi\hbar c^3} |\langle \phi_f | \mathbf{r} | \phi_i \rangle|^2 \int_0^\pi \int_0^{2\pi} \sin^3 \theta d\phi d\theta \\ &= \frac{\omega_\lambda^3 e^2}{2\pi\hbar c^3} |\langle \phi_f | \mathbf{r} | \phi_i \rangle|^2 \left(\frac{8\pi}{3} \right) = \frac{4\omega_\lambda^3 e^2}{3\pi\hbar c^3} \langle \phi_f | \mathbf{r} | \phi_i \rangle^2. \end{aligned}$$

For the total spontaneous decay rate it follows

$$P_i = \sum_f P_{i \rightarrow f}^{\text{se}} = \frac{4e^2}{3\pi\hbar^4 c^3} \sum_f (E_f - E_i)^3 |\langle \phi_f | \mathbf{r} | \phi_i \rangle|^2.$$

If atomic units are used and the total radiative decay is called γ , the radiative decay reads

$$\gamma_i = \frac{4}{3} \alpha^3 \sum_f (E_f - E_i)^3 |\langle \phi_f | \mathbf{r} | \phi_i \rangle|^2, \quad (6)$$

where α is the fine structure constant, that in atomic units is given by

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{c}.$$

Complex Rotation Method

If the initial state is a resonance $|\phi_f\rangle$ represented by the complex scaled state vector $|\psi_{f\theta}\rangle$ then both the energy and the matrix element of the position vector has to be replaced as follows [32]

$$(E_f - E_i)^3 |\langle \phi_f | \mathbf{r} | \phi_i \rangle|^2 \longrightarrow (\text{Re}(E_f) - E_i)^3 \text{Re}(\langle \phi_{f\theta} | \mathbf{r} | \phi_i \rangle^2).$$

E_i is real because only the radiative decay from a resonance to a bound state is considered and those states have real eigenvalues. A justification for using only the real part of the dipole matrix element is going to be developed in appendix A.2.

A.1.2 2D Helium Atom

For the planar case, the only differences with the 3D case is that the position vector of the electrons are restricted to the plane x - y and therefore wave functions depend on these two coordinates. There are still two possible polarization vectors $\hat{\pi}_1$ and $\hat{\pi}_2$ perpendicular to one another and to the wave vector polarization vector $\hat{k}$. Then, after projecting the position vectors $\mathbf{r}_i$ in the plane $\hat{\pi}_1$ - $\hat{\pi}_2$ and integrating over all possible directions we obtain the same expression for the radiative decay rate (6)

$$\begin{aligned} \gamma_n &= \frac{4\omega^3 \alpha^3}{3\pi} \pi \sum_i (x_{nf}^2 + y_{nf}^2), \\ &= \frac{\omega^3 \alpha^2}{2} \sum_f (\langle \psi_n | x_1 + x_2 | \psi_f \rangle^2 + \langle \psi_n | y_1 + y_2 | \psi_f \rangle^2). \end{aligned}$$

If the initial state $\langle \psi_f |$ is a resonance $|\psi_{n\theta}\rangle$ using the complex rotation method then the total decay rate is

$$\gamma_n = \frac{4\alpha^3}{3} \sum_f (\text{Re}(E_n) - E_f)^3 \text{Re}(\langle \psi_{n\theta} | x_1 + x_2 | \psi_{f\theta} \rangle^2 + \langle \psi_{n\theta} | y_1 + y_2 | \psi_{f\theta} \rangle^2), \quad (7)$$

where E_f is real because only bound states are considered in the sum.

A.2 Channel Theory

In this section the justification for the fluorescence expression (7) is given in the frame of the complex rotation method. In order to achieve this we need to arrive to the equivalence between the real part of the square of $\text{Re}(\langle \psi_n | D | \phi_i \rangle^2)$ and the square modulus of the dipole matrix element between the bound part of the wave function $|\varphi\rangle$ and the initial state $|\phi_i\rangle$, i.e. $|\langle \varphi | D | \phi_i \rangle|^2$. To describe the decay channels of a doubly excited atom the main results of the channel theory from [32, 42, 43] are summarized in this section and in section A.2.1, where the configuration interaction between bound and unbound states is taken into account. The physical system into consideration is described by a bound state $|\varphi\rangle$ and a non resonant continuum state $|\psi_E\rangle$ with energies E_φ and E , respectively. In the zero approximation, that is when the interaction potential is neglected, the eigenstates of the operators $\mathcal{Q}H\mathcal{Q}$ and $\mathcal{P}H\mathcal{P}$ are $|\varphi\rangle$ and $|\psi_E\rangle$, respectively, where $\mathcal{Q}$ and $\mathcal{P}$ are the projection operators to bound and non resonant continuum states. The matrix elements of these states are given by

$$\begin{aligned}\langle \varphi | H | \varphi \rangle &= E_\varphi, \\ \langle \psi_{E'} | H | \varphi \rangle &\equiv \langle \psi_{E'} | V | \varphi \rangle = V_{E'}, \\ \langle \psi_{E'} | H | \psi_E \rangle &= E \delta(E' - E).\end{aligned}$$

The non diagonal terms of the hamiltonian matrix, i.e. the configuration interaction, in terms of the projection operators $\mathcal{Q}$ and $\mathcal{P}$ is given by

$$V = \mathcal{P}H\mathcal{Q} + \mathcal{Q}H\mathcal{P}.$$

The corresponding eigenvector to be determined, which diagonalizes the portion of energy matrix that belongs to the subset of states $|\varphi\rangle$ and $|\psi_E\rangle$, is a combination of the bound and continuum states

$$|\phi_E\rangle = a(E) |\varphi\rangle + \int b_{E'}(E) |\psi_{E'}\rangle dE'. \quad (8)$$

The coefficients can be found and an important quantity, the autoionization rate, is introduced

$$\Gamma(E) = 2\pi |V_E|^2. \quad (9)$$

Analysing the interaction between the channels that generate the resonances one can show that the photoionization cross section is proportional to the oscillator strength [29]

$$|\langle \phi_E | D | \phi_i \rangle|^2 = |\langle \psi_E | D | \phi_i \rangle|^2 \left| \frac{\epsilon + q}{\epsilon + i} \right|^2 = |\langle \psi_E | D | \phi_i \rangle|^2 \frac{(\epsilon + q)^2}{\epsilon^2 + 1}, \quad (10)$$

where the dependence of the cross section on the energy exhibits the typical asymmetrical shape of a Beutler-Fano profile. In the last equation, D is the dipole operator, $|\phi_i\rangle$ is an initial state and the asymmetry parameter q and the energy ϵ of the resonance respect to its center position in units of half width are given by

$$\epsilon = \frac{E - E_\varphi - F}{\Gamma/2}, \quad q = \frac{\langle \Phi | D | \phi_i \rangle}{\pi V_E^* \langle \psi | T | \phi_i \rangle}, \quad (11)$$

where

$$F(E) = P \int \frac{|V_{E'}|^2}{E - E'} dE',$$

F is the energy shift due to the finite bound-continuum coupling, P is the Cauchy principal value of the integral and $|\Phi\rangle$ denotes the state $|\varphi\rangle$ modified by an admixture of the continuum state $|\psi_E\rangle$

$$\Phi = \varphi + P \int \frac{V_{E'} \psi_{E'}}{E - E'} dE'$$

If Γ , F , and q are assumed to be constant in the energy interval defined by the resonance, the integrated photoionization cross section of a resonance [42] is given by

$$\sigma(E) = |\langle \psi_E | D | \phi_i \rangle|^2 \left[\frac{(\epsilon + q)^2}{\epsilon^2 + 1} - 1 \right],$$

can be written as

$$\begin{aligned} \int \sigma(E) dE &= \int |\langle \psi_E | D | \phi_i \rangle|^2 \left[\frac{(\epsilon + q)^2}{\epsilon^2 + 1} - 1 \right] dE, \\ &= \int (|\langle \phi_E | D | \phi_i \rangle|^2 - |\langle \psi_E | D | \phi_i \rangle|^2) dE. \end{aligned}$$

where the first line is derived taking into account the results from the fano profile analysis of the interaction between a bound state and a pure continuum state [95, 96]. The last line can be obtained from the relation between $|\langle \phi_E | D | \phi_i \rangle|^2$ and $|\langle \psi_E | D | \phi_i \rangle|^2$ in (10). The integration over the energy interval $[-a, a]$ of the resonance is calculated in the limit $a \rightarrow \infty$. This can be justified for isolated resonances since the subintegral function does not significantly contribute to the integral outside the interval and the variable of integration is changed from E to ϵ

$$\epsilon = \frac{E_g + \omega_0 - E}{\Gamma/2}, \quad d\epsilon = \frac{dE}{\Gamma/2},$$

$$\int \sigma(\epsilon) \frac{\Gamma}{2} d\epsilon = \frac{\Gamma}{2} |\langle \psi_E | D | \phi_i \rangle|^2 \int_{-\infty}^{\infty} \left[\frac{(\epsilon + q)^2}{\epsilon^2 + 1} - 1 \right] d\epsilon \quad (12)$$

$$= \frac{\Gamma}{2} |\langle \psi_E | D | \phi_i \rangle|^2 \int_{-\infty}^{\infty} \left[\frac{\epsilon^2 + 2q\epsilon + q^2 - \epsilon^2 - 1}{\epsilon^2 + 1} \right] d\epsilon \quad (13)$$

$$= \frac{\Gamma}{2} |\langle \psi_E | D | \phi_i \rangle|^2 \int_{-\infty}^{\infty} \left[\frac{q^2 + 2q\epsilon - 1}{\epsilon^2 + 1} \right] d\epsilon \quad (14)$$

$$= \pi \frac{\Gamma}{2} |\langle \psi_E | D | \phi_i \rangle|^2 (q^2 - 1). \quad (15)$$

of (9) and (11) it follows that

$$\langle \Phi | D | \phi_i \rangle = q\pi V_E^* \langle \psi_E | D | \phi_i \rangle, \quad \frac{\Gamma}{2} = \pi |V_E|^2,$$

Inserting these relations [42] into the integrated photoionization cross section (12) we obtain

$$\begin{aligned} \int \sigma(\epsilon) \frac{\Gamma}{2} d\epsilon &= \pi \frac{\pi |V_E|^2}{\pi^2 |V_E|^2} |\langle \Phi | D | \phi_i \rangle|^2 - \pi \frac{\Gamma}{2} |\langle \psi_E | D | \phi_i \rangle|^2, \\ &= |\langle \Phi | D | \phi_i \rangle|^2 - \frac{\pi \Gamma}{2} |\langle \psi_E | D | \phi_i \rangle|^2, \\ \int \sigma(\epsilon) \frac{\Gamma}{2} d\epsilon &\equiv |\langle \varphi | D | \phi_i \rangle|^2. \end{aligned} \quad (16)$$

The integral over the resonance energy must be equal to $|\langle \varphi | D | \phi_i \rangle|^2$ because the transformation that diagonalizes the hamiltonian is unitary (8) and therefore cannot affect the total transition probability.

A.2.1 Photoionization Cross Section

The Fermi golden rule applied to the photoionization process leads to the expression for the cross section [29]

$$\sigma(\omega_0) = 4\pi^2\omega_0 \sum_j |\langle \phi_{jE} | D(\hat{e}_0) | \phi_i \rangle|^2,$$

where $|\phi_i\rangle$ is the bound initial atomic state with energy E_i , ω_0 is the transition energy, $|\phi_{jE}\rangle$ is the energy normalized continuum eigenstate with energy $E = E_i + \omega_0$, and $\hat{e}_0$ is the polarization vector of the incident photon beam. When using the complex scaling method the photoionization cross section is given by [32]

$$\sigma(\omega_0) = \frac{4\pi\omega_0}{c} \text{Im} \sum_j \frac{\overline{\langle \varphi_{j\theta} | R(\theta) D | \phi_i \rangle}^2}{E_{j\theta} - E}.$$

To prove that this expression is equivalent to a fano profile lets define the oscillator strength as a complex number

$$\overline{\langle \varphi_{j\theta} | R(\theta) D | \phi_i \rangle} = B_j + iC_j,$$

replacing this result into the expression for the partial photoionization cross section

$$\begin{aligned} \sigma_j &= \frac{4\pi\omega_0}{c} \text{Im} \left(\frac{\overline{\langle \varphi_{j\theta} | R(\theta) D | \phi_i \rangle}^2}{E_{j\theta} - E} \right) \\ &= \frac{4\pi\omega_0}{c} \text{Im} \frac{(B_j + iC_j)^2}{E_{j\theta} - E} \\ &= \frac{4\pi\omega_0}{c} \text{Im} \frac{(B_j^2 - C_j^2)A_j - \Gamma_j C_j B_j + i(2C_j B_j A_j + \frac{\Gamma}{2}(B_j^2 - C_j^2))}{A_j^2 + \frac{\Gamma^2}{4}}, \end{aligned}$$

where

$$E_{j\theta} = E_j - i\frac{\Gamma}{2} \quad \text{and} \quad A_j = E_j - E = E_j - E_g - \omega_0$$

taking the imaginary part of the partial cross section we obtain

$$\sigma_j = \mu_j^2 \left[\frac{(\epsilon_j + q_j)^2}{\epsilon_j^2 + 1} - 1 \right].$$

with

$$\epsilon_j = \frac{E_g + \omega_0 - E_j}{\Gamma_j/2}, \quad q_j = -\frac{B_j}{C_j}, \quad \mu_j^2 = \frac{8\pi\alpha\omega_0 C_j^2}{\Gamma_j}.$$

If we compare the last expression for the photoionization cross section with

$$\sigma \propto |\langle \psi_E | D | \phi_i \rangle|^2 \frac{(\epsilon + q)^2}{\epsilon^2 + 1},$$

then it can be seen that

$$|\langle \psi_E | D | \phi_i \rangle|^2 \propto \mu_j^2, \quad \text{then} \quad |\langle \psi_E | D | \phi_i \rangle|^2 \propto C_j^2,$$

where $|\psi_E\rangle$ is the continuum part of the resonance. Therefore, the square of the real part of the matrix element is proportional to the dipole coupling between the initial state and the quasi bound part (the modified bound part) of the resonance

$$B_j^2 \propto |\langle \Phi | D | \phi_i \rangle|^2.$$

Integrating the partial photoionization cross section we obtain

$$\begin{aligned} \int dE \sigma_j(E) &= \frac{\Gamma_j}{2} \int_{-\infty}^{\infty} d\epsilon_j \sigma_j(\epsilon_j), \\ &= \frac{\Gamma_j}{2} \int_{-\infty}^{\infty} d\epsilon_j \mu_j^2 \left[\frac{(\epsilon_j + q_j)^2}{\epsilon_j^2 + 1} - 1 \right], \\ &= 4\pi^2 \alpha \omega_0 [B_j^2 - C_j^2], \\ &= 4\pi^2 \alpha \omega_0 \operatorname{Re} \langle \psi_{j\theta} | D | \psi_{i\theta} \rangle^2. \end{aligned}$$

According to the result obtained in the (12), the real part of the square of the complex scaled matrix element $\operatorname{Re} \langle \psi_{n\theta} | D | \psi_{i\theta} \rangle^2$ is therefore equal to the transition matrix element where the configuration interaction between the bound and continuum part is neglected $|\langle \varphi | D | \phi_i \rangle|^2$. According to this equivalence almost the same result would be obtain in the framework were doubly excited resonance states were considered as true bound states. A qualitative argument can be given to justify (7). As the autoionization process arises from the interaction term, therefore the fluorescence as a first approach can be calculated considering that the main contribution to the radiative decay process is related to the bound part of the wave function $|\varphi\rangle$ (i.e a non interacting electron system which interacts with the external field).

A.3 Coupling to further Frozen Planet States

To study the coupling between BS with $L = 1$ and FPS with $L = 0$, we focus our analysis on FPS converging to I_4 and I_5 . These FPS are trivially not coupled to the the ground state of planar helium ${}_0\mathcal{G}$ due to the selection rules of the dipole operator. It is worth to mention that ${}_0\mathcal{G}$ is neither coupled to any $L = 1$ FPS (${}_1\mathcal{F}_k^N$) [23]. Therefore, to populate $L = 0$ or $L = 1$ FPS from the ground state it is necessary at least a two-photon transition. Here we explore the possibility of populating $L = 0$ FPS ${}_0\mathcal{F}_k^N$ by a two-photon excitation process using as intermediate states the BS ${}_1\mathcal{B}_i$. For this, we show the results used to analyse the coupling between the first six bound states ${}_1\mathcal{B}_i$ to the FPS ${}_0\mathcal{F}_n^i$ below the ionization thresholds I_4 and I_5 . We present the graphs of the photoionization cross section near the energies of the FPS with different initial bound states. In order to find a qualitative explanation for the coupling strengths between the states mentioned above, we also show different projections of the probability density in the configuration space of both BS and FPS.

The analysis for the differences in the coupling between BS and FPS can be extended for any other state, but here we give the details only for the FPS ${}_0\mathcal{F}_2^4$. The PCS near the energy of ${}_0\mathcal{F}_2^4$ is presented in figure 10(b). For ${}_0\mathcal{F}_2^4$ the stronger coupling is from ${}_1\mathcal{B}_6$ but there is also a contribution from ${}_1\mathcal{B}_5$. In order to explain the different coupling strengths we analyse the projections of the corresponding wave functions in configuration space. This will help us to understand the coupling between these states through the oscillator strength $\langle \phi_i | R(-\theta) B(x_1 + x_2) | \phi_f \rangle$, which actually will be non-zero when the initial and final states overlap. For that purpose it is important to notice that

each of the series of states, ${}_1\mathcal{B}_i$ and ${}_0\mathcal{F}_k^4$, respectively converge to the same ionization threshold. Therefore, all states of one of these series share the same excitation of the inner electron, which implies that the electrons will occupy the same region of the configuration space. For this reason we only consider the projections of the outer electron in the x_1 - y_1 plane.

In figure 10(d), for example, we show these projections for ${}_0\mathcal{F}_2^4$ and BS ${}_1\mathcal{B}_i$, $i = 1 \dots 6$. The position of the inner electron is fixed at coordinates corresponding to the maximum of the probability density at $(0.2, 0)$ for ${}_1\mathcal{B}_i$ and at $(8.1, 0)$ for ${}_0\mathcal{F}_2^4$. We see that the overlap between BS and FPS is large for the same states where the coupling is also large. However, a larger overlap does not imply a larger coupling in the PCS because, according to the expression for the oscillator strengths, it is more important the product of the initial and final state functions. For example, ${}_0\mathcal{F}_2^4$ has the largest overlap with ${}_1\mathcal{B}_5$, however, it exhibits a stronger coupling to ${}_1\mathcal{B}_6$ and yet the overlap of the latter is smaller. This can be understood comparing the maxima of the probability densities.

Figure 11(f) compares the transversal sections of the probability densities of ${}_0\mathcal{F}_2^4$ and BS. These sections are obtained from the projections of 10(d) for $y_1 = 0$ ⁶. We observe that in figure 10(f) the largest peak of ${}_0\mathcal{F}_2^4$ is localized around the largest peak of ${}_1\mathcal{B}_5$ and ${}_1\mathcal{B}_6$. As the maximum of the probability density of the latter is the largest of these BS, the coupling to ${}_0\mathcal{F}_2^4$ is stronger which is consistent with figure 10(b). The same analysis applies for the rest of FPS shown in figures 10-13.

⁶The FPS probability density maximum is typically smaller than the maxima for BS. Therefore, in order to get a better insight in panels (e) and (f) of figures 10–12 the FPS density has been rescaled.

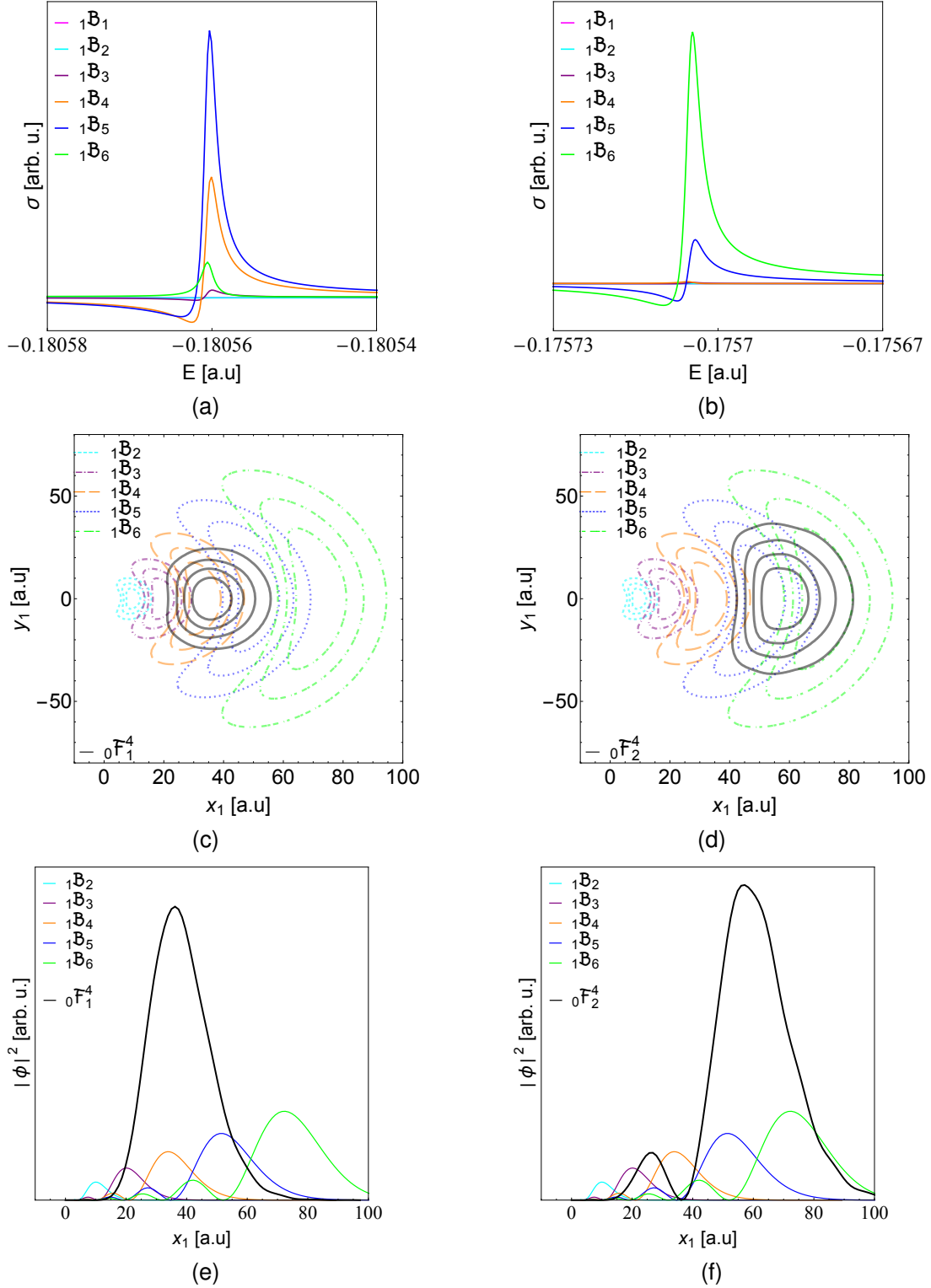


Figure 10: (a) and (b) PCS near the energies of ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_2^4$, respectively. (c) and (d) Contour plot of the electronic density $|\phi|^2$ into the configuration subspace of the outer electron of the BS ${}_1\mathcal{B}_i$ $i = 2$ to 6 and ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_2^4$, respectively. The projection correspond to the probability distribution for the outer electron, keeping the inner electron coordinates fixed at the maximum of the probability density, (0.2, 0) for BS and (8.1, 0) for ${}_0\mathcal{F}_k^4$. (e) and (f) $|\phi|^2$ of BS and ${}_0\mathcal{F}_1^4$ and ${}_0\mathcal{F}_2^4$, respectively, as a function of the outer electron coordinate x_1 keeping $y_1 = 0$ fixed and the inner electron coordinates fixed at the maximum of the electronic density.

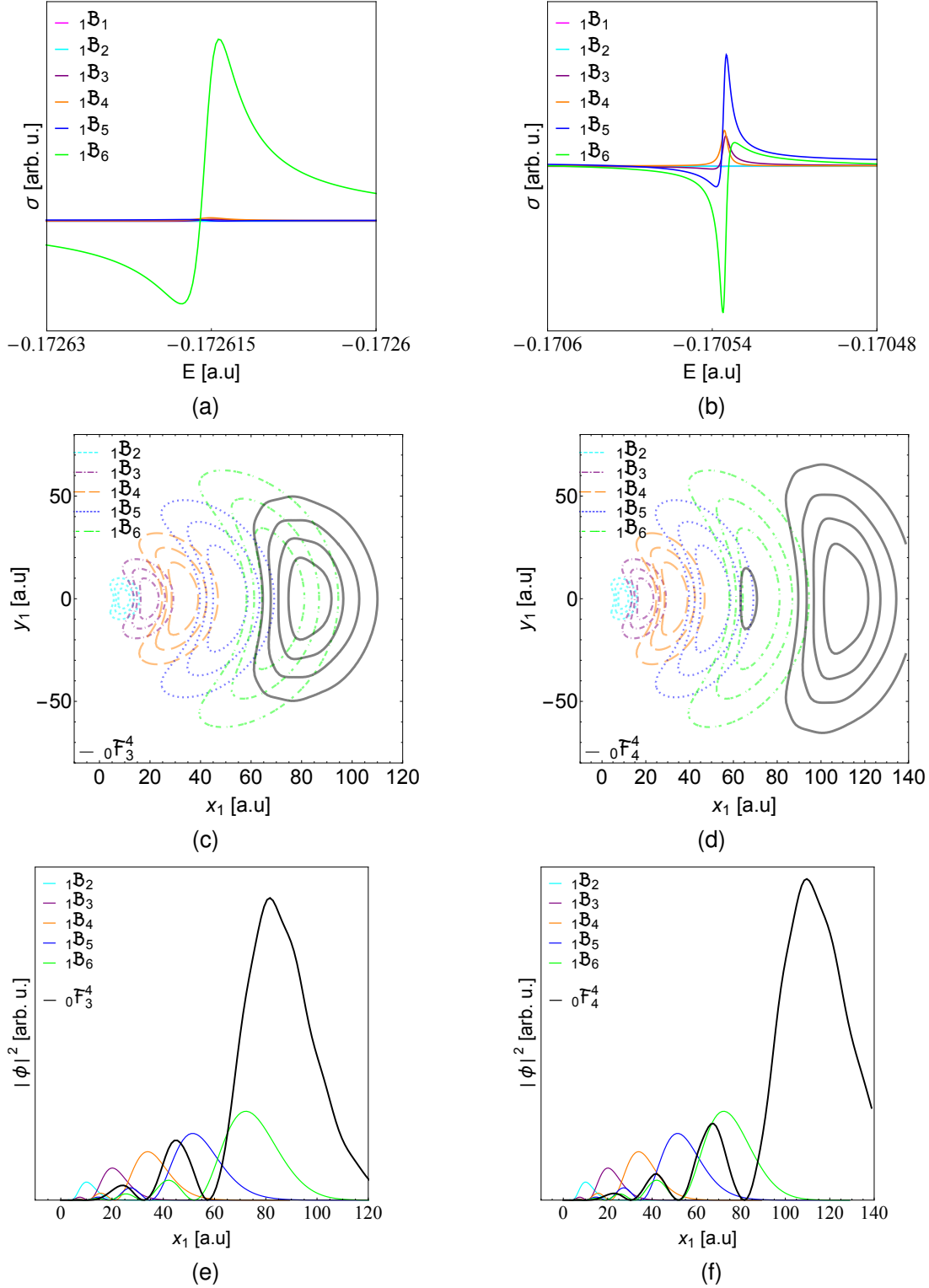


Figure 11: (a) and (b) PCS near the energies of ${}_0F_3^4$ and ${}_0F_4^4$, respectively. (c) and (d) Contour plot of the electronic density $|\phi|^2$ into the configuration subspace of the outer electron of the BS ${}_1B_i$ $i = 2$ to 6 and ${}_0F_3^4$ and ${}_0F_4^4$, respectively. The projection correspond to the probability distribution for the outer electron, keeping the inner electron coordinates fixed at the maximum of the probability density, $(0.2, 0)$ for BS and $(8.1, 0)$ for ${}_0F_k^4$. (e) and (f) $|\phi|^2$ of BS and ${}_0F_3^4$ and ${}_0F_4^4$, respectively, as a function of the outer electron coordinate x_1 keeping $y_1 = 0$ fixed and the inner electron coordinates fixed at the maximum of the electronic density.

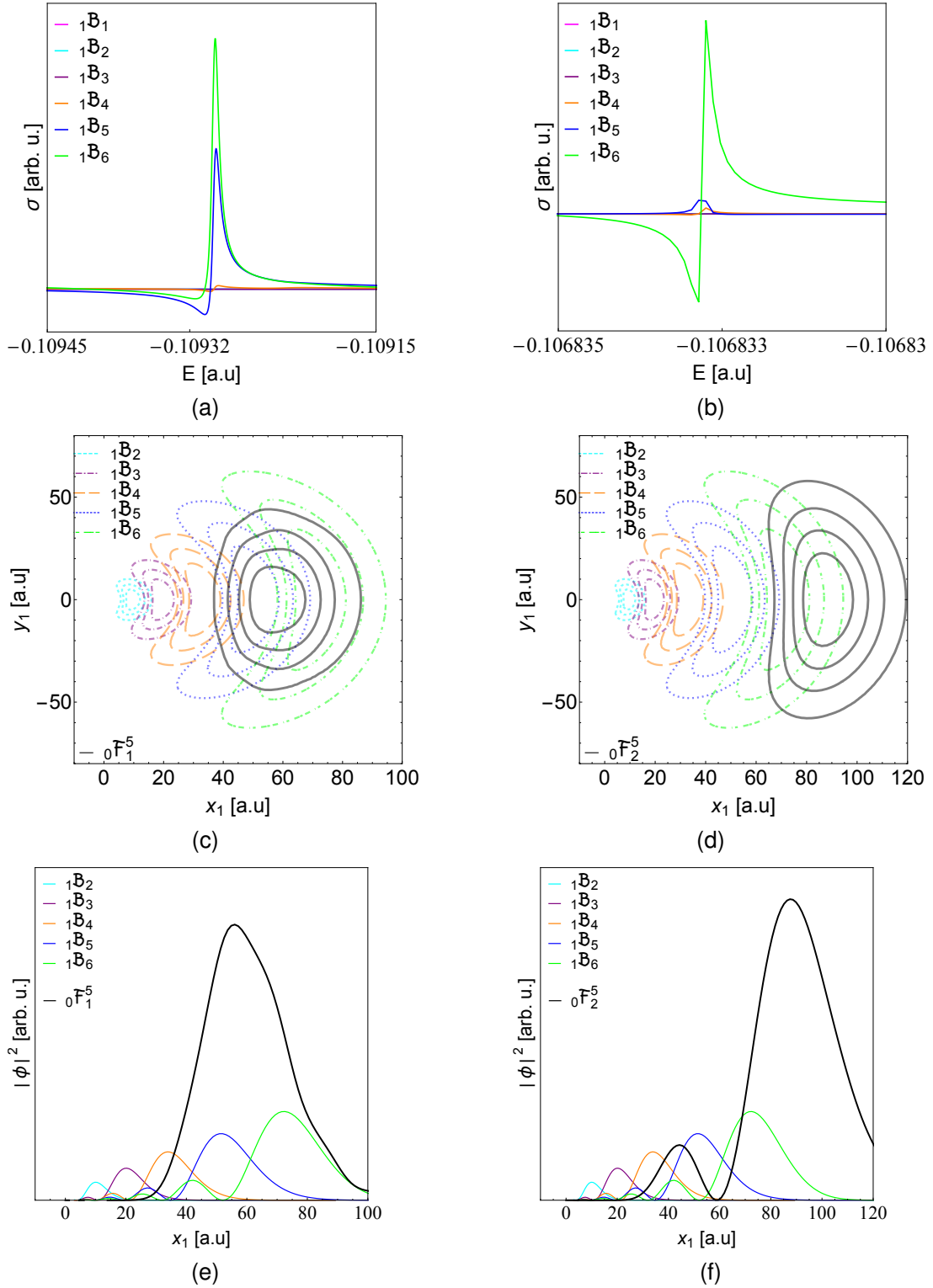
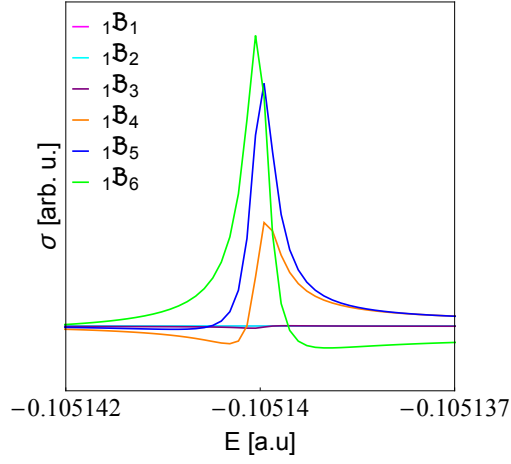
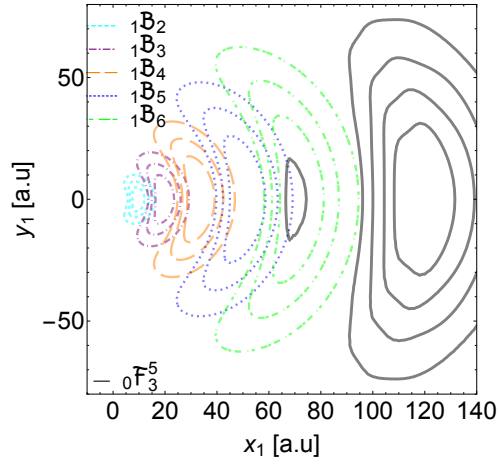


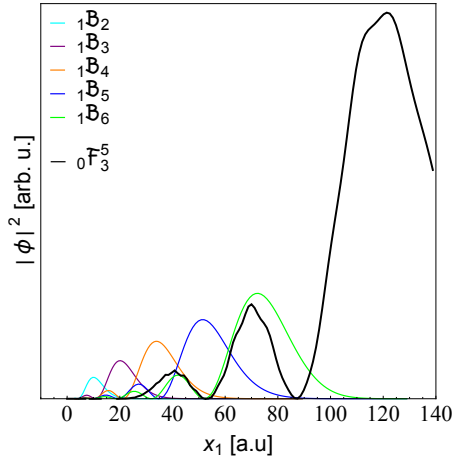
Figure 12: (a) and (b) PCS near the energies of $0F_1^5$ and $0F_2^5$, respectively. (c) and (d) Contour plot of the electronic density $|\phi|^2$ into the configuration subspace of the outer electron of the BS $1B_i$ $i = 2$ to 6 and $0F_1^5$ and $0F_2^5$, respectively. The projection correspond to the probability distribution for the outer electron, keeping the inner electron coordinates fixed at the maximum of the probability density, (0.2, 0) for BS and (15, 0) for $0F_k^5$. (e) and (f) $|\phi|^2$ of BS and $0F_1^5$ and $0F_2^5$, respectively, as a function of the outer electron coordinate x_1 keeping $y_1 = 0$ fixed and the inner electron coordinates fixed at the maximum of the electronic density.



(a)



(b)



(c)

Figure 13: (a) PCS near the energy of ${}_0\mathcal{F}_3^5$. (b) Contour plot of the electronic density $|\phi|^2$ into the configuration subspace of the outer electron of the BS ${}_1\mathcal{B}_i$ $i = 2$ to 6 and ${}_0\mathcal{F}_3^5$. The projection correspond to the probability distribution for the outer electron, keeping the inner electron coordinates fixed at the maximum of the probability density, $(0.2, 0)$ for BS and $(15, 0)$ for ${}_0\mathcal{F}_3^5$. (c) $|\phi|^2$ of BS and ${}_0\mathcal{F}_3^5$ as a function of the outer electron coordinate x_1 keeping $y_1 = 0$ fixed and the inner electron coordinates fixed at the maximum of the electronic density.

References

- [1] G. Tanner, K. Richter, and J. M. Rost. The theory of two-electron atoms: between ground state and complete fragmentation. *Rev. Mod. Phys.*, 72:497, 2000.
- [2] Johannes Eiglsperger and Javier Madroñero. Highly doubly excited states of planar helium: Fluctuations in photoionization cross sections. *Phys. Rev. A*, 80:022512, 2009.
- [3] Y. H. Jiang, R. Püttner, D. Delande, M. Martins, and G. Kaindl. Explicit analysis of chaotic behavior in radial and angular motion in doubly excited helium. *Phys. Rev. A*, 78(2):021401, 2008.
- [4] M. Domke, K Schulz, G Remmers, G Kaindl, and D Wintgen. High-resolution study of $1p^o$ double-excitation states in helium. *Phys. Rev. A*, 53:1424, 1996.
- [5] Johannes Eiglsperger, Tobias Kramer, and Javier Madroñero. Fluctuations in the spectra of open few-body systems. *New J. Phys.*, 13:063033, 2011.
- [6] K. Richter and D. Wintgen. Stable planetary atom configurations. *Phys. Rev. Lett.*, 65:1965, 1990.
- [7] K Richter, J S Briggs, D Wintgen, and E A Solovev. Novel dynamical symmetries of asymmetrically doubly excited two-electron atoms. *J. Phys. B*, 25:3929, 1992.
- [8] Madroñero J. *Spectral Properties of Planar Helium under Periodic Driving*. PhD thesis, LMU München, 2004.
- [9] Johannes Eiglsperger, Bernard Piraux, and Javier Madroñero. Spectral representation of the three-body coulomb problem. i. nonautoionizing doubly excited states of high angular momentum in helium. *Phys. Rev. A*, 81(4):042527, Apr 2010.
- [10] V N Ostrovsky and N V Prudov. Planetary atom states: adiabatic invariant theory. *J. Phys. B*, 28:4435, 1995.
- [11] Harald Friedrich and Johannes Trost. Working with wkb waves far from the semiclassical limit. *Phys. Rep.*, 397:359, 2004.
- [12] J. G. Leopold and I. C. Percival. The semiclassical two-electron atom and the old quantum theory. *J. Phys. B*, 13:1037, 1980.
- [13] U. Eichmann, V. Lange, and W. Sandner. Positional correlation in laser-excited three-body coulomb systems. *Phys. Rev. A*, 64:274, 1990.
- [14] M. Coreno, K. C. Prince, R. Richter, M. de Simone, K. Bučar, and M. Žitnik. Branching ratios in the radiative decay of helium doubly excited states. *Phys. Rev. A*, 72:052512, Nov 2005.
- [15] Chien-Nan Liu, Ming-Keh Chen, and C. D. Lin. Radiative decay of helium doubly excited states. *Phys. Rev. A*, 64:010501, May 2001.
- [16] Andrej Mihelič and Matja Žitnik. *Ab Initio* calculation of photoionization and inelastic photon scattering spectra of he below the $n = 2$ threshold in a dc electric field. *Phys. Rev. Lett.*, 98:243002, Jun 2007.
- [17] Thomas Ward Gorczyca, Jan-Erik Rubensson, Conny Sâthe, Magnus Ström, Marcus Agâker, Dajun Ding, Stefano Stranges, Robert Richter, and Michele Alagia. Radiative and relativistic

- effects in the decay of highly excited states in helium. *Phys. Rev. Lett.*, 85:1202–1205, Aug 2000.
- [18] Johan Söderström, Marcus Agåker, Anna Zimina, Raimund Feifel, Stefan Eisebitt, Rolf Follath, Gerd Reichardt, Olaf Schwarzkopf, Wolfgang Eberhardt, Andrej Mihelič, Matja Žitnik, and Jan-Erik Rubensson. Radiative decay spectra of selected doubly excited states in helium. *Phys. Rev. A*, 77:012513, Jan 2008.
 - [19] M. K. Odling-Smee, E. Sokell, P. Hammond, and M. A. MacDonald. Radiative decay of doubly excited states in helium below the He^+ ($N = 2$) ionization threshold. *Phys. Rev. Lett.*, 84:2598–2601, Mar 2000.
 - [20]
 - [21] L. Hilico, B. Grémaud, T. Jonckheere, N. Billy, and D. Delande. Quantum three body coulomb problem in two dimensions. *Phys. Rev. A*, 66:022101, 2002.
 - [22] J. Madroñero, P. Schlagheck, L. Hilico, B. Grémaud, D. Delande, and A. Buchleitner. Decay rates of planar helium. *Europhys. Lett.*, 70:183, 2005.
 - [23] Johannes Eiglsperger and Javier Madroñero. Fluctuations in photoionization cross sections of singlet planar helium. *Phys. Rev. A*, 82(3):033422, Sep 2010.
 - [24] Javier Madroñero and Andreas Buchleitner. Ab initio quantum approach to planar helium under periodic driving. *Phys. Rev. A*, 77:053402, 2008.
 - [25] S. Graffi, V. Grecchi, and H. J. Silverstone. Resonances and convergence of perturbation theory for n -body atomic systems in external ac-field. *Ann. Inst. Henri Poincaré*, 42:215, 1985.
 - [26] J. Aguilar and J. M. Combes. A class of analytic perturbations for one-body schrödinger hamiltonians. *Comm. Math. Phys.*, 22(4):269–279, 1971.
 - [27] E. Balslev and J. M. Combes. Spectral properties of many-body schrödinger operators with dilatation-analytic interactions. *Comm. Math. Phys.*, 22(4):280–294, 1971.
 - [28] Y. K. Ho. The method of complex coordinate rotation and its applications to atomic collision processes. *Phys. Rep.*, 99:1, 1983.
 - [29] Harald Siegfried Fiedrich. *Theoretical Atomic Physics*. Springer, 2006.
 - [30] Eiglsperger J. *Highly Doubly Excited States of Two-electron Atoms: Spectra, Cross Sections, and Localization Properties*. PhD thesis, TU München, 2010.
 - [31] A. Buchleitner, B. Grémaud, and D. Delande. Wavefunctions of atomic resonances. *J. Phys. B*, 27:2663, 1994.
 - [32] Mihelič Andrej. *Fluorescence of Doubly Excited States of Helium in Homogeneous Electric Field*. PhD thesis, University of Ljubljana, 2006.
 - [33] C. Lanczos. An iteration method for the solution of the eigenvalue problem of linear differential and integral operators. *J. Res. Natl. Bur. Stand.*, 45:225, 1950.
 - [34] B. N. Parlett and D. S. Scott. The lanczos algorithm with selective orthogonalization. *Math. Comput.*, 33:217, 1979.

- [35] T. Ericsson and A. Ruhe. The spectral transformation lanczos method for the numerical solution of large sparse generalized symmetric eigenvalue problems. *Math. Comput.*, 35:1251, 1980.
- [36] A. Krug. *Alkali Rydberg states in electromagnetic fields: computational physics meets experiment*. Dissertation, Ludwig-Maximilians-Universität München, 2001.
- [37] D. Wintgen, K. Richter, and G. Tanner. The semiclassical helium atom. *Chaos*, 2:19, 1992.
- [38] K. Richter and D. Wintgen. Stable planetary atom configurations. *Phys. Rev. Lett.*, 65:1965, 1990.
- [39] Peter Schlagheck and Andreas Buchleitner. Stable classical configurations in strongly driven helium. *Physica D*, 131:110, 1999.
- [40] C. D. Lin. Classification and supermultiplet structure of doubly excited states. *Phys. Rev. A*, 29:1019–1033, Mar 1984.
- [41] https://www.rp-photonics.com/ultraviolet_light.html. Accessed: 2015-08-31.
- [42] U Fano. Effects of configuration interaction on intensities and phase shifts. *Phys. Rev.*, 124:1866, 1961.
- [43] U. Fano and J. W. Cooper. Line profiles in the far-uv absorption spectra of the rare gases. *Phys. Rev.*, 137:A1364–A1379, Mar 1965.



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SISTEMA INTEGRAL DE GESTION DE PROYECTOS

CERTIFICADO DE REQUISITOS

CÓDIGO DEL PROYECTO: 42793

TITULO: Formation and control of cold molecules

ENTIDAD: Universidad del Valle

CONVOCATORIA: 658-2014 CONVOCATORIA PARA PROYECTOS DE INVESTIGACIÓN EN CIENCIAS BÁSICAS

PROGRAMA: PROGRAMA NACIONAL DE CIENCIAS BÁSICAS

RELACIÓN DE REQUISITOS Y DOCUMENTOS ADJUNTOS

Nº	Definición del requisito	Nombre del archivo adjunto	Tamaño
1	Autorización de uso de datos personales- Anexo 5	06-USODATOS.pdf	1442715 Bytes
2	Carta de aceptación términos de referencia- Anexo 7	10-IP-BL_anexo7.pdf	568849 Bytes
3	Carta de aprobación comité de ética con acto administrativo	07-COMITE_ETICA.pdf	1876114 Bytes
4	Carta de presentación, aval y aceptación de compromisos; relacionando que este proyecto no está siendo presentado por otra convocatoria y no está siendo financiado, -Anexo 2.	02-AVAL.pdf	546301 Bytes
5	Carta para certificación de la contrapartida aportada por entidad. -Anexo 4	05-CONTRAPARTIDA.pdf	181017 Bytes
6	Modelo de intención de Acuerdo de propiedad intelectual-Anexo 6	09-ACUERDO_PI-ICESI_Univalle.pdf	251362 Bytes
7	Relaciona los proyectos financiados por COLCIENCIAS en los últimos cinco años.- Anexo 3.	03-PROYECTOSColciencias.pdf	28454 Bytes
8	Otros adjuntos	Otros-FullProject-Control-Molecules.pdf	146978 Bytes

TOTAL: 8 ARCHIVOS ADJUNTOS

Certificado generado a los 18 días del mes de June de 2014 por el Departamento Administrativo de Ciencia, Tecnología e innovación - COLCIENCIAS



SISTEMA INTEGRAL DE GESTIÓN DE PROYECTOS

PRESENTACIÓN DEL PROYECTO

[Generalidades](#)
[Entidades del proyecto](#)
[Entidad Representante](#)
[Descripciones](#)
[Palabras clave](#)
[Cronograma](#)
[Resultados formación](#)
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GENERALIDADES DEL PROYECTO

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Tipo de Proyecto	PROYECTO		
Título	Formation and control of cold molecules		
Convocatoria	658-2014 CONVOCATORIA PARA PROYECTOS DE INVESTIGACIÓN EN CIENCIAS BÁSICAS		
Programa	PROGRAMA NACIONAL DE CIENCIAS BÁSICAS		
Línea Temática	INVESTIGACIÓN FUNDAMENTAL		
Tipo de financiación	RECUPERACIÓN CONTINGENTE		
Duración en meses	36		
Investigador principal	Beatriz Elena Londoño	CEDULA DE CIUDADANIA:	32108113
Lugar ejecución	CALI - VALLE DEL CAUCA		
Dirección electrónica	rector@univalle.edu.co		

ENTIDADES DEL PROYECTO (2)

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Nombre de la entidad	Rol
Universidad del Valle	EJECUTOR
Universidad Icesi	COEJECUTOR

ENTIDAD EJECUTORA

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Nit	890399010	Dígito de verificación	6
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Dirección electrónica	rector@univalle.edu.co		
Representante legal			

Nombre	Iván Enrique Ramos Calderón		
Tipo de identificación	CEDULA DE CIUDADANIA	Número de identificación	14989446
Clasificación			
Sector	EDUCATIVO		
Tipo de entidad	UNIVERSIDAD PUBLICA		

Grupos de investigación (Total: 3)[Menú entidad](#)

Código	COL0015366	Nombre	Grupo de Química Teórica y Computacional
Código	COL0008497	Nombre	Grupo de Física Teórica del Estado Sólido
Código	COL0014215	Nombre	Óptica Cuántica

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Información general			
Entidad	Universidad Icesi		
NIT	890316745	Dígito de verificación	5
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Dirección	Calle 18 No. 122-135 Pance		
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Dirección electrónica	frapie@icesi.edu.co		
Representante legal			
Nombre	Francisco Piedrahita Plata		
Tipo de identificación	CEDULA DE CIUDADANIA	Número de identificación	14934246
Datos de contacto			
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Clasificación		
Sector	PRIVADAS SIN ÁNIMO DE LUCRO	
Dirección	Calle 18 No. 122-135 Pance	
Teléfono	5725552334	
Tipo de entidad	CENTRO DE INVESTIGACIÓN	
Información adicional		
Exporta	NO	
Actividad económica	M08050 - EDUCACION SUPERIOR	
Capital		
Nacional	Público	0
	Privado	0
Extranjero	Público	0
	Privado	0
Ventas del último año	0	

Grupos (Total: 1)[Menú entidad](#)

Código	COL0093872	Nombre	Natura
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Entidad 2 de 2

[Información general](#) [Grupos](#)
[Menú del proyecto](#)

[Menú entidad](#)

Información general			
Entidad	Universidad del Valle		
NIT	890399010	Dígito de verificación	6
País	COLOMBIA	Ciudad	CALI - VALLE DEL CAUCA
Dirección	Ciudad Universitaria Meléndez, Calle 13 No 100-00		
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Representante legal			
Nombre	Iván Enrique Ramos Calderón		
Tipo de identificación	CEDULA DE CIUDADANIA	Número de identificación	14989446
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	Teléfono	5723212257
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Clasificación		
Sector	EDUCATIVO	
Dirección	Ciudad Universitaria Meléndez, Calle 13 No 100-00	
Teléfono	5723212100	
Tipo de entidad	UNIVERSIDAD PUBLICA	
Información adicional		
Exporta	No	
Capital		
Nacional	Público	0
	Privado	0
Extranjero	Público	0
	Privado	0
Ventas del último año	0	

Grupos (Total: 3)[Menú entidad](#)

Código	Nombre
COL0015366	Grupo de Química Teórica y Computacional
COL0008497	Grupo de Física Teórica del Estado Sólido
COL0014215	Óptica Cuántica

DESCRIPCIONES DEL PROYECTO (Total: 15)[Ir al menú](#)**Descripción 1 de 15****CONFORMACIÓN DEL EQUIPO DE INVESTIGACIÓN**

Research team.

Name - Group - COLCIENCIAS code - Function- Time commitment (Hours per week).

1. Beatriz Elena Londoño Flórez - Óptica Cuántica - COL0014215 - Lead researcher (objectives 5-7) - 10 hours/week.
2. Karem Cecilia Rodríguez Ramírez - Física Teórica del Estado Sólido - COL0008497 - Researcher (objectives 8-10) - 5 hours/week.
3. Carlos Alberto Arango Mambuscay - Natura - COL0093872 - Researcher (objectives 5-7) - 4 hours/week.
4. Julio César Arce Clavijo - Química Teórica y Computacional - COL0015366 - Researcher (objectives 1-4) - 8 hours/week.
5. José Guillermo López Sotelo - Química Teórica y Computacional - COL0015366 -Researcher (objectives 1-4) - 5 hours/week.
6. Estudiante 1 - Student (objectives 1-7) - 40 hours/week.
7. Estudiante 2 - Student (objectives 8-10) - 40 hours/week.

Descripción 2 de 15**ANTECEDENTES Y RESULTADOS PREVIOS DEL EQUIPO DE INVESTIGACIÓN SOLICITANTE EN LA TEMÁTICA ESPECÍFICA DEL PROYECTO**

Background and previous results.

The dynamics of molecular photoexcitation by femtosecond laser pulses using the alkali molecule RbCs as a model system were analyzed in reference [1]. In this scheme, the molecules are initially produced by photoassociation or magnetoassociation into bound vibrational levels close to the first dissociation threshold. Two different approaches are used: the "wavepacket" method, which is global, and the "level-by-level" method, which is restricted in the sense that the number of vibrational levels is limited to a small subset. The comparison between the results of the two approaches produced qualitative insights into the complex dynamics of the high-field regime. In particular, the important role of far-from-resonance levels, which are adiabatically excited through vertical transitions with large Franck-Condon factors, and the outstanding excitation blockade, due to the presence of a quasi-degenerate level in the lower electronic state, were clarified. Moreover, a selective transfer with femtosecond pulses in the low-field regime was observed and the accumulation of population with a coherent train of low-intensity femtosecond pulses was achieved.

Furthermore, the enhancement of photoassociation in RbCs due to spin-orbit resonance coupling, which depends on nuclear separation, was observed [2]. In addition, the influence of the variation with nuclear separation of the transition dipole moments on the electronic transitions was quantified, and the theoretical predictions about the preferential population of levels close to the first threshold in the lowest triplet state after photoexcitation followed by spontaneous emission were seen to agree with the experimental observations [2].

The dynamics of molecules (classical, semiclassical and quantum), and the coherent control of chemical reactions have been studied. In particular a molecular rotor in combined pulses with the aim to produce oriented or aligned molecules, with respect to the coherent control was analyzed. Atom-atom collisions forming diatomic molecules are controlling by the phase control of the dynamics of molecules, studied systems motivated for their biological interest [3-4].

A vast experience on strongly correlated many-body systems has been achieved on the frame work of ultra-cold quantum gases in low-dimensional optical lattices [5-8]. Out-of-equilibrium dynamical problems using both hard-core and soft-core bosons are studied in references [5-6]. Front-wave knowledge in quantum magnetism studying spinor Fermi-gases were been developed in [7] and spinor Bose-gases in [8]. Density matrix renormalization group (DMRG) codes based on matrix product states (MPS) formulation for these problems were developed. The codes allow the numerical calculation of local and non-local observables such as population, magnetization, correlation functions, critical exponents, among others, in both ways statically and dynamically.

In reference [9] the energies and lineshapes of some of the resonances associated with centrifugal-barrier tunneling (quasibound) states that arise at high values of the rotational quantum number J in the rovibrational eigenspectrum, within the ground electronic state, of molecular hydrogen (H_2) were determined. In addition, the cross-sections for the quadrupole O-, Q- and S-branch transitions from vibrational states close to the dissociation threshold into these resonances were evaluated and found to be up to three orders of magnitude larger than the fundamental S-branch transition $v''=0, J''=0$ toward $v'=1, J'=2$. These preliminary results strongly indicate that the direct, i.e. within the ground electronic state, photoassociation of diatomic molecules through orbiting resonances is a quite plausible mechanism. These calculations were performed employing an optical-potential real-time wavepacket propagation method [9-11], which allows the treatment of bound, quasi-bound and continuum states on the same footing and the determination of an eigen or an optical spectrum in a single calculation.

In reference [12] it was shown that a treatment of photoejection processes in terms of wavepackets is more convenient than the one in terms of scattering eigenstates, not only because it allows a dynamical description of the phenomena, but because the cross-sections and other observables can be extracted from the time-dependent wavefunction. Since a direct photoassociation process is, in a sense, the inverse of a photoejection one, analogous consideration should be applicable in this case.

Molecular dynamics was studied in complex system such as $Ne + Ar_2$ by quantum and classical point view. This has allowed explored the implementation of the Wigner function as a straightforward way to incorporate the most important quantum mechanical effects in classical simulations of collisions involving cold weakly bound complexes. [13]

Descripción 3 de 15**RESUMEN EJECUTIVO**

Short summary.

The success and efficiency of the coherent control of chemical reactions requires preparation of the reactants, which can be molecules or atoms, in specific states. Cold molecules formation from cold atoms by external fields and their dynamics must be analyze, this demands the knowledge of precise details about the molecular structure and collisions processes between

atoms. The rapid progress in the technology of radiation sources and nanoscale engineering give us access to much accuracy information on this cold matter. We need to study and understand this information with the expectation to obtain control over the quantum processes; in fact it is a major role of the theoretical counter part of the field.

For the first time in Colombia, a group has combined experiences and knowledge from different areas on topics like: control of chemical reaction by light, collision of atoms, creation of molecules, strongly correlated many-body systems, and molecular reaction dynamics, to do contributions in a new and excited research area on Cold Molecules.

The current mechanism to produce cold molecules from photoassociation of pair of cold atoms involves two or more steps [14-17]. The one-step process, which is proposed here using cold alkali atoms initially trapped in orbiting resonances, to go on translational cold molecules in their ground electronic states are an original proposal in the cold molecules field. Chirped laser pulses to control the population transfer during the process are used. We focus in molecules of experimental interest for example KRb.

After the formation of molecule by above proposal or another, the transferring of the molecule toward specific rovibrational states are studied. Methodologies well established experimentally like STImulated Raman Adiabatic Passage - STIRAP [14-17] and Stark-induced Adiabatic Raman Passage - SARP [17] are theoretically explored, to obtain real parameters of pulses to get the control over internal degrees of freedom of molecule. We expect that the methodology performed of project is extended to other polar molecules as LiCs, RbCs.

Due to photoassociation mechanism the triplet-rovibrational excited state has high probability to be populated [2, 14-17], thus STIRAP process involves passage from triplet to singlet-rovibrational ground state. Hence, it is interesting to analyze the coherent direct-transfer population between the singlet and triplet sublevels of the rovibrational of the Mott-Insulator molecular ground-state [26] as a function of the Coulomb on-site and nearest-neighbor interactions. For which on a strongly interacting many-body molecular gas loaded on one-dimensional optical lattices are studied.

Some spectroscopic details of the molecule are taken from literature, such as electronic potentials, long-range contributions, van Der Waals coefficients, scattering lengths, electronic dipoles, spin-orbit couplings, among others. Those are necessary to calculate the properties here we propose. The methodology to obtain precise potentials and dipole transfer moments was acquired in previous works. In general in this project several analytic and numerical methods are combined to study the dynamics of the molecule, which enriches the analyzing.

The expectations from this project are concentrated in two points: formation of the students and publication of the papers in which the main conclusions are shown.

Descripción 4 de 15

PLANTEAMIENTO DEL PROBLEMA

Problem.

Nowadays, the cold molecules field is a hot topic. Continuous experimental successful go in hand a big theoretical effort to analyze, to propose scenarios, to use this system to achieve dreams of scientists: to control the evolution of a quantum system at the ultimate limit. Control over evolution of every internal and external degrees of freedom of a quantum system is a possible situation in cold matter.

In this project the studied points are: (I) photoassociation of cold alkali atoms to create molecules, (II) the control of molecular internal states, (III) the study of collective processes of a molecular gas loaded on optical lattices.

In the case of cold molecules formation (I) a direct, one-step mechanism for the production of cold diatomic molecules is proposed, entailing the stimulated photoassociation of cold ground-state atoms, initially trapped in orbiting resonances, into translationally cold molecules in their ground electronic states. Moreover, we will attempt to control the population transfer during the process by means of chirped laser pulses. The whole scheme will be implemented computationally employing numerical time-dependent methods.

Using the previous technique or any other that allows us to obtain molecules in the absolute ground state [14-17], specific rovibrational states (v , J , M) or linear combinations of the M -states [17], kipping in mind the objective to be closer to the coherent control of chemical reactions. Theoretical study of the process to prepare KRb molecules in specific rovibrational states is studied. (II) The well-established experimental STIRAP and SARP [15-17] methodologies are analyzed.

Once the molecules are stabilized in the rovibrational ground state, this strongly interacting many-body molecular gas is loaded on a one-dimensional optical lattice (III), The aim is to analyze the coherent direct-transfer population between the singlet and triplet lowest states of the molecules.

The specific problem here is how can we find new routes or improve the existing techniques to create molecules, getting to desired target states and controlling the internal and collective processes in the molecular dynamics?

Descripción 5 de 15

JUSTIFICACIÓN

Justification.

The cold molecules field represents attractive structures to achieve the control of the evolution of a quantum system. Since its origin two decades ago, the field has been quickly developed because of the many applications which motivated the world wide community such as controlled molecular dynamics, cold chemistry, high resolution spectroscopic, test of fundamental laws, quantum information, quantum simulators and coherent control. The rapid advance of electromagnetic sources and nanoscale technologies allow trapping and creating molecules in well-defined internal states. Such progress clearly benefited from a continuous exchange between theory and experiment, either for predictions or for interpretations of observed results.

Cold molecules are a new and very promising area because the huge scientific and technological impact; this combined with expertise of the theoretical research proponents motivates the current proposal, making of this project a good opportunity to create interdisciplinary areas in Colombia in front-wave science. The country science is measurable by the contributions made by their researchers and the researches of the present project are working on important topics for the international community, which allow us to be quickly spotted.

The group working on the current project proposal has vast experience on theoretical aspects, which allow us to contribute in the prediction and interpretation of topics related with cold molecules, specifically in the three points mentioned in Problem section. In our knowledge for the first time in Colombia a research on Cold Molecules is led.

Every expectation above mentioned is relevant to the current Science, Technology and Innovation law in Colombia. Projects in theoretical basic science are promoting the achievement of objectives in article 3 of 1286 law, 2009, specially 1, 5, 6 and 7 which are related to the increasing and strengthening of the scientific ability, the promotion of education and the use of human capacity. Moreover the objectives of this project are relevant for the priorities as: less poverty, more jobs, international connection and innovation that established the Strategic Plan 2011-2014 of COLCIENCIAS by the creation of skills in science, technology and innovation of the community. The coordinated and articulated science, technology and innovation guidelines for regional, national and international implementation, consolidation of scientific, technological and innovation community through a set of tools, strategies and strengthening of the human capital. Strengthen of master, doctoral degrees in Colombia; promote the post-doctoral research and national and international mobility.

Descripción 6 de 15

MARCO CONCEPTUAL

Theoretical framework.

The new area of cold quantum matter involving ultracold and quantum degenerate molecular gases is currently on the focus of interest within the atomic physics, molecular physics and physical chemistry communities. Researches on cold molecules started mainly with the formation of alkali dimers, as alkali atoms are the most widely used species for laser cooling. A detailed knowledge of their structure is necessary for appropriate manipulation of these species in the course of their formation and control process.

The laser cooling techniques that have been developed for atoms [18] do not work for molecules, due to the presence of rovibrational degrees of freedom and the cluttering of quantum states. After indirect methods like photoassociation, the translational cooling of atoms is keeping then the molecular internal degrees of freedom can be cooled [18-21]. In the photoassociation of pre-cooled atoms, the motion of the center of mass is essentially unaffected, thereby preserving the translational temperature of the recombining atoms [19]. The photoassociation process employed in Julienne's laboratory [20] entails an initial free-bound excitation into a weakly-bound vibrational level of an excited electronic state, followed by a bound-bound spontaneous emission into the ground electronic state. This scheme has the disadvantages that the final vibrational state may be an incoherent mixture of vibrational levels, and, moreover, weakly bound, in which case the molecule may dissociate into atoms which leave the trap. To channel the populations into robust final molecular states, adiabatic passage and pump-dump schemes that involve stimulated emission from the intermediate excited electronic state have been proposed by various groups [21]. STIRAP and SARP [15-17] process have caught the molecule in a specific rovibrational state. Again these processes conserve the translational cooling while the molecule has been driven to the lowest rovibrational state.

A recently intense scientific interest come from polar molecules because they can be situate inside lattices to study many-body dynamics, which provide highly controllable, long-lived and strongly interacting dipolar systems, a first experimental observation is reported in [22]. Hence, it is possible to explore a way to transfer in a coherent and direct way the molecular population between the singlet and triplet sublevels of the rovibrational Mott-Insulator ground molecular state [26] as a function of the Coulomb on-site and nearest-neighbor interactions.

In a general way the main theoretical aspects to perform these problems come from atomic and molecular physics, dynamical studies of the molecular internal degree of freedom in the presence of radiation and evolution of many-body strongly correlated systems

Descripción 7 de 15**ESTADO DEL ARTE**

State of knowledge in the problem area.

The revolution in cold matter begun with cooling of atoms by laser - The Nobel Prize in Physics 1997 S. Chu, C. Cohen-Tannoudji and W. D. Phillips - and the first successful was Bose-Einstein Condensate (BEC) of Rb and Na atoms - The Nobel Prize in Physics 2001 E. A. Cornell, W. Ketterle, y C. E. Wieman. The BEC temperature is of the order of nano Kelvin, and the cloud is trapped by magneto-optical fields in almost perfect vacuum (10^{-14} bar).

Laser cooling of atoms relies on a closed-level radiative transition scheme which allows the atoms to undergo many absorption-spontaneous emission cycles until they are stopped in the laboratory frame. Such closed-level schemes are not expected to be easily found in molecules because they have many internal degrees of freedom: vibrations, rotations and hyperfine structure.

Production of ultra-cold molecules either by cooling thermal gases (direct methods) or by linking ultra-cold atoms (indirect methods) is still in continuous improving. The successful association of two pre-cooled atoms to form molecules has been achieved using photoassociation and magnetoassociation. These process are the most known indirect methods at the current time and they take advantage from Feshbach resonance to control the interaction between atoms, this allowed to get the molecular BEC in 2003 [23].

Cold molecules have attracted growing interest in last times, due to their potential utility in several areas: cold chemistry, quantum dipolar system, quantum information. In many of these applications completed evolve the molecular system in a robust target quantum state is desirable; hence the control in all degrees of freedom (electronic, vibrational, rotational, hyperfine and external motion) is required [24].

Due to the atom-atom association mechanism the triplet-rovibrational excited state has higher probability to be populated [2, 17] and further technique as STIRAP must be implemented to undergo the singlet-rovibrational ground state. Although this technique is experimentally complex, it is highly efficient and state-selective [16]. Nevertheless, it can only be applied once per experimental realization, limiting the ultimate number of ground state molecules. An alternative to the use of STIRAP step is to ramp up an optical lattice, this step provides no further heating [25-26] and once the loading of the ultracold molecules is performed, the system becomes deeply bound [27] and strongly correlated and finally can be used as a quantum simulator.

Descripción 8 de 15**OBJETIVO GENERAL**

General objective.

To propose and implement computationally new mechanisms for the formation of cold alkali molecules, involving the laser control of collisions between cold atoms, the subsequent dynamics of the internal molecular degrees of freedom and ultracold lattice molecules.

Descripción 9 de 15**OBJETIVOS ESPECÍFICOS**

Specific objectives:

1. To calibrate the ab-initio potential energy curves for alkali molecules reported in the literature, in order to obtain a good agreement between theory and experiment of spectroscopic properties and scattering lengths.
2. To determine the energies and lifetimes of the orbiting resonances arising in the ground electronic state of the target diatomic alkali molecule at high J.
3. To calculate the cross-sections for stimulated photoassociation of two colliding ground-state atoms into the vibrational states of the electronic ground state of the target diatomic molecule, taking as initial states the orbiting resonances determined in specific objective 2.
4. To simulate the coherent quantum dynamics, and possible control, of the stimulated photoassociation processes described in objective 3, employing chirped laser pulses.
5. To propose a theoretical scheme using multiple laser pulses to produce alkali diatomic molecules in specific rovibrational

states.

6. To determine the role of different intermediate states to efficiently obtain KRb molecules by STIRAP in the ground vibrational state from Feshbach molecules.

7. To design SARP laser pulses to generate KRb molecules on specific rovibrational states (v , J , M) or superposition of sublevels M .

8. To establish the effective Hamiltonian that exhibits the relevant low-energy physical phenomena of the tightly bound ultracold lattice molecules in the triplet- and singlet-rovibrational ground-state in the Mott-insulator regime.

9. To identify the relevant and necessary local- and non-local-observables, critical exponents and correlations to be measured from the lattice molecules obtained in objective 8 and perform the respective numerical implementations.

10. To find how to stabilize a coherent transfer population between the singlet and triplet sublevels of the rovibrational Mott-Insulator molecular ground-state as a function of the Coulomb on-site and nearest-neighbor interactions, using the obtained information from objective 9.

Descripción 10 de 15

METODOLOGÍA

Methodology for achieving each objective.

The general objective in this project involves time-dependent calculations to analyze the dynamic of molecules.

To achieve 1-4 objectives we propose an alternative scheme based on the following physical picture: Since the majority of the atomic collisions that occur in the dilute, cold gas are binary and involve high impact parameters, i.e. high rotational quantum numbers J , a sizable fraction of them occur with energies that coincide with the energies of orbiting resonances in the center-of-mass frame. As these resonances are rovibrational quasibound states located just above the dissociation threshold, the cross-sections for optical transitions from them into bound vibrational levels are much higher than those from free scattering states [9]. Hence, by tuning the laser field to these quasibound to bound transitions, we can stimulate the formation of the diatomic molecule. This scheme has the advantage that it entails a direct one-step process, in which the laser can be finely tuned to any desired final vibrational state, within the J values allowed by the rotational selection rule. Moreover, we intend to control the population transfers during such transitions employing chirped laser pulses. The resonances and cross-sections will be computed by means of the optical-potential real-time wavepacket propagation method [9-11]. The coherent, unitary quantum dynamics of the photoassociation processes will be simulated by numerical integration of the time-dependent Schrödinger equation [1-4, 12], taking as initial conditions incoming wavepackets with a range of energies and widths consistent with the low temperatures of the phenomenon. The prototype systems will be alkali molecules, for which the potential-energy curves and dipole transition moments are well known [1, 2].

(5-7 objectives) To determine the molecular structure (vibrational energy levels, and oscillator strengths between vibrational levels), the numerical method used to solve the time independent Schrödinger equation is called "Mapped Fourier Grid Hamiltonian Representation Method" (MFGHR) [2]. Using this numerical method we can obtain for each vibrational state of a chosen electronic state the transition probabilities toward lower vibrational levels and the respective values of the lifetimes. The respective potentials and molecular electronic dipole are calculated in the Laboratory Aimé Cotton in Orsay, France, and constitute our raw material for the construction of respective tables with numerical values of transition probabilities and lifetimes. From these available numerical tables, we proceed to make graphs that allow us to analyze information, draw conclusions for each dimer and to compare results for different molecules.

To determine the dynamics induced in the molecule in the presence of a laser pulse, two different approaches are used to solve the time dependent Schrödinger equation. By using the 'wave-packet method', we calculate globally the evolution of the vibrational wave-packets created on the electronic states coupled by the laser pulses. The time-dependent Schrödinger equation is solved by polynomial expansion in Chebychev basis. By using the "level by level method", we determine the instantaneous amplitudes of population of a restricted number of vibrational levels explicitly supposed to be involved in the excitation process. [1].

(8-10 objectives) The description of the ultracold strongly correlated molecules loaded on one-dimensional optical lattices is performed by means of two methods depending on the length of the lattice. Focusing on few-sites quantum-state systems (around 10 sites) we are going to use Exact Diagonalization (ED) like the Lanczos algorithm [28]. To analyze longer systems (more than 20 sites) we are going to use the Matrix Product State (MPS) technique [29]. The latter has been chosen because the MPS representation efficiently approximates the ground state of 1D local Hamiltonians. The formalism is highly recommended when the amount of entanglement in the system is limited reducing the calculation complexity from an original exponential to an algebraic growing of the Hilbert space. This method allows us to study the molecular quantum ground-state properties via the calculations of local and non-local operators, correlations and critical exponents.

Descripción 11 de 15**RESULTADOS ESPERADOS DE LA INVESTIGACIÓN**

Expected results (knowledge).

The development of this project allows knowledge about spectroscopic properties of alkali molecules as KRb. This is important to get full control over system and the implemented control mechanics allow us understanding on control protocols over cold di-alkali molecules.

Expected results (products).

- Products related to achievement of new knowledge:

5 - Research papers (review A1).

- Products related to profit of social knowledge:

5 - Internal seminars. Departamento de Física y química -Univalle - ICESI.

1 - International meeting, 2 - National meeting.

- Products related to the formation and skill achievement of persons:

2 - Research work (Master student).

Descripción 12 de 15**TRAYECTORIA DEL EQUIPO DE INVESTIGACIÓN**

Trajectory of the researchers.

The researchers of this project have vast experience on theoretical studies about collisions between atoms, formation of molecules, used of laser to control chemical reactions, molecular dynamics, atom-diatom collisions and dynamical of many particles. The project gathers researchers from different groups and areas: physics and chemistry hence the vision from different areas and expertise of the researchers are an advantage to get successful results.

For first time this working team perform a research proposal with the expectation to create and lead a new line of research in Colombia on Cold Molecules.

Descripción 13 de 15**POSIBLES EVALUADORES**

Suggested evaluators.

1. Jordi Mur Petit - jordi.murino@gmail.com - google-sites: <https://sites.google.com/site/jordimurpetit/> - Instituto de Estructura de la Materia Serrano, 123 Room 138 Madrid 28006 (Spain).

2. Rosario González Férez - rogonzal@ugr.es - web-page: <http://www.ugr.es/~rogonzal/> - Departamento de Física Atómica, Molecular y Nuclear . Instituto Carlos I de Física Teórica y Computacional. Universidad de Granada - Facultad de Ciencias Avenida de Fuentenueva, S/N 18071 Granada (Spain).

Descripción 14 de 15**IMPACTO AMBIENTAL DEL PROYECTO**

Environmental impact .

This research is purely theoretical and on basic science hence there is not directly and measurable environmental impact which is produced during its development. Analytic and numerical calculations are our main activity. Thus at present time and near future the expected impact of this project is the same to daily human activity like: to use the car or the electric spending. The current possibility to reduce this impact comes from the individual consciousness.

In the future, the possible impact of industrial production which can derivate from results on this research is more speculative

hence it is not relevant do now.

Descripción 15 de 15

BIBLIOGRAFÍA

References.

- [1] B. E. Londono, A. Derevianko, J. E. Mahecha, A. Crubellier and E. Luc-Koenig. Femtosecond pulses and dynamics of molecular photoexcitation: RbCs example. *Phys. Rev. A*. 85, 033419 (2012).
- [2] B. Londoño, J. E. Mahecha, E. Luc-Koenig, and A. Crubellier, Lifetime of vibrational levels from Fourier grid calculations: RbCs example. DOI: 10.1039/C1CP21167F. *Phys. Chem. Chem. Phys.* 13, 18738 (2011). B. Londoño, J. E. Mahecha, E. Luc-Koenig, and A. Crubellier, Resonant coupling effects on the photoassociation of ultracold Rb and Cs atoms. *Phys. Rev. A* 80, 032511 (2009).
- [3] Arango, C., Shapiro, M., Brumer, P. Coherent control of collision process: Penning versus associative ionization. *The Journal of Chemical Physics* 125, 094315 (2006).
- [4] Arango, C., Shapiro, M., Brumer, P. Cold Atomic Collisions: Coherent Control of Penning and Associative Ionization. *Physical Review Letters* 97, 193202 (2006)
- [5] K. Rodríguez, S. R. Manmana, M. Rigol, R. M. Noack, and A. Muramatsu, "Coherent matter waves emerging from Mott-insulators", Invited paper to a special issue on Cold Atoms in Optical Lattices, *New J. Phys.* 8, 169 (2006).
- [6] K. Rodríguez, A. Argüelles and L. Santos, "Correlation dynamics of strongly-correlated bosons in time-dependent optical lattices", *ArXiv:0905.3312 [cond-mat.quantgas]* (2009).
- [7] K. Rodríguez, A. Argüelles, M. Colomé-Tatché, T. Vekua and L. Santos, "Mott-Insulator Phases of Spin-3/2 Fermions in the Presence of Quadratic Zeeman Coupling", *Phys. Rev. Lett.* 105, 050402 (2010).
- [8] K. Rodríguez, A. Argüelles, A. K. Kolezhuk, L. Santos and T. Vekua, "Field-induced phase transitions of repulsive spin-1 bosons in optical lattices", *Phys. Rev. Lett.* 106, 105302 (2011).
- [9] J.C. Arce. Real-time wavepacket propagation method for the spectroscopy of simple systems: pure quadrupole vibration-rotation spectra of molecular hydrogen. *Rev. Col. Fís.* 31, 65 (2000).
- [10] D.F. Montaña, J.C. Arce and N. Porrás-Montenegro, Quantum states and interband optical spectra in spherical GaAs-(Ga,Al)As quantum dots doped with on-centre shallow donor impurities: a real-time wavepacket propagation method. *J. Phys. Condens. Matter* 12, 9917 (2000).
- [11] P.W. Langhoff, J.C. Arce, and J.A. Sheehy. Dynamical theory of molecular photoionization: electron ejection kinematics and angular distributions from molecules fixed in space. *J. Electron Spectrosc. Relat. Phenom.* 123, 117 (2002).
- [12] M.L. Zambrano and J.C. Arce, Stark-resonance densities of states, eigenfunctions, and lifetimes for electrons in GaAs/(Al,Ga)As quantum wells under strong electric fields: An optical-potential wave-packet propagation method. *Phys. Rev. B* 66, 155340 (2002).
- [13] J. G. López and A. B. McCoy. Classical treatments of quantum mechanical effects in collisions of weakly bound complexes. *Chem. Phys.* 308, 267 (2005)
- [14] C D Bruzewicz, M. Gustavsson, T. Shimasaki and D DeMille. Continuous formation of vibronic ground state RbCs molecules via photoassociation. *New Journal of Physics* 16, 023018 (2014).
- [15] Debatin, M., Creation of Ultracold RbCs Ground-State Molecules, D. Sc. Dissertation, Faculty of Mathematics, Computer Science and Physics, University of Innsbruck, Innsbruck July 2013.
- [16] Mukherjee, N., Dong, W., Zare, R., Coherent superposition of M-states in a single rovibrational level of H₂ by Stark-induced adiabatic Raman passage, *The Journal of Chemical Physics* 140, 074201 (2014).
- [17] Gaubatz, U., Rudecki, P., Becker, M., Schiemann, S., Külz, M., Bergmann, K., Population switching between vibrational levels in molecular beams, *Chem. Phys. Lett.* 149, 463 (1988).
- [18] W. D. Phillips, Nobel Lecture: Laser cooling and trapping of neutral atoms. *Rev. Mod. Phys.* 70, 721 (1998).
- [19] M. Viteau, A. Chotia, M. Allegrini, N. Bouloufa, O. Dulieu, D. Comparat, P. Pillet. Optical Pumping and Vibrational Cooling of Molecules. *Science* 321, 232 (2008).
- [20] K. M. Jones, E. Tiesinga, P. D. Lett, P.S. Julienne. Publisher's Note: Ultracold photoassociation spectroscopy: Long-range molecules and atomic scattering. *Rev. Mod. Phys.* 78, 483 (2006).
- [21] C. P. Koch and M. Shapiro, Coherent Control of Ultracold Photoassociation. *Chem. Rev.* 112, 4928 (2012).
- [22] Bo Yan, S. A. Moses, B. Gadway, J. P. Covey, K. R. A. Hazzard, A. M. Rey, D. S. Jin & Jun Ye. Observation of dipolar spin-exchange interactions with lattice-confined polar molecules. *Nature* 501, 521 (2013)
- [23] S. Jochim, et al., Bose-Einstein condensation of molecules, *Science* 302, 2101 (2003); M. Greiner, C. A. Regal and D. S. Jin, Emergence of a molecular Bose-Einstein condensate from a Fermi gas, *Nature* 426, 537 (2003); M. W. Zwierlein, et al., Observation of Bose-Einstein condensation of molecules, *Phys. Rev. Lett.* 91, 250401 (2003).
- [24] N. Balakrishnan and A. Dalgarno, Chemistry at ultracold temperatures. *Chem. Phys. Lett.* 341, 652 (2001); R. V. Krems, Viewpoint: Ultracold controlled chemistry, *Physics* 3, 10 (2010).
- [25] T. Rom, T. Best, O. Mandel, A. Widera, M. Greiner, T. W. Hänsch, and I. Bloch. State Selective Production of Molecules in Optical Lattices. *Phys. Rev. Lett.* 93, 073002 (2004).

[26] T. Volz, N. Syassen, D. M. Bauer, E. Hansis, S. Dürr, and G. Rempe, Preparation of a quantum state with one molecule at each site of an optical lattice, *Nature Phys.* 2, 692 (2006).

[27] Johann G Danzl, Manfred J Mark, Elmar Haller, Mattias Gustavsson, Russell Hart, Andreas Liem, Holger Zellmer and Hanns-Christoph Näger, Deeply bound ultracold molecules in an optical lattice. *New J. Phys.* 11, 055036 (2009).

[28] Golub, G. H., Van Loan, C. F. (1989), *Matrix computations*. Johns Hopkins University Press, 2nd edition.

[29] F. Verstraete, J. J. García-Ripoll and J. I. Cirac. Matrix Product Density Operators: Simulation of Finite-Temperature and Dissipative Systems. *Phys. Rev. Lett.* 93, 207204 (2004); G. Vidal. Efficient Simulation of One-Dimensional Quantum Many-Body Systems. *Phys. Rev. Lett.* 93 040502 (2004).

PALABRAS CLAVE (Total: 6)[Ir al menú](#)

- quantum control
- resonances
- optical lattice
- photoassociation
- Cold molecules
- strongly correlated system

CRONOGRAMA (Total: 22)[Ir al menú](#)

Número	Actividad	Desde	Hasta	Tiempo
01	Calibration of electronic potentials of KRb molecule (objective 1)	1	2	Meses
02	Calculation of vibrational energies, lifetime, cross-section, dipole transition moments (objectives 2,3,6,7,8)	2	6	Meses
03	Characterization of orbiting resonances on KRb molecule (objective 3)	4	9	Meses
04	Preparation of paper (objectives 1,2)	10	12	Meses
05	Implementation of a chirped pulse to control the orbiting resonances on KRb molecule (objetives 3,4)	13	17	Meses
06	Study and analyzed of mechanics to vibrational cooling (objectives 3,4)	17	20	Meses
07	Implementation of process to create cold KRb molecule from orbiting resonances in the cold collision of K and Rb atoms (objective 4)	21	28	Meses
08	Preparation of paper (objectives 3,4)	28	31	Meses
09	Determination of the interesting rovibrational states to implement the STIRAP and SARP and comparison with experimental reports to date (objectives 5,6,7)	7	14	Meses
10	Analysis of the rovibrational dynamic in wavepacket created by pulse (objectives 6,7)	14	23	Meses
11	Preparation of paper (objectives 6,7)	24	26	Meses
12	Implementation of optimal pulse to control STIRAP process (objective 6)	26	31	Meses
13	Implementation of optimal pulse to control SARP process (objective 7)	29	34	Meses
14	Implementation of a scheme to obtain the KRb molecule in a specific rovibrational state (objective 5)	28	34	Meses
15	Preparation of paper (objective 5)	31	34	Meses

16	Determination of effective Hamiltonian of lattice KRb polar molecule (objectives 8,9,10)	6	9	Meses
17	Determination of the observables, correlations, critical exponents of the determined Hamiltonian for lattice molecule (objective 9)	9	16	Meses
18	Numerical implementation to solve the dynamics of determined Hamiltonian for lattice molecule (objectives 9,10)	17	26	Meses
19	Analysis a mechanics to obtain coherent transfer population between the singlet and triplet rovibrational sublevels in KRb molecule (objectives 10)	21	30	Meses
20	Preparation of paper (objectives 8,9,10)	29	33	Meses
21	Preparation of reports (objectives 1-10)	34	36	Meses
22	Discussions between researchers and/or international partners. (Continuous activity during the development of the project) (objectives 1-10)	1	36	Meses

RESULTADOS FORMACIÓN (Total: 1)[Ir al menú](#)

Formación	Descripción	Personas	Beneficiario
MAESTRIA	Research work of Master students	2	students, university and country

RESULTADOS PUBLICACIONES (Total: 1)[Ir al menú](#)

Publicación	Descripción	Cantidad	Beneficiario
PONENCIAS	1 - International meeting 2 - National meeting	3	community

OTROS RESULTADOS (Total: 1)[Ir al menú](#)

Resultado	Descripción	Cantidad	Beneficiario
ARTICULO EN REVISTA A1, A2, B, C Y D	5	7	university, country, cientific intrenational community

COBERTURA(1)[Ir al menú](#)

Nombre	Porcentaje de cobertura
VALLE	100

TIPO PERSONAL (Total: 3)[Ir al menú](#)

Rol en el Proyecto	Cantidad
ESTUDIANTE MAESTRIA	2
INVESTIGADOR	4
INVESTIGADOR PRINCIPAL	1

PERSONAS (Total: 7)[Ir al menú](#)**Persona 1 de 7**

Entidad	Universidad Icesi
Rol en el proyecto	INVESTIGADOR
Primer apellido	Arango
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Tipo de identificación	CEDULA DE CIUDADANIA
Número	94398430
Responsabilidades	Desarrollo de objetivos 5-7
Dedicación horas semanales	4
Número de meses	36

Persona 2 de 7

Entidad	Universidad del Valle
Rol en el proyecto	INVESTIGADOR
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Tipo de identificación	CEDULA DE CIUDADANIA
Número	52517246
Responsabilidades	Desarrollo de objetivos 8-10
Dedicación horas semanales	5
Número de meses	36

Persona 3 de 7

Entidad	Universidad del Valle
Rol en el proyecto	INVESTIGADOR
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Responsabilidades	Desarrollo de objetivos 1-4
Dedicación horas semanales	8
Número de meses	36

Persona 4 de 7

Entidad	Universidad del Valle
Rol en el proyecto	INVESTIGADOR
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Número	94382084
Responsabilidades	Desarrollo de objetivos 1-4
Dedicación horas semanales	5
Número de meses	36

Persona 5 de 7

Entidad	Universidad del Valle
Rol en el proyecto	INVESTIGADOR PRINCIPAL
Primer apellido	Londoño
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Género	Femenino
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País	COLOMBIA
Correo electrónico	beatriz.e.londono.f@correounivalle.edu.co
Tipo de identificación	CEDULA DE CIUDADANIA
Número	32108113
Responsabilidades	Desarrollo de objetivos 5-7
Dedicación horas semanales	10
Número de meses	36

Persona 6 de 7

Entidad	Universidad del Valle
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Rol en el proyecto	ESTUDIANTE MAESTRIA
Primer apellido	NN
Segundo apellido	NN
Nombres	NN
País	COLOMBIA
Responsabilidades	Desarrollo de objetivos 1-7
Dedicación horas semanales	40
Número de meses	24

Persona 7 de 7

Entidad	Universidad del Valle
Rol en el proyecto	ESTUDIANTE MAESTRIA
Primer apellido	NN
Segundo apellido	NN
Nombres	NN
País	COLOMBIA
Responsabilidades	Desarrollo de objetivos 8-10
Dedicación horas semanales	40
Número de meses	24

PRESUPUESTO GLOBAL(Total: 5)[Ir al menú](#)

Rubros	Financiado	Contrapartida		Total
		Ejecutora(s)	Otras	
EQUIPOS	15,000,000	13,000,000	2,000,000	30,000,000
GASTOS DE OPERACIÓN	17,652,251	0	0	17,652,251
PERSONAL CIENTÍFICO	120,000,000	115,926,617	26,788,320	262,714,937
SEGUIMIENTO Y EVALUACION	5,825,243	0	0	5,825,243
VIAJES	41,522,506	0	0	41,522,506
Totales	200,000,000	128926617	28788320	357,714,937

RESUMEN POR RUBROS (Total: 5)[Ir al menú](#)

Rubros	Financiado	%	Especie	%	Efectivo	%	Total
EQUIPOS	15000000	50%	15,000,000	50%	0	0%	30,000,000
GASTOS DE OPERACIÓN	17652251	100%	0	0%	0	0%	17,652,251
PERSONAL CIENTÍFICO	120000000	45,68%	142,714,937	54,32%	0	0%	262,714,937
SEGUIMIENTO Y EVALUACION	5825243	100%	0	0%	0	0%	5,825,243
Totales	200,000,000	55.91	157,714,937	44.09	0	0.00	357,714,937

Rubros	Financiado	%	Especie	%	Efectivo	%	Total
VIAJES	41522506	100%	0	0%	0	0%	41,522,506
Totales	200,000,000	55.91	157,714,937	44.09	0	0.00	357,714,937

PRESUPUESTO POR ENTIDAD (Total: 2)[Ir al menú](#)**Entidad 1 de 2 Universidad Icesi**

Rubro	Descripción	Entidad financiadora	Financiado	%	Contrapartida				Total
					Especie - %		Dinero - %		
EQUIPOS	Estaciones de trabajo y una impresora	COLCIENCIAS	0	0	2,000,000	100,00	0	0	2,000,000
PERSONAL CIENTÍFICO	Carlos Alberto	COLCIENCIAS	0	0	26,788,320	100,00	0	0	26,788,320
Totales			0	0.0	28,788,320	100.0	0	0.0	28,788,320

Entidad 2 de 2 Universidad del Valle

Rubro	Descripción	Entidad financiadora	Financiado	%	Contrapartida				Total
					Especie - %		Dinero - %		
EQUIPOS	Estaciones de trabajo y una impresora	COLCIENCIAS	0	0	0	0	0	0	0
EQUIPOS	Estaciones de trabajo y una impresora	COLCIENCIAS	15,000,000	53,57	13,000,000	46,43	0	0	28,000,000
GASTOS DE OPERACIÓN	gastos Universidad	COLCIENCIAS	17,652,251	100,00	0	0	0	0	17,652,251
PERSONAL CIENTÍFICO	NN	COLCIENCIAS	60,000,000	100,00	0	0	0	0	60,000,000
PERSONAL CIENTÍFICO	NN	COLCIENCIAS	60,000,000	100,00	0	0	0	0	60,000,000
PERSONAL CIENTÍFICO	José Guillermo	COLCIENCIAS	0	0	15,145,000	100,00	0	0	15,145,000
PERSONAL CIENTÍFICO	Beatriz Elena	COLCIENCIAS	0	0	38,682,000	100,00	0	0	38,682,000
PERSONAL CIENTÍFICO	Karem Cecilia	COLCIENCIAS	0	0	19,667,617	100,00	0	0	19,667,617
PERSONAL CIENTÍFICO	Julio Arce	COLCIENCIAS	0	0	42,432,000	100,00	0	0	42,432,000
SEGUIMIENTO Y EVALUACION	seguimiento COLCIENCIAS	COLCIENCIAS	5,825,243	100,00	0	0	0	0	5,825,243
VIAJES	Cali	COLCIENCIAS	13,000,000	100,00	0	0	0	0	13,000,000
VIAJES	Nacional y/o internacional	COLCIENCIAS	28,522,506	100,00	0	0	0	0	28,522,506
Totales			200,000,000	60.8	128,926,617	39.2	0	0.0	328,926,617

PRESUPUESTO DETALLADO (Total: 5)[Ir al menú](#)**Cuadro 1 de 5 EQUIPOS**

Descripción	Justificación	Cantidad	Valor unitario	Entidad	Financiado	Contrapartida		Total
						Especie	Dinero	
Estaciones de trabajo y una impresora	Cálculos numéricos, impresión de material bibliográfico y documentos.			Universidad Icesi	0	2,000,000	0	2,000,000
Estaciones de trabajo y una impresora	Cálculos numéricos, impresión de material bibliográfico y documentos.			Universidad del Valle	0	0	0	0
Estaciones de trabajo y una impresora	Cálculos numéricos, impresión de material bibliográfico y documentos.			Universidad del Valle	15,000,000	13,000,000	0	28,000,000
Totales					15,000,000	15,000,000	0	30,000,000

Cuadro 2 de 5 PERSONAL CIENTÍFICO

Nombre	Función en el proyecto	Tipo de vinculación	Dedicación Hora/Semana	Entidad	Financiado	Contrapartida		Total
						Especie	Dinero	
Carlos Alberto Arango	Desarrollo de objetivos 5-7	EN PLANTA	4	Universidad Icesi	0	26,788,320	0	26,788,320
NN NN	Desarrollo de objetivos 1-7	POR CONTRATO	40	Universidad del Valle	60,000,000	0	0	60,000,000
NN NN	Desarrollo de objetivos 1-7	POR CONTRATO	40	Universidad del Valle	60,000,000	0	0	60,000,000
José Guillermo López	Desarrollo de objetivos 1-4	EN PLANTA	5	Universidad del Valle	0	15,145,000	0	15,145,000
Totales					120,000,000	142,714,937	0	262,714,937

Nombre	Función en el proyecto	Tipo de vinculación	Dedicación Hora/Semana	Entidad	Financiado	Contrapartida		Total
						Especie	Dinero	
Beatriz Elena Londoño	Desarrollo de objetivos 5-7	EN PLANTA	10	Universidad del Valle	0	38,682,000	0	38,682,000
Karem Cecilia Rodríguez	Desarrollo de objetivos 8-10	EN PLANTA	5	Universidad del Valle	0	19,667,617	0	19,667,617
Julio Arce Arce	Desarrollo de objetivos 1-4	EN PLANTA	8	Universidad del Valle	0	42,432,000	0	42,432,000
Totales					120,000,000	142,714,937	0	262,714,937

Cuadro 3 de 5 GASTOS DE OPERACIÓN

Descripción	Justificación	Entidad	Financiado	Contrapartida		Total
				Especie	Dinero	
gastos Universidad	procesos internos universidad Operación	Universidad del Valle	17,652,251	0	0	17,652,251
Totales			17,652,251	0	0	17,652,251

Cuadro 4 de 5 VIAJES

Lugar / Justificación	Nº días / Nº personas	Pasaje por persona	Estadía por persona	Entidad	Financiado	Contrapartida		Total
						Especie	Dinero	
Cali / Visitas de experto a Cali durante 2 semanas/Fortalecimiento del intercambio y la formación científicos	20 / 2	2,500,000	200,000	Universidad del Valle	13,000,000	0	0	13,000,000
Nacional y/o internacional / Pasantías de los investigadores y/o los estudiantes del proyecto a laboratorios internacionales /Fortalecimiento del intercambio y la formación científicos y/o Participación en eventos nacionales y/o internacionales de los investigadores y los estudiantes/ Divulgación de los avances científicos	5 / 4	3,000,000	826,125	Universidad del Valle	28,522,506	0	0	28,522,506
Totales					41,522,506	0	0	41,522,506

Cuadro 5 de 5 SEGUIMIENTO Y EVALUACION

Descripción	Justificación	Entidad	Financiado	Contrapartida		Total
				Especie	Dinero	
seguimiento COLCIENCIAS	COLCIENCIAS	Universidad del Valle	5,825,243	0	0	5,825,243
Totales			5,825,243	0	0	5,825,243

PRESUPUESTO GLOBAL TOTAL (Total: 2 entidades)[Ir al menú](#)

Entidad	Financiado	Contrapartida Especie	Contrapartida Dinero	Total
Universidad Icesi	0	28,788,320	0	28,788,320
Universidad del Valle	200,000,000	128,926,617	0	328,926,617
Totales	200,000,000	157,714,937	0	357,714,937

PRESUPUESTO GLOBAL POR AÑO (Total: 5 rubros)[Ir al menú](#)

Rubro	Financiado	Año 1	Año 2	Año 3	Total
EQUIPOS	30,000,000	30,000,000	0	0	30,000,000
GASTOS DE OPERACIÓN	17,652,251	17,652,251	0	0	17,652,251
PERSONAL CIENTÍFICO	262,714,937	87,571,646	87,571,646	87,571,645	262,714,937
SEGUIMIENTO Y EVALUACION	5,825,243	5,825,243	0	0	5,825,243
VIAJES	41,522,506	6,522,506	20,000,000	15,000,000	41,522,506
Totales	357,714,937	147,571,646	107,571,646	102,571,645	357,714,937



XIV Encuentro Nacional de Óptica
y V Conferencia Andina y del Caribe
en Óptica y sus Aplicaciones
Santiago de Cali, Noviembre 16 - 20, 2015



INTERNATIONAL
YEAR OF LIGHT
2015

La Sociedad Red Colombiana de Óptica y la Universidad del Valle

certifican que:

Isabel Guzmán Naranjo

con número de identificación 1144037200,

Participó en el XIV Encuentro Nacional de Óptica & V Conferencia Andina y del Caribe en Óptica y sus Aplicaciones realizado en la Universidad del Valle del 16 al 20 de Noviembre de 2015.



**Prof. Efraín Solarte Rodríguez, Dr.rer.nat.
Presidente**

XIV Encuentro Nacional de Óptica
V Conferencia Andina y del Caribe en Óptica y sus
Aplicaciones



**Prof. Beatriz Elena Londoño Flórez
Jefe del departamento de Física (e)
Universidad del Valle**



XIV Encuentro Nacional de Óptica
y V Conferencia Andina y del Caribe
en Óptica y sus Aplicaciones
Santiago de Cali, Noviembre 16 - 20, 2015



INTERNATIONAL
YEAR OF LIGHT
2015

La Sociedad Red Colombiana de Óptica y la Universidad del Valle

certifican que:

Isabel Guzmán Naranjo

presentó la ponencia Poster

*“Coupling of frozen planet states of helium to its bound states: towards the preparation of two-electron
nondispersive wave packets”*
I. Guzmán, A. González, J. Madroñero

En el marco del XIV Encuentro Nacional de Óptica & V Conferencia Andina y del Caribe en Óptica y sus Aplicaciones
realizado en la Universidad del Valle del 16 al 20 de Noviembre de 2015.



**Prof. Efraín Solarte Rodríguez, Dr.rer.nat.
Presidente
XIV Encuentro Nacional de Óptica
V Conferencia Andina y del Caribe en Óptica y sus
Aplicaciones**



**Prof. Beatriz Elena Londoño Flórez
Jefe del departamento de Física (e)
Universidad del Valle**



VICERRECTORÍA DE
INVESTIGACIONES
Programa de Apoyo a
la Investigación

PROGRAMA SEMILLEROS DE INVESTIGACIÓN
FORMATO DE VERIFICACIÓN DE CUMPLIMIENTO DE
REQUISITOS PARA ACCEDER AL PROGRAMA

Fecha: Día 18 Mes 02 Año 2015

Identificación:

Código del estudiante:	1130962
Nombre del estudiante:	Jhoan Sebastian Ortiz Giron
Código y nombre del Programa académico:	3146 - Física

Verificación de requisitos

Estudiante regular del programa académico	Si <u>X</u>	No <u> </u>
El estudiante ha aprobado mínimo el 40% de los créditos del programa en el que está matriculado?	Si <u>X</u>	No <u> </u>
El promedio acumulado es igual o superior a 3.5:	Si <u>X</u>	No <u> </u>
Ha cursado asignaturas equivalentes al seminario de investigación formativa?	Si <u> </u>	No <u>X</u>

Firma director del programa académico:

[Firma manuscrita]

Datos del grupo al que se vincula ¹:

Nombre del grupo de investigación al que se vincula:	QUANTIC
Nombre del Tutor:	Javier Modroñero
Código y nombre del proyecto de investigación en el que desarrollara sus actividades:	7973 Teoría de Floquet para estudios de correlaciones en sistemas atómicos dependientes del tiempo

Firma del director de grupo:

[Firma manuscrita]

VoBo del Vicedecano de Investigaciones de la Facultad u homólogo:

Los estudiantes que estén vinculados a actividades de investigación a través de monitorías pagadas por proyectos de investigación pertenecerán al programa pero no deben matricular las asignaturas PASANTIA I y II



VICERRECTORÍA DE INVESTIGACIONES
Área Administrativa

SOLICITUD DE VINCULACIÓN DE PERSONAL DE APOYO

Fecha

Día	Mes	Año
10	9	2015

1. DATOS DEL PROYECTO (Todos los campos son obligatorios)

NOMBRE DEL PROYECTO:	Teoría de Floquet para el estudio de correlaciones en sistemas atómicos dependientes periódicamente en el tiempo		
Centro de Información:	7973		
Fuente de Financiación:	RUBRO:	Gastos de Personal	
Recursos del Proyecto ☒	SUBRUBRO:		
Recursos de Contrapartida ☐		N/A ☐	

2. DATOS PERSONALES DEL ESTUDIANTE (Todos los campos son obligatorios)

Nombre del estudiante:	Jhoan Sebastian Ortiz Girón		
No. de cédula del estudiante:	1113663866		
Código del estudiante:	1130962		
Dirección:	Calle 41 No. 15-85, Palmira, Valle del Cauca		
Teléfono(s):	2813690		
Email:	jhoan.ortiz@correounivalle.edu.co		
Tipo de Vinculación:	NUEVA ☐ PRORROGA ☐ ADICIÓN ☐ MONITORIA ☒ ASISTENTE DE INVESTIGACIÓN Maestría ☐ Doctorado ☐		

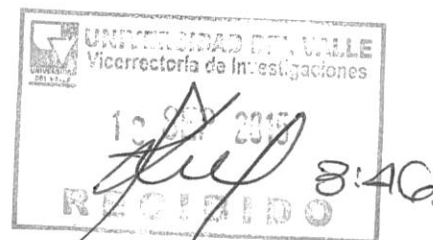
3. CRONOGRAMA DE ACTIVIDADES (Todos los campos son obligatorios)

ACTIVIDADES	PERIODO DE VINCULACIÓN		VALOR TOTAL
	INICIO (dd/mm/aaaa)	FINAL (dd/mm/aaaa)	
Desarrollo de modelos de transporte y localización en redes ópticas desordenadas unidimensionales	15/09/2015	11/12/15	\$ 1,071,720.00

OBSERVACIONES:

Interventor y/o supervisor del contrato

Nombre	Karem Cecilia Rodríguez Ramírez
Firma	<i>Karem Cecilia Rodríguez Ramírez</i>
Cédula No.	52517246
E-mail	karem.c.rodriguez@correounivalle.edu.co
Teléfono	3153564





Fecha

Día	Mes	Año
13	3	2015

1. DATOS DEL PROYECTO (Todos los campos son obligatorios)

NOMBRE DEL PROYECTO:	Teoría de Floquet para el estudio de correlaciones en sistemas atómicos dependientes periódicamente en el tiempo		
Centro de Información:	7973		
Fuente de Financiación:	☒	RUBRO:	Gastos de Personal
Recursos del Proyecto	☐	SUBRUBRO:	N/A ☐
Recursos de Contrapartida			

2. DATOS PERSONALES DEL ESTUDIANTE (Todos los campos son obligatorios)

Nombre del estudiante:	Juan Pablo Villada		
No. de cédula del estudiante:	10634116		
Código del estudiante:	540545		
Dirección:	Calle 71D# 4n-100 B.Los guaduales.		
Teléfono(s):	3833017		
Email:	juán.villada.palacios@correounivalle.edu.co		
Tipo de Vinculación:	☒ NUEVA ☐ PRORROGA ☐ ADICIÓN	☒ MONITORIA	☐ ASISTENTE DE INVESTIGACIÓN Maestría ☐ Doctorado ☐

3. CRONOGRAMA DE ACTIVIDADES (Todos los campos son obligatorios)

ACTIVIDADES	PERIODO DE VINCULACIÓN		VALOR TOTAL
	INICIO (dd/mm/aaaa)	FINAL (dd/mm/aaaa)	
Colaboración en el desarrollo de algoritmos usando interpolación polinómica y desarrollar códigos en MATLAB para calcular variables de control de sistemas atómicos.	16/03/2015	15/6/2015	\$ 700.000,00

OBSERVACIONES:

Interventor y/o supervisor del contrato

Nombre	Karem Cecilia Rodríguez Ramírez
Firma	
Cédula No.	52517246
E-mail	karem.c.rodriguez@correounivalle.edu.co
Teléfono	3153564





Fecha de Radicación del Proyecto en la Unidad
Académica

Día	Mes	Año
5	Junio	2014

I- UNIDAD ACADÉMICA

FACULTADES	
Artes Integradas	☐
Ciencias Nat. y Exactas	☒
Ciencias de la Adm.	☐
Salud	☐
Ciencias Soc. y Eco.	☐
Humanidades	☐
Ingeniería	☐

INSTITUTOS ACADEMICOS	
Educación y Pedagogía	☐
Psicología	☐

II- NOMBRE DEL PROYECTO, OBRA O CREACIÓN:

Teoría de Floquet para el estudio de correlaciones en sistemas atómicos dependientes periódicamente del tiempo

Objeto Principal del Proyecto o Tema General de la Obra o Creación:

El objetivo general de este proyecto consiste en estudiar la dinámica tanto de átomos de helio en presencia de campos electromagnéticos como de bosones en redes ópticas con dependencia periódica del tiempo usando teoría de Floquet.

III- TIPO DE PRODUCTO INTELECTUAL:

Proyecto de Investigación ☒

Proyecto de Producción Artística ☐

Consultoría y/o Asesoría ☐

Otro ☐ Especifique _____

IV- CLASE DE OBRA:

1. Obra Individual ☐

(producida por una persona natural)

3. Obra Colectiva ☐

(producida por un grupo bajo la orientación de una persona natural o jurídica que divulga y publica bajo su nombre)

5. Obra por encargo ☐

(obra creada en ejecución de un contrato de prestación de servicios)

2. Obra en Colaboración ☒

(producida por dos o mas personas)

4. Obra Derivada ☐

(creación autónoma que resulta de la adaptación, traducción y otra transformación de una obra originaria)

6. Otra ☐

Especifique _____

V- AUTORES, COAUTORES E INVENTORES

NOMBRE Y APELLIDOS	DOCUMENTO DE IDENTIFICACIÓN	P/E/I E ¹	FECHA DE INGRESO AL PROYECTO	HORAS SEMANA DEDICACIÓN	CALIDAD EN LA QUE PARTICIPA ²
Karem Cecilia Rodriguez Ramirez	CC 52.517.246	P	17 de junio de 2014	10	IP
Guillermo Javier Madroñero P.	CC 87.714.245	P	17 de junio de 2014	10	CI
Alejandro González Melan	CC 16.378.002	E3	17 de junio de 2014	40	T

¹ Señale P: si es Profesor; E1: si es Estudiante de Pregrado; E2: si es Estudiante de Maestría; E3: Estudiante de Doctorado; IE: Investigador Externo.



²Calidad en que participa en la obra intelectual, de acuerdo a la función asignada así: D: Director del Proyecto; IP: Investigador Principal; CI: Coinvestigadores; CA: Coautores; CP: Coordinador del proyecto, T: Tesis o Trabajo de Grado.

En caso de abandono o no cumplimiento de las actividades de Propiedad Intelectual, debe ser certificado por el investigador o autor principal.

VI- PRODUCTOS ESPERADOS DE ESTE TRABAJO INTELECTUAL (numérico):

1. Derechos de Autor				
Tipo de producto	Científico	Técnico	Artístico	Humanístico
1. Obras Literarias				
2. Obras Musicales				
3. Obras Artísticas				
4. Obras Audiovisuales				
5. Registro de Software				
6. Fonogramas				
7. Contratos				
8. Artículos de Comunicación Corta	1			
9. Otros				

2. Propiedad Industrial			
Patente ☐	Modelo de utilidad ☐	Diseño Industrial ☐	
Innovación Tecnológica ☒	Adaptación Tecnológica ☐	Know How ☐	

VII- FINANCIACIÓN

ORGANISMOS FINANCIADORES

No ☐

Si ☒

Otro ☐

Especifique _____

Nombre de la entidad financiadora: _____

Aporte financiación externa: _____

\$58.447.000,00

Contraprestación Universidad del Valle: _____

VIII- GARANTÍAS Y RESPONSABILIDAD

El presente acuerdo se registrará por la Ley colombiana y comunitaria que sea aplicable. Las controversias derivadas de derecho de propiedad intelectual serán sometidas al Comité de Propiedad Intelectual y al Comité de conciliación de la Universidad del Valle antes de pasar a la jurisdicción ordinaria. Todas los participantes profesores, estudiantes, servidores, funcionarios de entidades públicas y privadas manifiestan que conocen y aceptan lo dispuesto en el Estatuto de Propiedad Intelectual de la Universidad del Valle y demás normas que lo modifiquen, adicionen o aclaren. Y aceptan lo dispuesto en las siguientes cláusulas:

a) Derechos de Propiedad Intelectual:

Calidad en que participa en la obra intelectual, de acuerdo a la función asignada así: D: Director del Proyecto; DT: Director Trabajo de Grado o Tesis de investigación; IP: Investigador Principal; CI: Coinvestigadores; CA: Coautores; CP: Coordinador del proyecto, T: Tesis o Trabajo de Grado

Los derechos morales: la titularidad del derecho moral corresponden a los profesores, estudiantes y servidores en su calidad de autores, coautores, directores, investigadores o coinvestigadores; **Los derechos patrimoniales:** Comprenden el derecho de reproducción y comunicación pública. Es el beneficio sobre la explotación económica de la obra o producto intelectual, corresponden conforme a la Ley 23 de 1982 a la Universidad, salvo estipulación expresa en caso de participación de organismos financiadores, entidades públicas o privadas, en los términos del contrato, convenio o proyecto suscrito.



b) **Grado de autonomía y responsabilidad para designar colaboradores:** La Universidad y los organismos financieros, reconocen el grado de autonomía y de responsabilidad que tienen tanto el autor, investigador principal o director del proyecto como los coinvestigadores, o coautores o codirectores del proyecto para proponer sus colaboradores. La designación y participación de éstos, en todo caso se establecerá de conformidad con las normas vigentes de la Universidad.

c) **Obligación de Informar Modificaciones:** Con el fin de definir derechos de propiedad entre los intervinientes, éstos se comprometen a hacer constar expresamente en escrito que se anexará al Acta de Acuerdo de propiedad intelectual las modificaciones que surjan durante el desarrollo de la actividad o proyecto. Así mismo se expresarán las causales de retiro y exclusión del director, coordinador, coinvestigador, o coautor: por retiro voluntario o por incumplimiento de sus obligaciones u otros causales que lo desvinculen del proyecto.

d) **Cronograma de actividades:** El desarrollo de la obra, proyecto o consultoría se efectuará de conformidad con el cronograma de actividades aprobado en el proyecto que se anexa a ésta acta.

e) **Cláusula de confidencialidad:** Los docentes y estudiantes participantes, además de cumplir con sus obligaciones, se comprometen a guardar la reserva de la información que han obtenido a través del desarrollo de la obra o del proyecto de investigación, especialmente cuando el resultado esperado sea una invención, un modelo de utilidad, un diseño industrial o creaciones similares, aún después de su desvinculación del proyecto, para evitar que se puedan violar los derechos de propiedad intelectual y la obligación de confidencialidad, por lo menos durante un periodo no menor a dos años.

En constancia de aceptación se firma esta Acta por los que en ella intervienen, en Santiago de Cali a los 5 días del mes de junio de 2014 y se envía una copia al Comité de Propiedad Intelectual de la Universidad del Valle.

FIRMAS AUTORES, COAUTORES E INVENTORES

(Javier Madroero)

(Alejandro González)

(Karen Rodriguez)

Firma del Investigador Principal

Vo.Bo Vicedecano de Investigaciones o Similar



VICERRECTORÍA DE INVESTIGACIONES
Oficina de Transferencia de Resultados de Investigación
OTRI

**MODIFICACIÓN ACTA DE PROPIEDAD INTELECTUAL
DE TITULARIDAD DE DERECHOS
- AUTORES, COAUTORES E INVENTORES**

Modificación No. _____

Fecha de Radicación de la
Modificación del Acta

DÍA	MES	AÑO
04	MAR	2015

Mediante la presente acta se modifica el numeral V del Acta de Propiedad Intelectual del siguiente Proyecto:

Título: **Teoría de Floquet para el estudio de correlaciones en sistemas atómicos dependientes periódicamente en el tiempo**

Fecha de Registro en la Vicerrectoría: _____

CI: 7973

Investigador principal: Karem Cecilia Rodríguez Ramírez

VINCULACIONES

AUTORES, COAUTORES E INVENTORES					
NOMBRE Y APELLIDOS	DOCUMENTO DE IDENTIDAD	P/E/ IE¹	FECHA DE INGRESO AL PROYECTO	HORAS SEMANA DE DEDICACIÓN	CALIDAD EN LA QUE PARTICIPA²
Isabel Guzmán Naranjo	cc 1144037200	E1			T
Manuel Humberto Muñoz	cc 1144065124	E1			T
Juan Pablo Villada	cc 10634116	E1			T

RETIROS

AUTORES, COAUTORES E INVENTORES				
NOMBRE Y APELLIDOS	DOCUMENTO DE IDENTIDAD	P/E/ IE¹	FECHA DE RETIRO DEL PROYECTO	CAUSAL³

¹ Señale P: si es Profesor; E1: si es Estudiante de Pregrado; E2: si es Estudiante de Maestría; E3: Estudiante de Doctorado; IE: Investigador Externo.

² Calidad en que participa en la obra intelectual, de acuerdo a la función asignada así: D: Director del Proyecto; IP: Investigador Principal; CI: Coinvestigadores; CA: Coautores; CP: Coordinador del proyecto, T: Tesis o Trabajo de Grado.

³ En caso de que haya renuncia a continuar en el proyecto, señale la causal: D: Desistir, R: Renuncia, A: Abandono.

En caso de abandono o no cumplimiento de las actividades de Propiedad Intelectual, debe ser certificado por el investigador o autor principal.

Certifico: _____

Los aquí firmantes declaran que conocen los términos del acta original la cual permanece sin modificación en los numerales no mencionados en la presente acta.

En constancia de aceptación se firma esta Acta por los que en ella intervienen, en Santiago de Cali a los _____ días del mes de _____ de 20 _____ y se envía una copia al Comité de Propiedad Intelectual de la Universidad del Valle.

FIRMAS AUTORES, COAUTORES E INVENTORES

manuel muñoz
Isabel Guzmán
Juan P. Villada P

Firma del Investigador Principal

Vo.Bo. Vicedecano de Investigaciones o Similar

Fecha: _____

Anexo: Few-level model for the driven 2D helium

We consider the helium atom in presence of an external electromagnetic field. In the dipole approximation and without consider relativistic corrections, the Hamiltonian for the driven atom reads

$$\begin{aligned} H &= H_0 + F(x_1 + x_2) \cos(\omega t) \\ H &= H_0 - \frac{F}{i\omega} \left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) \sin(\omega t) \end{aligned} \quad (1)$$

in the position and velocity gauge, respectively. Here, H_0 is the unperturbed Hamiltonian and the field is a periodic with amplitude F and frequency ω , linearly polarized along the x direction.

Floquet theory

Since the Hamiltonian is periodic in time, with period $T = 2\pi/\omega$, the Floquet theorem guarantees that the solutions of the Schrodinger equation associated with can be expressed as superpositions of time periodic wave functions

$$|\psi(t)\rangle = \sum_j c_j e^{-i\varepsilon_j t} |\phi_{\varepsilon_j}(t)\rangle, \quad |\phi_{\varepsilon_j}(t+T)\rangle = |\phi_{\varepsilon_j}(t)\rangle$$

where ε_j and $|\phi_{\varepsilon_j}(t)\rangle$ are eigenvalues and eigenstates of the Floquet operator $\mathcal{H}_F = H - i\frac{\partial}{\partial t}$, and are called *quasienergies* and *Floquet states*, respectively.

The Floquet states are periodic in time, so they can be expanded in Fourier series

$$|\phi_{\varepsilon_j}(t)\rangle = \sum_{k=-\infty}^{\infty} e^{-ik\omega t} |\phi_{\varepsilon_j}^k\rangle$$

in tis way, the the eigenvalue problem is written as

$$(H_0 + k\omega) |\phi_{\varepsilon_j}^k\rangle + \frac{F}{2} (x_1 + x_2) (|\phi_{\varepsilon_j}^{k+1}\rangle + |\phi_{\varepsilon_j}^{k-1}\rangle) = \varepsilon_j |\phi_{\varepsilon_j}^k\rangle \quad (2)$$

$$(H_0 + k\omega) |\phi_{\varepsilon_j}^k\rangle + \frac{F}{2\omega} \left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) (|\phi_{\varepsilon_j}^{k+1}\rangle - |\phi_{\varepsilon_j}^{k-1}\rangle) = \varepsilon_j |\phi_{\varepsilon_j}^k\rangle \quad (3)$$

in the position and velocity gauge, respectively. So the time dependence has been eliminated and we have a new quantum number k . It can be shown that in the semiclassical limit, the quantum number k counts the number of photons exchanged between the atom and the field.

Rotated Floquet operator in parabolic coordinates

To extract the resonant states and their decay rates we use the complex rotation method. Additionally we introduce a dilation described by the unitary operator

$$D_{\alpha_c} = \exp \left(i(\log \alpha_c) \frac{\vec{r} \cdot \vec{p} + \vec{p} \cdot \vec{r}}{2} \right) \quad (4)$$

where α_c is a positive real number. In this way the cartesian coordinates and momenta transform according to

$$\begin{aligned} \vec{r} &\rightarrow \alpha_c \vec{r} e^{i\theta} \\ \vec{p} &\rightarrow \frac{1}{\alpha_c} \vec{p} e^{-i\theta} \end{aligned} \quad (5)$$

The spectra of the Hamiltonian H is not affected by the dilation, however, when the basis is truncated, the spectrum does depend on the parameter α_c if the basis set is not large enough. So that, α_c can be used as a variational parameter.

Again, the regularization of or is carried out by multiplication with the Jacobian. Thus, after complex rotation and dilation, we obtain¹

$$(\mathcal{H}_0^{(\alpha)}(\theta) - k\omega J)|\phi_{\varepsilon_j}^k\rangle + \mathcal{F}^{(\alpha)}(\theta)(|\phi_{\varepsilon_j}^{k+1}\rangle + \eta|\phi_{\varepsilon_j}^{k-1}\rangle) = \varepsilon_j J|\phi_{\varepsilon_j}^k\rangle \quad (6)$$

where $\mathcal{H}_0^{(\alpha)}(\theta) = -Te^{-2i\theta}/2\alpha^8 + Ve^{-i\theta}/\alpha^4$, $\eta = \pm 1$ in the position and velocity gauge, respectively, and

$$\mathcal{F}^{(\alpha)}(\theta) = \begin{cases} \frac{F\alpha^4}{2}e^{i\theta}(x_1 + x_2)J, & \text{in the position gauge,} \\ \frac{F}{2\omega\alpha^4}e^{-i\theta}J\left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2}\right), & \text{in the velocity gauge.} \end{cases} \quad (7)$$

The expressions for $\mathcal{F}^{(\alpha)}(\theta)$ are polynomial functions in the parabolic coordinates and their partial derivatives.

Few-level model

For unperturbed 2D helium, angular momentum is a conserved quantity, $\Delta l = 0$. The action of an electromagnetic field couples a state of angular momentum l to states of angular momentum $l - 1$ or $l + 1$, i.e. $\Delta l = \pm 1$. Additionally the field operator couples states where the photon quantum number k differs by ± 1 . Thus, in comparison with the unperturbed problem, in the driven system the matrices involved are very large and their dimensions dramatically increases with the number of angular momenta included as well as with the order of the multiphoton excitation process induced by the external field.

¹A dilation by α_c in Cartesian coordinates is equivalent to a dilation by α_c^4 in parabolic coordinates, so onwards we denote $\alpha = \alpha_c^4$.

This defines a computational problem of major proportions, for instance, the matrices to diagonalize requires an amount of RAM memory of the order of 500GB. Fortunately, previous work on one dimensional helium suggest that only a relative small number of resonances of the unperturbed atom that take part in the formation of NDWP. This means that with an appropriate filtering of the atomic states we can reduce the size of the matrices involved in the driven system, and thus avoid the use of supercomputers.

In order to implement this approach, we do not solve the complete driven problem, instead, we consider a model system in which a reduced number of atomic states is studied under the action of an external electromagnetic field. Hence, first we solve the unperturbed system²

$$\mathcal{H}_0^{(\alpha)}(\theta)|\varphi_j^l\rangle = \epsilon_j^l J |\varphi_j^l\rangle \quad l = l_{\min}, \dots, l_{\max} \quad (8)$$

where the index l represent the angular momentum. The states $|\varphi_j^l\rangle$ are given in the basis set of harmonic oscillators

$$|\varphi_j^l\rangle = \sum_n \varphi_{jn}^l |n\rangle_l, \quad |n\rangle_l = |n_1, n_2, n_3, n_4\rangle_l \quad (9)$$

and satisfy

$$\langle \varphi_i^l | J | \varphi_j^{l'} \rangle = \delta_{i,j} \delta_{l,l'} \quad (10)$$

The next step is to select the resonance states that can contribute to the formation of the NDWP. The number of states to be included depends with the number of angular momenta involved and with the order of the multiphoton excitation process induced by the external field. The initial filtering criteria that we are using is to select the states with energy around the FPS of interest. Once we have the contributing states, we construct the basis set

$$|\varphi_j^{l,k}\rangle = |\varphi_j^l\rangle \otimes |k\rangle \quad (11)$$

where the photon quantum number k was introduced in a trivial way. In this basis, the Floquet states that solves the driven system (6), are expressed as

$$|\phi_{\varepsilon_i}^k\rangle = \sum_l \sum_j \phi_{\varepsilon_i l j}^k |\varphi_j^{l,k}\rangle \quad (12)$$

Replacing the expansion (12) in (6), we obtain

$$(\epsilon_j^l J - k\omega J) |\varphi_j^{l,k}\rangle + \mathcal{F}^{(\alpha)}(\theta) (|\varphi_j^{l,k+1}\rangle + \eta |\varphi_j^{l,k-1}\rangle) = \varepsilon_j J |\varphi_j^{l,k}\rangle \quad (13)$$

The computation of the matrix elements $\langle \varphi_i^{l,k} | \mathcal{F}^{(\alpha)}(\theta) | \varphi_j^{l',k'} \rangle$, is given in terms of the of

²The energies ϵ_j^l depend on the angle θ and in case of a truncated basis, also depend on the parameter α , however in order to simplify the notation this dependency will not be explicitly.

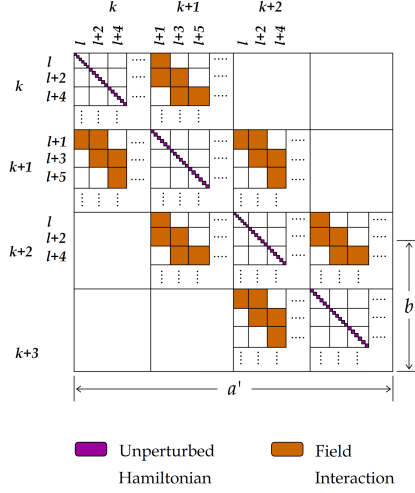


Figure 1: General form of the complex symmetric matrix $\mathcal{A}$

the matrix elements in the harmonic oscillators basis $\langle m | \mathcal{F}^{(\alpha)}(\theta) | n \rangle$, for which there are analytic expressions

$$\begin{aligned}
 \langle \varphi_i^{l,k} | \mathcal{F}^{(\alpha)}(\theta) | \varphi_j^{l',k'} \rangle &= \sum_{m,n} \langle \varphi_i^{l,k} | m \rangle \langle m | \mathcal{F}^{(\alpha)}(\theta) | n \rangle \langle n | \varphi_j^{l',k'} \rangle \\
 &= \sum_{m,n} \varphi_{i,m}^{*l,k} \varphi_{j,n}^{l',k'} \langle m | \mathcal{F}^{(\alpha)}(\theta) | n \rangle
 \end{aligned} \tag{14}$$

The matrix representation of (13) in the basis (11) is written as

$$\mathcal{A} \mathcal{X}_i = \varepsilon_i \mathcal{X}_i$$

where $\mathcal{A}$ is the block matrix

$$\mathcal{A} = \begin{pmatrix}
 \ddots & \vdots & \vdots & \vdots & \\
 \cdots & \epsilon_j^l - (k-1)\omega & \eta \mathcal{F} & 0 & \cdots \\
 \cdots & \mathcal{F} & \epsilon_j^l - k\omega & \eta \mathcal{F} & \cdots \\
 \cdots & 0 & \mathcal{F} & \epsilon_j^l - (k+1)\omega & \cdots \\
 & \vdots & \vdots & \vdots & \ddots
 \end{pmatrix}$$

and $\mathcal{X}$ is the column vector which represents $|\varphi_i^{l,k}\rangle$. The matrix $\mathcal{A}$ is a banded matrix with the general form depicted in figure .