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Time-Dependent Many-body Perturbation Theory: Possibilities and Limitations

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Division of Mathematical Physics
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Abstract

This dissertation investigates the possibilities and limitations of time-dependent many-body perturbation theory by studying small Hubbard clusters for which the exact solution is available.

The first part of the thesis is comprised of a short introduction to the concepts and methodologies used. The second part consists of a review of the main findings of the thesis and a short summary of four original papers.

In paper I we study the dynamics of short Hubbard chains within many-body perturbation theory and compare to the exact solution. The main outcomes are that the T-matrix approximation works well in the low filling regime and that all approximations which involve correlation effects develop an unphysical steady state.

In paper II we present the methodology used in paper I. We find that the correlation-induced damping appears even in the presence of leads and that there are multiple steady and quasi steady states.

In paper III we make a review of the status of time-dependent density functional theory for lattice models. In particular we find that a non-perturbative adiabatic local density approximation describes strong correlations quite well while many-body perturbation theory accounts better for non-adiabatic effects.

In paper IV we propose a method to obtain the double occupancy from the Kadanoff-Baym equations. We show that the positiveness condition may be violated in the GW or the second Born approximation but fulfilled in the T-matrix approximation. We apply this method to obtain the local entanglement entropy.

Key words: Real-time Green's functions, many-body perturbation theory, Hubbard model, correlation functions

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Till Marta och Nil
Jag älskar er
Us estimo

This thesis is based on the following publications:

- I Marc Puig von Friesen, Claudio Verdozzi and Carl-Olof Almbladh
  Succecces and failures of Kadanoff-Baym dynamics in Hubbard nanoclusters
  Physical Review Letters **103**, 176404 (2009).
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- II Marc Puig von Friesen, Claudio Verdozzi and Carl-Olof Almbladh
  Kadanoff-Baym dynamics of Hubbard clusters: Performance of many-body schemes, correlation-induced damping and multiple steady and quasi-steady states
  Physical Review B **82**, 155108 (2010).
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- III Claudio Verdozzi, Daniel Karlsson, Marc Puig von Friesen, Carl-Olof Almbladh and Ulf von Barth
  Some open questions in TDDFT: Clues from Lattice Models and Kadanoff-Baym Dynamics
  Submitted to Chemical Physics

- IV Marc Puig von Friesen, Claudio Verdozzi and Carl-Olof Almbladh
  Can we always get the entanglement entropy from the Kadanoff-Baym equations? The case of the T-matrix approximation
  Submitted to Europhysics Letters

Other papers not included in the thesis:

1. Marc Puig von Friesen, Claudio Verdozzi and Carl-Olof Almbladh
   Artificial damping in the Kadanoff-Baym dynamics of small Hubbard chains
   Journal of Physics: Conference Series **220**, 012016 (2010).

2. Marc Puig von Friesen, Magnus Ögren and Sven Åberg
   Quantum chaos and regularity in ultracold Fermi gases
   Physical Review E **76**, 057204 (2007).

Preface

This thesis is about interacting, quantum mechanical systems out of equilibrium, which, by the mere sound of the words seems absolutely frightening but at the same time immensely intriguing. After some four years of work, entailing hard trials but also many moments of joy, I have now come to end of this journey. When I now look back at what I have learned and experienced during this period I want to thank the people which have, in one way or the other, stood by my side.

Not many Phd students have had the fortune of having not only one but two fantastic supervisors. I wish to thank Carl-Olof Almbladh and Claudio Verdozzi for introducing me to the mesmerising world of diagrams, contours and hopping electrons. You supported me not only at the beautiful blackboards but also by plunging into the muddy backyards of the codes. No matter what the future will bring, I will always look back at these years with great gratification.

Jag vill tacka Ulf och Daniel för den tid vi kunnat arbeta ihop. Tack Sven för att bjuda in mig till Matematisk Fysik och inleda mitt forskaräventyr. Tack Magnus för ditt sammarbete, men framförallt för din vänskap. Tack Maria och Sara för att ha varit underbara kontorskamrater och vänner.

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Merci Rodrigo per tot, que sense tu ja saps que no sóc res. Gràcies també, Miquel i els altres de física per compartir els durs inicis de física a Barcelona.

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Jag vill rikta ett stort tack till min polska familj och alla mina andra vänner i Sverige för att alltid vara där i també als amics catalans, que tot i la distància sempre hi heu sigut.

Jag vill tacka min svenska familj: Magge, Jutta, Stina och alla andra.

Vull donar les gràcies a la meva familia catalana: Pau, Rina, Ingrid i August però també Rosa, Jaume i Albert.

Finalment vull donar-vos les gràcies a vosaltres, Marta i Nil, per compartir la meva vida.

Lund, in March 2011
Marc Puig von Friesen

Contents

Popular Science Summary

One of the most subtle concepts in physics is "**interaction**". In common usage, interaction means that separate entities (being electrons, people or galaxies) influence[1] one another. Due to this influence, these entities may form "emergent" systems with novel collective properties, far beyond the simple characteristics of the individual parts. Under such circumstances, "the whole is greater than the sum of its parts", as Aristotle put it. Let us, for simplicity, consider a potato. This fantastic vegetable is formed by a multitude of interacting cells, but is immensely more complex than just a mere collection of cells. Similarly, the cells are built of molecules which in turn are made of atoms and so on... It is easy to imagine that describing each step in this increasing complexity requires special efforts such as the introduction of new concepts and methodologies. In fact, in physics one often refers to the description of such interacting systems as the "many-body problem".

The everyday world surrounding us – that we can see, touch, smell and taste directly with our senses – is perfectly described by classical physics.[2] However, when we try to describe very small objects, such as atoms or nanometer size structures, the classical physics fails, not only quantitatively but even qualitatively. We need to make use of "**quantum mechanics**". It is striking that the fundamental axioms, on which all our physical theories are based, are not only different but actually in contradiction when we compare classical and quantum physics. Classical physics says that the physical reality exists independently of the observer while quantum mechanics claims that there is an inevitable influence of the observer on the physical reality. Where classical physics tells us that a quantity has a certain well-defined value, quantum physics says no: it has only a probability of attaining a certain value. Classical physics endows particles with precise positions and velocities in space but quantum physics forbids such a procedure – a particle is to be represented by an extended wave

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[1] In physics this influence corresponds to a force.

[2] This is, of course, strictly speaking not true as all macroscopic systems are ultimately made of particles which obey the laws of quantum physics. In fact, according to recent theories, the way our nose interprets different molecules as different smells can not be described within classical physics.

function. When classical physics says that a quantity, such as energy, can have any value within a certain interval, quantum physics says no: only certain discrete (quantised) values are allowed. That classical and quantum physics give contradictory answers on some principal questions does, however, not imply that they are not reconcilable. In fact, in the limit of large systems, the equations of quantum mechanics become the same as the classical ones.

Another very important concept in physics is "**non-equilibrium**". Being out of equilibrium means that something changes in time. The wind that blows, the current that flows and the glass which falls are all examples of non-equilibrium dynamics. The very essence of life is intrinsically linked to non-equilibrium, in fact the capacity to utilise the non-equilibrium is one of the basic properties of living organisms. Equilibrium is the opposite: everything stays unchanged, nothing happens.[3]

Whenever a system goes out of equilibrium, such as when a cold spoon is put into a warm cup of tea, the natural tendency of the system is to relax to the equilibrium state. If we just leave a potato alone it will finally end up as an inert and boring lump. In order for a system to be driven out of equilibrium there has to be something that changes (a gradient) in space. In the case of the spoon, the tea has a higher temperature than the spoon and, therefore, to re-establish the equilibrium, there will be a flow of heat into the spoon until it acquires the same temperature as the tea. In fact, the whole universe may slowly be going towards an equilibrium which ultimately leads to the so-called thermal death, i.e. when all that can fall has fallen, when all the chemical reactions have taken place and everything is lukewarm, then nothing will ever be able to happen...

The problem that we deal with in this thesis incorporates all the three aspects mentioned above, i.e. interaction, quantum mechanics and non-equilibrium. We treat this problem by using an approximate[4] methodology called many-body perturbation theory, which is widely used in many different fields in physics.

The central object of many-body perturbation theory is the Green's function which gives the probability amplitude that a particle added (or removed) to a system at a given position and time propagates to another position at a different time. With this information one can obtain knowledge of certain important properties of the system, such as the particle density, the currents and the energy. In many-body perturbation theory one approximates the Green's function in a clever way which guarantees the fulfilment of certain physical laws, such as the conservation of energy and matter.

The problem of a time-dependent interacting quantum mechanical system

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[3] The constituent microscopic parts may fluctuate in time but the macroscopic system as a whole does not change on the average.

[4] An approximate method means that it is intrinsically approximative and thus even if one had a computer with infinite capacity, one could only obtain approximate results.

is a very difficult one. Therefore, instead of trying to describe a real physical system with all its complicated details (which is at present not technically feasible but will ultimately be the goal of this kind of research) we replace it by a model system. A model is a simplified version of reality,[5] where one neglects many complicated and hopefully irrelevant aspects and keeps only what one can hope to be able to treat, all along longing that the model resembles the real system.[6]

Apart from actually being technically manageable and having some relation to the real world, model systems do sometimes admit exact solutions. This is, of course, delightful. Exact solutions are an invaluable source of to gain insight of the reliability of approximate schemes such as, e.g. many-body perturbation theory.

The goal of this thesis is to study how well many-body perturbation theory works to describe time-dependent phenomena. This is done by considering simple model systems, where one has full control of the exact solution which can therefore be used as a benchmark.

The many-body perturbation theory as used here optimises some properties, specifically the fulfilment of basic conservation laws. A main outcome of this thesis is that many-body perturbation theory can in some cases give quite a successful description of the non-equilibrium dynamics. However, in other situations it may give rise to unphysical results for other properties. The understanding of these unphysical results is crucial as they put severe boundaries on the applicability of time-dependent many-body perturbation theory.

Hopefully, our work will be useful in future efforts to remedy these shortcomings.

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[5] Note that we always refer to the physical reality and that we do not dare to even consider any metaphysical true reality...

[6] This view is a bit exaggerated, as models have in many cases reproduced the real physics not only qualitatively but actually quantitatively.

Populärvetenskaplig sammanfattning

Ett av de mest subtila begrepp i fysik är "**växelverkan**". I en alldaglig mening betyder växelverkan att skilda entiteter (som elektroner, människor eller galaxer) påverkar[1] varandra. När dessa entiteter växelverkar kan de skapa "emergenta" system med nya, kollektiva egenskaper långt utöver de individuella delarna. Under dessa omständigheter är "helheten mycket mer än summan av sina delar" som Aristoteles en gång framställde det. Ta för enkelhetens skull en potatis. Denna fantastiska rotfrukt är byggd av en mängd växelverkande celler, men är oerhört mycket mer komplex än blott en grupp celler. På liknande vis är dessa celler byggda av molekyler som i sin tur består av atomer och så vidare... Det är lätt att föreställa sig att beskrivningen av varje steg av denna ökande komplexitet kräver stora ansträngningar som till exempel införandet av nya begrepp och metodologier. Beskrivningen av växelverkande system brukar benämnas som "mångkropparproblemet".

Den vardagliga världen som omger oss – som vi kan se, röra, lukta och smaka direkt med våra sinnen – beskrivs väl av den klassiska fysiken.[2] Men när vi försöker studera mycket små saker, som atomer eller nanometer-stora strukturer, då misslyckas den klassiska fysiken, inte bara kvantitativt utan även kvalitativt. Vi måste använda "**kvantmekaniken**". Det är verkligen slående att de grundläggande axiomen, på vilka alla våra fysiska teorier är baserade, inte bara är annorlunda utan även motsäger varandra när vi jämför klassisk fysik med kvantmekaniken. Klassik fysik säger att den fysiska verkligheten existerar oberoende av observatören medan kvantmekaniken menar att det finns en ofrånkomlig påverkan av observatören på den fysiska verkligheten. Där klassisk fysik säger oss att en kvantitet har ett givet väldefinierat värde säger kvantmekaniken nej: den har endast en sannolikhet att anta ett visst värde. I klas-

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[1] I fysiken motsvaras denna påverkan av en kraft.

[2] Detta är, uppenbarligen, egentligen inte sant eftersom alla makroskopiska system består ytterst av partiklar som lyder kvantmekanikens lagar och faktiskt kan inte sättet vår näsa uppfattar olika molekyler som olika lukter, beskrivas av klassik fysik.

sisk fysik har partiklarna bestämda positioner och hastigheter i rummet men kvantmekaniken förbjuder detta – en partikel måste beskrivas av en utbredd vågfunktion. När klassik fysik säger att en kvantitet, som till exempel energin, kan ha vilket värde som helst inom ett givet intervall säger kvantmekaniken nej: bara vissa diskreta (kvantiserade) värden är tillåtna. Att klassisk fysik och kvantmekaniken ger motsägande svar på några grundläggande frågor betyder inte att de är oförenliga. I gränsen för stora system ger kvantmekaniken samma förutsägelser som klassisk fysik.

Ett annat mycket viktigt begrepp inom fysiken är “**icke jämvikt**”. Att vara utom jämvikt betyder att något förändras i tiden. Vinden som blåser, strömmen som flödar och glaset som faller är alla exempel på dynamik utom jämvikt. Livets innersta väsen är ohjälpligt bundet till icke jämvikt; att kunna använda saker och ting utom jämvikt är faktiskt en grundläggande egenskap hos levande organismer. Jämvikt är själva motsatsen: Allt förblir oförändrat, ingenting händer.[3]

När ett system hamnar utanför jämvikt, som till exempel när en kall sked sätts ner i en kopp hett te, är den naturliga utvecklingen att systemet återgår till jämvikt. Om vi bara lämnar en potatis åt sig själv så kommer den slutgiltigen brytas ner och förvandlas till en intetsägande klump. För att ett system skall drivas ut från jämvikt måste det finnas något som ändras (en gradient) i rummet. I fallet med skeden har teet en högre temperatur än skeden och därför kommer det flöda in värme in i skeden tills skeden får samma temperatur som teet. Faktum är att hela universum kanske sakta går mot en jämvikt som till slut leder till det som kallas för den termiska döden, alltså när allt som kan falla har fallit, när alla kemiska reaktioner har ägt rum och allt är lagom, då kan ingenting någonsin hända...

Problemet vi behandlar i den här avhandlingen innefattar alla tre beskrivna aspekter, nämligen växelverkan, kvantmekanik och icke jämvikt. Vi behandlar detta problem med en approximativ[4] metodologi som kallas mångpartikelteori och som används mycket i vitt skilda fält i fysiken.

Det centrala objektet inom mångpartikelteori är Greensfunktionen som ger sannolikheten för att en partikel som lagts till (eller dragits bort) i systemet vid en given position och vid en viss tid, kommer till en annan position vid en annan tid. Med den informationen kan man få fram viktig kunskap om systemets egenskaper som till exempel dess täthet, strömmar och energi. I mångpartikelteorin approximerar man Greensfunktionen på ett sätt som garanterar att vissa grundläggande fysikaliska lagar uppfylls, som till exempel bevarandet av energi och materia.

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[3] De mikroskopiska delarna som utgör system kan fluktuera i tiden men det makroskopiska systemet ändras inte i snitt.

[4] En approximativ metod betyder att den är approximativ till sin natur, det vill säga att även om man hade en dator med oändlig kapacitet skulle man endast få approximativa resultat.

Att beskriva ett växelverkande kvantmekaniskt system utanför jämvikt är mycket svårt. Istället för att försöka beskriva ett riktigt fysikaliskt system (vilket idag inte är tekniskt möjligt, men som i själva verket är det slutgiltiga målet för denna typ av forskning) ersätter vi det därför med ett modellsystem. En modell är en förenklad version av verkligheten,[5] där man helt enkelt bortser från en mängd komplicerade och förhoppningsvis oviktiga detaljer och lämnar endast kvar det som man tro sig kunna lösa samtidigt som man hoppas att modellen skall efterlikna det riktiga systemet.[6]

Förutom att faktiskt vara tekniskt hanterbara och ha viss motsvarighet till verkligheten kan modellsystem i vissa fall ha exakta lösningar. Detta är självfallet fantastiskt. Exakta lösningar är ovärderliga källor för att få grundläggande kunskap om approximationers, till exempel mångpartikelteorins, tillförlitlighet.

Målet för denna avhandling är att utforska hur bra mångpartikelteorin fungerar för att beskriva tidsberoende fenomen. Detta görs genom att studera enkla modellsystem, där man också har tillgång till exakta resultat.

Mångpartikelteorin som den används här optimerar vissa egenskaper, specifikt att grundläggande konserveringslagar uppfylls. Ett huvudresultat av avhandlingen är att mångpartikelteorin kan i vissa fall ge en bra beskrivning av dynamiken. I andra fall kan metoden emellertid ge ofysikaliska resultat för andra egenskaper. Förbättrad förståelse av dessa ofysikaliska egenskaper är avgörande eftersom de begränsar användbarheten av den tidsberoende mångpartikelteorin.

Förhoppningsvis kan resultaten presenterade här ge uppslag till framtida arbeten med syfte att överbrygga dessa svårigheter.

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[5] Lägg märke till att vi alltid diskuterar den fysiska verkligheten och att vi inte ens vågar röra vid någon metafysisk verklighet...

[6] Denna beskrivning är lite väl överdriven eftersom modellsystem i många fall har reproducerat riktiga fysikaliska system inte bara kvalitativt utan även kvantitativt.

Resum divulgatiu

Un dels conceptes més subtils de la física és "**la interacció**". En termes comuns, interacció vol dir que diferent entitats (siguin electrons, persones o galàxies) s'influencien[1] les unes a les altres. Quan aquestes entitats interactuen, poden formar sistemes "emergents" amb noves propietats col.lectives molt més enllà de les característiques de les entitats inicials. En aquestes circumstàncies, tal com deia Aristòtil: "el tot és més que la suma de les seves parts". Com a exemple senzill ens podem imaginar una patata. Aquest fantàstic tubercle està format per una multitud de cèl.lules interactuant però és immensament més complex que un simple conjunt de cèl.lules. De manera similar, les cèl.lules estan formades per molècules que en si estan fetes d'àtoms i així fins a l'avorriment... És fàcil imaginar-se que descriure cada pas d'augment de complexitat requereix grans esforços com ara la introducció de nous conceptes i metodologies. De fet, en física, se sol referir a la descripció de sistemes interactuants com el "problema dels molts cossos".

El món del dia a dia que ens envolta, que podem veure, tocar, olorar i tastar directament amb els nostres sentits, es pot descriure perfectament amb la física clàssica.[2] Quan intentem, però, descriure objectes molt petits, com ara àtoms o estructures a l'escala nanomètrica, la física clàssica l'erra no només quantitativament sinó també qualitativament i necessitem utilizar la "**mecànica quàntica**". És molt impactant que els axiomes fonamentals, que són la base de totes les teories de la física, no només són diferents sinó també que són contradictoris quan comparem la física clàssica amb la quàntica. La física clàssica diu que la realitat física existeix independentment de l'observador mentres que la quàntica diu que hi ha una influència inevitable de l'observador i la realitat física. Allà on la física clàssica diu que una quantitat té un valor ben definit, la física quàntica diu que només té una probabilitat d'adoptar un cert valor. A la física clàssica les partícules tenen posicions i velocitats a l'espai ben deter-

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[1] En la física aquesta influència correspon a una força.

[2] De fet això, òbviament, no es estrictament veritat ja que tots els sistemes macroscòpics estan en el fons constituïts per partícules que estan sotmeses a les lleis de la física quàntica. De fet, la manera que el nostre nas interpreta certes molècules com a diferents olors, no es pot descriure amb física clàssica.

minades però la quàntica ho prohibeix; una partícula és representada per una funció d'ona extensa. Quan la física clàssica diu que una quantitat, com per exemple l'energia, pot tenir qualsevol valor en un cert interval, la quàntica diu que tan sols alguns valors discrets (quantitzats) són permesos. Que la física clàssica i la quàntica es contradiguin en algunes preguntes fonamentals no vol dir que no siguin reconciliables. De fet, al límit de sistemes grans, les equacions de la mecànica quàntica esdeven les mateixes que les clàssiques.

Un altre concepte important en física és el de "**no equilibri**". Trobar-se fora de l'equilibri vol dir que alguna cosa canvia en el temps. El vent que bufa, el corrent que flueix i el got que cau són exemples de dinàmica fora de l'equilibri. La pròpia essència de la vida està intrínsicament lligada al no equilibri i, de fet, la capacitat d'utilitzar coses fora de l'equilibri és una de les propietats fonamentals dels organismes vius. L'equilibri és el contrari, tot es queda igual, no passa res.[3]

Sempre que un sistema surt fora de l'equilibri, com per exemple quan es posa una cullera freda en un got de te calent, la tendència natural és de tornar a l'equilibri. Si deixem una patata tota sola, al final esdevindrà una massa inerta i avorrida. Perquè un sistema surti de l'equilibri, cal que hi hagi alguna cosa que canviï (un gradient) a l'espai. En el cas de la cullera, el te té una temperatura més alta que la de la cullera i, degut a això, fluirà calor del te a la cullera fins que aquesta assoleixi la mateixa temperatura que el te. De fet, pot ser que l'univers estigui a poc a poc anant cap a un equilibri que finalment porti a la mort tèrmica, és a dir, quan tot el que pot caure hagi caigut, quan totes les reaccions químiques s'hagin produït i tot sigui tediosament tebi, llavors res podrà passar mai més...

El tema que tractem en aquesta tesi incorpora els tres aspectes descrits: la interacció, la mecànica quàntica i el no equilibri. Per afrontar aquest problema utilitzarem una metodologia aproximada[4] que s'anomena teoria de perturbació de molts cossos i que s'utilitza en molts àmbits de la física.

L'objecte central de la teoria de perturbació de molts cossos és la funció de Green que dóna la probabilitat que una partícula afegida (o extreta) al sistema en un punt en l'espai i en un instant donats, es mogui a un altre punt de l'espai en un altre instant. Tenint aquesta informació es poden obtenir coneixements sobre les propietats del sistema, com ara la densitat de partícules, els corrents i l'energia. La teoria de perturbació de molts cossos aproxima la funció de Green de tal manera que es garanteixi el compliment de certes lleis físiques, com ara la conservació de l'energia i de la matèria.

El problema d'un sistema quàntic interactuant fora de l'equilibri és molt complex. Per això, en comptes d'intentar descriure un sistema físic real (que

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[3] Les parts microscòpiques constituents poden fluctuar en el temps però el sistema macroscòpic no canvia en promig.

[4] Un mètode aproximat vol dir que és intrínsicament aproximatiu i, per tant, encara que es tingués un ordinator amb capacitat infinita, només s'obtindrien resultats aproximats.

a hores d'ara no és tècnicament factible però que és la fita final d'aquest tipus de reserca) el substituïm per un model. Un model és una versió simplificada de la realitat[5] on ens desfem d'un munt d'aspectes complicats i suposadament irrellevants i ens quedem només amb el que esperem poder tractar, sempre tenint la confiança que el model s'assembli al sistema real.[6]

Els models, a banda de ser tècnicament manejables i de tenir alguna relació amb el món real, de vegades es poden resoldre de manera exacte; això és, clarament, un gran avantatge. Les solucions exactes són una font inestimable per obtenir comprensió fonamental del grau de fiabilitat de diferents mètodes aproximats, com per exemple la teoria de perturbació de molts cossos.

L'objetiu d'aquesta tesi és el d'estudiar com funciona la teoria de perturbació de molts cossos per desciure fenòmens depenents del temps. Això es fa analitzant uns models senzills, on es té el control sobre la solució exacte i per tant serveix com a referent.

La teoria de perturbació de molts cossos, com és utilitzada aquí, optimitza algunes propietats, en concret el compliment de les lleis fonamentals de conservació. Un resultat principal d'aquesta tesi és que la teoria de perturbació de molts cossos pot, en certs casos, donar una bona descripció de la dinàmica del no equilibri. En altres situacions dóna resultats que violen altres lleis de la física; la comprensió d'aquestes propietats és primordial, ja que posen severes restriccions a l'aplicabilitat de la teoria de perturbació de molts cossos fora de l'equilibri.

Esperem que els nostres resultats obrin la porta a noves investigacions que puguin superar aquest problema.

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[5] Observa que sempre ens referim a la realitat física i ni tan sols ens atrevim a tocar cap realitat metafísica...

[6] Aquesta descripció és una mica exagerada ja que hi han molts casos on models han pogut descriure sistemes físics reals no tan sols qualitativament sinó també quantitativament.

Part A

Background

1

Introduction

Treating interacting systems with strong correlation effects out of equilibrium is a hard and largely unsolved problem in solid state physics. There are several different methods which try to tackle this question, all of them with their own pros and cons. Most approximate methodologies focus on certain physical aspects and this may lead to the deterioration of other properties. There are, however, also methods which are in principle exact, but these are usually very limited by the system size.[1]

This thesis is focused on the non-equilibrium Green's function or Kadanoff-Baym equations (KBE) technique [1, 2] within many-body perturbation theory (MBPT) [3]. The strength of this method is that one can build approximations of increasing complexity and that it incorporates memory, which can become essential when dealing with time-dependent phenomena [4, 5]. An other advantage of the KBE+MBPT technique is that it allows to treat non-homogenous and extended systems, in particular those of a quantum transport geometry, i.e. a central interacting region coupled to semi-infinite non-interacting leads [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. There are various limitations of the KBE+MBPT approach. One is that the methodology is only approximate,[2] which means that one has to compare to experiments or exact methods in order to assess its validity. An other restriction is that the Green's function is a two-point object[3] and the scheme is thus computationally very demanding. An additional restraint is that the procedure is of perturbative character which means that it will, in most cases, only be able to describe systems in which the interaction does not play too strong a role.

To appraise the performance of the KBE+MBPT procedure we have in this

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[1] In general one is only able to find exact solutions in two limiting cases: if the system is very small, where one can use exact numerical techniques, and in the limit of an infinite system where analytical methods play a key role in finding the exact solution as, e.g. in the case of the Bethe-Ansatz solution of the one dimensional Hubbard model.

[2] The formulation of MBPT is in principle exact, however, in practice it is used to find approximate Green's functions.

[3] Every point represents all space, spin and time variables; thus for a three dimensional system with spin 1/2 particles the Green's function depends on 10 variables.

thesis compared it to two other methods, namely exact diagonalisation [20] and one which combines time-dependent density functional theory (TDDFT) [22] with dynamical mean field theory (DMFT) [21]. The exact diagonalisation scheme has the advantage that it is an exact method but in practise it can only treat very small systems. The strength of TDDFT is that it depends on one-point functions, which makes the method computationally very convenient. The weakness, on the other hand, is that it is difficult to construct good approximations and that it is challenging to incorporate memory effects. The advantage of using DMFT is that it is not perturbative which means that it is more adapted to treat strongly correlated systems.

This thesis will deal with model systems. The reasons for studying a model system are basically three. The first one is that a model is much easier to handle than a real system. This makes it at all possible to study strongly correlated systems, also those which are not homogeneous in space and time. The second reason is that one can in some cases have access to the exact solution to benchmark the approximate schemes. The third one is that simple model systems, such as the Hubbard model [23], do have important aspects in common with the real systems of interest and can actually describe them quite well. In fact, various works [24] are able to describe real systems by fitting the model parameters to *ab initio*[4] calculations. In cold atom physics the real Hamiltonian can not only be described very accurately by the Hubbard model but one can actually experimentally tune the parameters of the model in a vast range of values.

The first two points, which are the basis of this thesis, are very important as they make it possible to scrutinise basic conceptual issues and principles without having to develop a full-fledged technical machinery as required by *ab initio* treatments. It should be clear, however, that the final aim of this kind of investigations, which is well beyond the scope of this thesis, is to assess criteria and develop methodologies for an *ab initio* description of realistic systems.

The actual systems studied in this thesis are small Hubbard clusters, isolated and coupled to semi-infinite, one-dimensional and non-interacting leads.

The general strategy we will follow to assess the scope of time-dependent MBPT is to study its performance for model systems by comparing to the exact solution and to the TDDFT+DMFT method.

The background material given in the following chapters is aimed at people with some general knowledge in physics and mathematics who would like to get some superficial notion of the concepts and methodologies studied in this thesis. To this end I will describe the main ideas without going into technical details. For a more extended discussion, the reader is referred to the original papers and the references therein.

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[4] *Ab initio* refers to the treatment of real systems with methods based on first principles.

2

Model systems

In physics it is very convenient and common to make use of models. In some circumstances the word "model" refers to a methodological and theoretical framework as, e.g. in the "standard model". In other contexts, such as in the field of solid state physics, a model refers to a "model system", i.e. an hypothetical system which is intended to share certain important characteristics with a real system. It is in this second sense that we will use the concept of model in this thesis.

Typically, a model includes effective parameters. If one wants to study a specific system one needs to fit these parameters, either experimentally or from *ab initio* calculations. This is however, not the only way one can use a model. In fact one can study the properties of a model system theoretically by tuning the parameters, and then, with modern nano technology one can very often build a system with some desired characteristics.

Another very important feature of model systems is that they sometimes admit exact solutions and can therefore be used as benchmark for addressing fundamental questions of certain approximative methodologies.

The general set-up we consider in this thesis is that of a generic quantum transport geometry,[1] namely a central region, C, contacted to leads, L. The Hamiltonian of the two parts and their mutual coupling read, in standard notation,

$$H = H_C + H_L + H_{LC}. \tag{2.1}$$

We will take the central region to be interacting and described by a Hubbard-like model [23], while the leads will be non-interacting[2] and described by the semi-infinite tight-binding model.

The Hubbard model, introduced in 1963,[3] is one of the most important

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[1] Note that, however, with very minor modifications, this method can be used for any generic subsystem connected to external reservoirs.

[2] The reason for taking the leads non-interacting is that it is at present not possible to deal with correlations in extended leads.

[3] The use of this model goes actually back far earlier in time. It appears that is was first considered by Van-Vleck [25] already in the late forties, and called the $U-T$ model. However,

models in solid state theory as it is the simplest model which incorporates interaction between particles in a lattice. It has been used to study diverse physical phenomena such as high-T$_c$ superconductivity, antiferromagnetism and ferromagnetism. For a good review see, e.g. [26].

The Hubbard model describes particles which live on discrete interconnected sites[4] which form a lattice. These particles can hop from one site to the other and if two particles happen to be on the same site they repel (attract) each other thus getting and energy penalisation (reward). The one band Hubbard Hamiltonian is:[5]

$$H_C = -V \sum_{\langle RR' \rangle,\sigma} a^\dagger_{R\sigma} a_{R'\sigma} + \sum_{R,\,\sigma} \epsilon_R \hat{n}_{R\sigma} + U \sum_{R} \hat{n}_{R\uparrow} \hat{n}_{R\downarrow} + \sum_{R,\,\sigma} w_R\,(t)\, \hat{n}_{R\sigma}. \tag{2.2}$$

Here, R, is the site label, $a^\dagger(a)$ are creation (annihilation) operators, $\hat{n}_{R\sigma} = a^\dagger_{R\sigma} a_{R\sigma}$, $\sigma = \uparrow, \downarrow$, and $\langle RR' \rangle$ denotes pairs of nearest neighbour sites. The $V = 1$ is the hopping parameter, ϵ_R are the on-site energies, U is the on-site interaction parameter and $w_R\,(t)$ is a local, spin-independent, external field which can be of any shape in time t and space. The parameters ϵ_R, U and $w_R\,(t)$ are given in units of V. Our approach is valid for systems which are compensated as well as uncompensated in spin. However, in what follows we will only consider clusters (with/out leads) with an equal average number of spin-up and -down electrons in the ground state; this will hold at all times during the dynamics, since H has no spin-flip terms. The leads are taken to be non-interacting, metallic and described by the semi-infinite, one-dimensional tight binding model:

$$H_L = \sum_{\alpha} \{ -V_{L_\alpha} \sum_{\substack{\langle R_\alpha R'_\alpha \rangle,\,\sigma \\ R_\alpha, R'_\alpha \in L_\alpha}} a^\dagger_{R_\alpha \sigma} a_{R'_\alpha \sigma} + w^B_{L_\alpha}\,(t) \sum_{\substack{R_\alpha,\,\sigma \\ R_\alpha \in L_\alpha}} \hat{n}_{R_\alpha \sigma} \}. \tag{2.3}$$

The coupling, H_{LC}, describes hopping between the central region and the leads,

$$H_{LC} = \sum_{\alpha} \{ -V_{L_\alpha C} \sum_{\substack{\langle R_\alpha R' \rangle,\,\sigma \\ R_\alpha \in L_\alpha, R' \in C}} a^\dagger_{R_\alpha \sigma} a_{R' \sigma} \} + h.c. \tag{2.4}$$

Here the hopping parameter, V_{L_α}, and the bias $w^B_{L_\alpha}$, in the α-th lead as well as the coupling to the central region, $V_{L_\alpha C}$ are similarly in units of V. The biases can have any shape in time but are restricted to be the same on all sites for a given lead.[6]

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due to the detailed analysis provided by Hubbard, the model is universally referred to as the Hubbard model.

[4] These sites may represent localised d- or f-orbitals in atoms, coupled quantum dots or traps in an optical lattice, etc.

[5] In its original form, the model did not include any time-dependent fields and considered only positive U:s.

[6] The reason for having a bias uniform in space is that this greatly simplifies the treatment.

3

Time-dependent many-body perturbation theory out of equilibrium

According to the laws of quantum mechanics, a system is completely determined by its wave function, Ψ. This means that if one possesses the wave function one has the full knowledge of all the possible physical properties of the system. The equation which governs the wave function, for a given Hamiltonian H, is the so-called Schrödinger[1] equation [27]:

$$i\hbar\partial_t\Psi = H\Psi. \tag{3.1}$$

When looking at equation 3.1 the path to follow seems clear: first one finds the Hamiltonian of the system, then one solves the Schrödinger equation and then finally one finds all the physical properties one is interested in. True but not true... The problem is that for any realistic system, the Schrödinger equation can simply not be solved, and furthermore, even if one had the full many-body wave function it would essentially be impossible to access the physical properties. The question of how to treat an interacting system is called the many-body problem and has attracted an enormous attention in the last five decades from the condensed matter community.

The reason why the Schrödinger equation can not be solved, and no physical properties extracted, for any realistic system, where there are typically 10^{23} particles,[2] is that the wave function is just too large. For a system with N particles, the wave function depends on N coordinates, where each coordinate contains space and spin variables. Non-interacting systems are relatively simple to treat as they are represented by simple Slater determinants, which are of single-particle nature. When the particles do interact, however, the wave

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[1] This is the case when the relativistic effects can be neglected. The equation which determines the relativistic wave function is the so-called Dirac equation.

[2] In fact it impossible to solve equation 3.1 even for some few hundreds of particles.

function becomes much more intricate and the phase space grows exponentially with the system size.[3]

In actual experiments one is normally interested in few-body correlations and therefore an attractive alternative to finding the many-body wave function is to consider the n-particle Green's function.[4] The n-particle Green's function is, contrary to the full many-body wave function, designed to explicitly yield the n-particle correlations. In particular the single-particle Green's function,[5] which describes a sudden addition or removal of a particle, gives important quantities such as the density, the currents and total energy.

The main advantage[6] of the Green's function is that it depends only on two coordinates, where these coordinates include spin, space and time. An other advantage is that when one possesses the Green's function it is very simple to obtain the corresponding physical quantities. A word of caution: finding the exact Green's function is as hard as solving the original Schrödinger equation. It is, however, much easier to find approximations for the Green's function.

The many-body perturbation theory (MBPT) is, as the name suggests, an approximate and perturbative methodology which attempts to describe the behavior of systems consisting of interacting particles. It is very convenient to formulate the MBPT in terms of the Green's function.[7] This is done by considering the integral equation to which the Green's function is the solution, the so-called the Dyson equation. The kernel of the Dyson equation is called the self energy and determines the Green's through self-consistency. The aim of MBPT is to construct approximations of the self energy based on a perturbative expansion in terms of the interaction strength. This expansion is generally not a simple order by order series in the interaction strength but rather, as will be seen in section 3.6, of partial sums to infinite order. This is done in a systematic way by using the Wick's theorem and Feynman diagrams [3] or, alternatively, by the Schwinger functional derivative technique [29]. Originally MBPT was developed for ground states. Later, Matsubara [30] generalised it to equilibrium ensembles and Baym, Kadanoff [2, 31, 32] and Keldysh [1] showed how the technique could be generalised to time-dependent phenomena.

There are many different ways of finding the ground-state or equilibrium Green's function by solving the Dyson equation. To determine the time-dependent Green's function, however, one needs to use the Keldysh formalism [1] and solve the Kadanoff-Baym equations [2] i.e. the equations of motion of

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[3] The phase space of the non-interacting wave function also increases exponentially with the system size but does so in a simple way as it is separable.

[4] Typically one is only interested in the one- or two-particle Green's function.

[5] Henceforth, "Green's function" will denote the single-particle Green's function, if not stated otherwise.

[6] As mentioned in the introduction, although if the Green's function is a great simplification with respect to the many-body wave function, it is still only possible to determine, even approximately, for very simple systems.

[7] Actually MBPT can be used without introducing the Green's function, as in, e.g. [28].

the Green's function.

There is a class of many-body approximations (MBA:s) called the conserving approximations [32], which guarantee that important quantities like the total energy or the number of particles are conserved when the system is subject to an external field. The use of conserving approximations when dealing with real-time evolution is of great importance as the violation of the conservation laws would compromise the results.

This chapter is structured as follows: The single-particle Green's function, the Keldysh contour and the general Dyson equation will be introduced in section 3.1, the equilibrium Dyson equation will be discussed in section 3.2, the Kadanoff-Baym equations will be described in section 3.3, how to embed an interacting region into a non-interacting one is examined in section 3.4, the topic of conserving many-body approximations is approached in section 3.5 and finally four specific MBA:s, namely the Hartree-Fock, the second Born, the GW and T-matrix approximations, will be presented in section 3.6.

3.1 Green's functions

It is not really possible to point out a specific work in which the Green's functions an other field theoretical methods were introduced in condensed matter physics. For an early review see, e.g. [33].

As already mentioned, the Green's function, G, does not provide us with full knowledge of the system but it does give access to important quantities such as densities, currents, excitation energies of a system with one added or removed particle as well as the total energy. There are many ways of introducing the Green's function. The way to motivate the definition of the Green's function in this thesis is to consider the time-dependent expectation value of a single-particle operator in the grand canonical ensemble.

3.1.1 Definition of the single-particle Green's function

One important aim of the single-particle Green's function, G, is to obtain the expectation value of a single-particle operator $\hat{O}$. The time-dependent observable is:

$$O\left(t\right)=\left\langle \Psi\left(t\right)\middle|\hat{O}\middle|\Psi\left(t\right)\right\rangle=\left\langle \Psi\left(0\right)\middle|\hat{U}\left(0,t\right)\hat{O}\hat{U}\left(t,0\right)\middle|\Psi\left(0\right)\right\rangle=\left\langle \hat{O}_H\right\rangle. \quad (3.2)$$

Here, $\hat{O}_H$, is the operator in the Heisenberg picture and $\Psi\left(0\right)$ is the initial, equilibrium wave function.[8] To evaluate the operators in the grand canonical

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[8] Note that in equation 3.2 we choose the initial time to be zero. This is convenient but obviously completely arbitrary.

ensemble[9] we write,

$$O(t) = \mathrm{Tr}\left\{\hat{\rho}_0 \hat{O}_H\right\}, \tag{3.3}$$

where

$$\hat{\rho}_0 = \frac{e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}}{\mathrm{Tr}\left\{e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right\}}. \tag{3.4}$$

Here Tr indicates trace, $1/\beta$ is the temperature,[10] μ is the chemical potential and $\hat{N}$ is the particle number operator.

If we now look at the Boltzmann factor, $e^{-\beta\hat{H}}$, we realise that it actually has the same form as an evolution operator in imaginary time, thus:

$$\hat{\rho}_0 = e^{\mu\hat{N}} \cdot \frac{\hat{U}(-i\beta, 0)}{\mathrm{Tr}\left\{e^{\mu\hat{N}}\hat{U}(-i\beta, 0)\right\}}. \tag{3.5}$$

By using the translational invariance in time, $\hat{U}(-i\beta, 0) = \hat{U}(-i\beta/2, i\beta/2)$, and the cyclic property of the trace, the final expression for the time-dependent observable becomes:

$$O(t) = \frac{\mathrm{Tr}\left\{e^{\mu\hat{N}}\hat{U}(-i\beta/2, 0)\,\hat{U}(0, t)\,\hat{O}\hat{U}(t, 0)\,\hat{U}(0, i\beta/2)\right\}}{\mathrm{Tr}\left\{e^{\mu\hat{N}}\hat{U}(-i\beta/2, i\beta/2)\right\}} \tag{3.6}$$

The above expression can be interpreted as follows: first we evolve the system from $i\beta/2$ to 0, then from 0 to t, then we perform the measurement with $\hat{O}$, then we evolve back from t to 0 and finally from 0 to $-i\beta/2$. At this point it becomes natural to introduce the Keldysh contour,[11] see Fig. 3.1.

We now define the single-particle Green's function as,

$$G(r_1 z_1, r_2 z_2) = -i\frac{\mathrm{Tr}\left\{e^{\mu\hat{N}}\mathcal{T}_\gamma\left[\hat{U}(-i\beta/2, 0)\,\hat{\psi}_H(r_1, z_1)\,\hat{\psi}_H^\dagger(r_2, z_2)\,\hat{U}(0, i\beta/2)\right]\right\}}{\mathrm{Tr}\left\{e^{\mu\hat{N}}\hat{U}(-i\beta/2, i\beta/2)\right\}}. \tag{3.7}$$

Here the time argument, z, lies on the Keldysh contour and may be either real, t, or imaginary, $i\tau$. $\mathcal{T}_\gamma$ is the Keldysh path ordering operator, i.e. it orders the field operators, ψ_H, according to the Keldysh contour in Fig. 3.1. This path ordering of the operators is a prerequisite for using the diagram technique

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[9] The careful reader will realise that in the following scheme, the contact with the bath is strictly broken once a perturbing field is switched on at t=0.

[10] We use natural units ($k_B = \hbar = 1$).

[11] Note that the contour in Fig. 3.1 is not the traditional one. The use of the contour in Fig. 3.1 is numerically favorable as discussed in paper II.

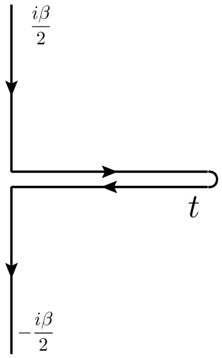

Figure 3.1: Keldysh contour.

which will be discussed in section 3.6. The time-dependent observable can now readily be found by:

$$O\left(z\right)=-i\,\mathrm{Tr}\left\{\hat{O}\left(z\right)G\left(z,z^{+}\right)\right\}. \tag{3.8}$$

Apart from the expectation values of all single-particle operators, the Green's function gives the excitation energies of a system if one adds or removes a particle. In addition one can obtain certain two-body correlation functions such as the total energy and the double occupancy, $\langle \hat{n}_{R\uparrow}\hat{n}_{R\downarrow}\rangle$, as discussed in paper II and IV respectively. The double occupancy can in turn be used to evaluate the entanglement entropy, which is a key quantity in the field of quantum information, see paper IV.

3.1.2 Physical interpretation

By inspecting the definition of the Green's function in Eq. 3.7 we see that for $z_1 > z_2$ the $\hat{\psi}_H^{\dagger}\left(r_2,z_2\right)$ creates a particle at the point r_2 at time z_2. The system with the extra particle then propagates to r_1 at time z_1. The Green's function therefore gives the probability amplitude that a particle added at r_2 at time z_2 is found at r_1 at time z_1. Similarly, for $z_1 < z_2$ the Green's function describes the propagation of a hole.

3.1.3 Dyson equation

To shed better light on the underlying structure in what follows we write the Green's function in a short-hand notation:

$$G(12)=-i\left\langle \mathcal{T}_{\gamma}\left[\psi_H(1)\psi_H^{\dagger}(2)\right]\right\rangle. \tag{3.9}$$

Here $1 = r_1\sigma_1 z_1$ represent all single-particle (space/spin) and time labels.

The Green's function obeys an integral equation which is called the Dyson equation,

$$G\left(12\right) = G_0\left(12\right) + \int_\gamma G_0\left(13\right)\Sigma\left(34\right)G\left(42\right)d34. \tag{3.10}$$

Here the non-interacting Green's function G_0 defined by

$$\left(i\partial_{z_1} - h\left(1\right)\right)G_0\left(12\right) = \delta\left(12\right), \tag{3.11}$$

where $h\left(z\right)$ is the non-interacting Hamiltonian. The kernel of the Dyson equation, Σ, is called the self energy and describes the effects of interactions and embedding, as discussed in sections 3.3 and 3.4. The self energy, which is non-local in space and time, is a functional of the Green's function, $\Sigma\left[G\right]$, and therefore the Dyson equation must be solved self-consistently.[12]

3.2 Equilibrium state

In equilibrium all quantities depend only on $z = z_2 - z_1$ and the equations are then most easily handled in the frequency domain, in terms of Fourier transformed quantities. The entire ground-state calculation can be performed using real times[13] and the resulting Dyson equation becomes

$$G\left(\epsilon\right) = G_0\left(\epsilon\right) + G_0\left(\epsilon\right)\Sigma\left(\epsilon\right)G\left(\epsilon\right), \tag{3.12}$$

where ϵ is a real frequency. In Fourier space the Dyson equation becomes a simple matrix equation in the single-particle basis, which can be solved directly by inversion.

In this thesis we will work in the zero temperature limit and use the correlated ground state as the initial, state for the time evolution [4].

3.3 Kadanoff-Baym equations

For a system which changes in time, the Green's function becomes intrinsically dependent on two times and the use of the Keldysh formalism becomes inevitable.

The generic Keldysh propagator, $\mathcal{K}$, has the following structure:

$$\mathcal{K}\left(12\right) = \mathcal{K}^{\delta}\left(12\right)\delta\left(z_1, z_2\right) + \Theta\left(12\right)\mathcal{K}^{>}\left(12\right) + \Theta\left(21\right)\mathcal{K}^{<}\left(12\right), \tag{3.13}$$

---

[12] The self energy in approximate treatments is generally also a functional of the Green's function and non-local in space and time.

[13] The use of real times and then going to Fourier space is only one of many possible ways of solving the Dyson equation.

where the greater, >, and lesser, <, propagators refer to the electron and hole part respectively and the $\mathcal{K}^{\delta}$ is the time-local part.[14] For real times we may also introduce a retarded

$$\mathcal{K}^{R}(12) = \mathcal{K}^{\delta}(12)\,\delta(t_1, t_2) + \Theta(t_1, t_2)\left[\mathcal{K}^{>}(12) - \mathcal{K}^{<}(12)\right], \tag{3.14}$$

and advanced propagators,

$$\mathcal{K}^{A}(12) = \mathcal{K}^{\delta}(12)\,\delta(t_1, t_2) - \Theta(t_2, t_1)\left[\mathcal{K}^{>}(12) - \mathcal{K}^{<}(12)\right]. \tag{3.15}$$

When both time arguments are imaginary, the Keldysh function reduces to the corresponding equilibrium Matsubara function:

$$\mathcal{K}^{M}(\tau - \tau') = -i\mathcal{K}(-i\tau, -i\tau'). \tag{3.16}$$

In Eq. (3.13), $\Theta(12)$ should be understood as $\Theta(z_1, z_2)$, i.e. a generalised Heaviside function for z_1, z_2 on the path ordered Keldysh contour. It is worth noting that when both time arguments lie on the imaginary (Matsubara) axis, the quantities represent the initial state, taken to be the equilibrium ensemble, as mentioned in the previous section, which depend only on the time differences.

From the definition of the single-particle Green's function and using Schrödinger equation for the field operators we can write the equations of motion of the Green's function:

$$(i\partial_{z_1} - h(1))\,G(12) = \delta(12) - i\int_{\gamma} u\left(1^{+}3\right) G^{II}\left(133^{+}2\right) d3, \tag{3.17}$$

$$(-i\partial_{z_2} - h(2))\,G(12) = \delta(12) - i\int_{\gamma} u\left(2^{+}3\right) G^{II}\left(133^{+}2\right) d3. \tag{3.18}$$

Here $u(12) = u(12)\,\delta(z_1 z_2)$ is the bare interaction, $1^{+} = r_1\sigma_1 z_1^{+}$ and G^{II} is the two-particle Green's function. Similarly, the equations of motion of the two-particle Green's function involve the three-particle Green's function, and so forth.[15] To close the equations we define the self energy Σ in Eq. 3.10 by:

$$\int_{\gamma} \Sigma(13)\,G(32)\,d3 = -i\int_{\gamma} u\left(1^{+}3\right) G^{II}\left(133^{+}2\right) d3 \tag{3.19}$$

$$\int_{\gamma} G(13)\,\Sigma(32)\,d3 = -i\int_{\gamma} u\left(2^{+}3\right) G^{II}\left(133^{+}2\right) d3. \tag{3.20}$$

---

[14] For the $\mathcal{K}$:s considered in this thesis, only Σ and W have time-local parts which are non zero.

[15] In fact this hierarchy can be used to generate approximations by, e.g. factorizing the three-particle Green's function in terms of one- and two-particle Green's function as done in [34].

The resulting equations of motion of the Green's function are called the Kadanoff-Baym equations (KBE),

$$\left(i\partial_{z_1} - h\left(1\right)\right) G\left(12\right) = \delta\left(12\right) + \int_\gamma \Sigma\left(13\right) G\left(32\right) d3, \tag{3.21}$$

$$\left(-i\partial_{z_2} - h\left(2\right)\right) G\left(12\right) = \delta\left(12\right) + \int_\gamma G\left(13\right) \Sigma\left(32\right) d3. \tag{3.22}$$

To simplify the transparency of the KBE we separate out the time-local Hartree-Fock self energy and include it into the single-particle Hamiltonian,

$$\Sigma = \Sigma_{HF} + \Sigma_{c/e}, \qquad \mathfrak{h} = h + \Sigma_{HF}. \tag{3.23}$$

The time non-local contribution, $\Sigma_{c/e}$, consist of two terms:

$$\Sigma_{c/e} = \Sigma_{corr} + \Sigma_{emb}. \tag{3.24}$$

The first describes correlations and the second is the embedding (lead) self energy, which will be discussed in the next section. Specialising on the derivative of the first argument with both arguments real we can then break the KBE into:

$$i\partial_{t_1} G^{\lessgtr}\left(t_1, t_2\right) = \mathfrak{h}\left(t_1\right) G^{\lessgtr}\left(t_1, t_2\right) + I_1^{\lessgtr}\left(t_1, t_2\right), \tag{3.25}$$

where

$$\begin{aligned} I_1^{\lessgtr}(t_1, t_2) =& \int_0^{t_1} d\bar{t} \left[\Sigma^R_{c/e}\left(t_1, \bar{t}\right) G^{\lessgtr}\left(\bar{t}, t_2\right) + \Sigma^{\lessgtr}_{c/e}\left(t_1, \bar{t}\right) G^A\left(\bar{t}, t_2\right)\right] \\ &+ \frac{1}{i}\int_0^{\beta/2} d\bar{\tau} \left[\Sigma^<_{c/e}(t_1, -i\bar{\tau}) G^>(-i\bar{\tau}, t_2) + \Sigma^>_{c/e}(t_1, i\bar{\tau}) G^<(i\bar{\tau}, t_2)\right], \end{aligned} \tag{3.26}$$

is a collision integral and describes the correlation and lead effects. The first integral represents the contribution of the real axis, i.e. the memory from the time evolution. The second integral embodies the effect of the correlations and embedding of the initial state.

3.4 Embedding procedure

For the scope of this thesis, one of the main advantages of the Green's function technique is that it is possible to include non-interacting leads,[16] with a space-homogeneous but time-dependent bias, in an exact way through an embedding

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[16] In general the embedding scheme can be used to treat any non-interacting region. An other example of embedding is presented in section. 4.3, where a single impurity is coupled to a non-interacting bath.

procedure.[17] The idea is that one separates the system into a central (possibly interacting) region and some non-interacting leads which are then projected into the central region. The net result is that the leads come in effectively as an embedding self energy [36, 37, 15, 16],

$$\Sigma_{emb}(z_1, z_2) = \sum_{\alpha} |V_{L_\alpha C}|^2 g_{L_\alpha}(z_1, z_2) \,. \tag{3.27}$$

Here $g_{L_\alpha}(z_1, z_2)$ is the non-interacting Green's function of the uncontacted, possibly biased, lead L_α.[18]

3.5 Conserving approximations

The Green's function based formulations for ground-state and excitation properties in terms of the one-particle Green's function and other few-particle correlation functions are formally exact, and so are the Kadanoff-Baym equations. However, in order to obtain the self-energy and other key quantities in practice, one has to resort to approximations. A large class of approximations within MBPT involves infinite partial summations or some clever decoupling scheme of the equations of motion. It is then very important to have some guiding principles in order to avoid unphysical results.

In the late fifties and early sixties, Luttinger, Ward, Nozières and others [38, 39, 40] provided microscopic justification of Landau's Fermi-liquid theory by infinite-order perturbation theory and could verify the existence of a sharp Fermi surface enclosing the correct number of particles as well as the conservation of particles, momentum, etc. An important ingredient in these works was the discovery that the exact self energy Σ can be considered a functional of the exact G, and that this functional has a vanishing curl. This means that the exact Σ is the gradient of some scalar functional $\Phi[G]$,

$$\Sigma\,(12) = \frac{\delta\Phi[G]}{\delta G\,(21)}. \tag{3.28}$$

Later, Kadanoff and Baym could identify some key properties that approximate self energies must fulfil in order to have important macroscopic conservations laws fulfilled, such as the conservation of particles, energy, and momentum, [32, 31]. In his 1962 paper, Baym [32] found that the necessary and sufficient condition for guaranteeing the conservation laws is that the approximate self energy must fulfil the same functional relationship in Eq. (3.28) as the

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[17] Similar embedding schemes can be used in wave function based approaches such as in time-dependent density functional theory [35].

[18] Eq. 3.27 stays the same if the bias is space dependent but the calculation of $g_{L_\alpha}(z_1, z_2)$ becomes much more complicated.

exact one. Different approximate generating functionals Φ generate different conserving approximations.

The conserving aspects play a less prominent role in equilibrium and might actually deteriorate the quality of some physical properties [41]. One example is the well-known GW approximation. This is a conserving approximation provided that Σ is computed self-consistently. However, in free-electron-like metals and in the electron gas, the already poor description of satellites is much worsened [42], and there is also evidence that the quasi-particle bands in semiconductors deteriorate [43]. If the quantity of interest is the spectral function one should probably use other summation criteria. These matters have been discussed, e.g. in [44, 45]. Out of equilibrium, however, it is essential to use conserving approximations, as an uncontrolled violation of the conservation laws would put serious limitations on the possible external fields.

3.6 Many-body approximations

The schemes we will consider in this thesis to calculate the Green's function are based on conserving MBPT. Loosely speaking, such schemes, can be said to be perturbative in character. However, at the same time it should be kept in mind that in conserving approximations one works with the self-consistent G, which brings in the interaction to all orders already in the simple Hartree-Fock approximation.[19]

An advantage of MBPT is its close relation to the Keldysh formalism which allows us to treat systems which are inhomogeneous both in space and in time. It is also possible to construct approximations of increasing degree of complexity in a systematic way, although the difficulties rapidly increase as more vertex corrections are added.

The self energy admits expansions in terms of the Green's function and the bare interaction [3, 46]. These terms become rapidly very intricate and difficult to handle. The use of the diagram technique,[20] where the terms in the perturbation series are represented by diagrams, becomes decisive.

Order by order perturbation theory leads to expansions in the non-interacting Green's function G_0 and the bare interaction u. Via infinite partial summations this may be converted into expansions involving the the interacting Green's function G and the bare u which defines a functional relationship $\Sigma[G, u]$ used in conserving approximations. The corresponding diagrams are usually called skeletonic and are fewer than those which occur in expansions with respect to G_0. In systems with long-range (Coulomb) interaction it is advantageous to perform yet another partial summation with respect to screening,

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[19] This obviously also applies to the other MBA:s.

[20] In the late forties Richard Feynman revolutionised many-body physics, by introducing the diagram technique [47] which made the whole treatment immensely simpler.

and this leads to an expansion in terms of G and the screened interaction W and a functional relationship $\Sigma[G, W]$. The GW approximation is the simplest approximation of this latter kind.

We will consider two types of MBA:s. In the first type, all diagrams with a given maximal number of interaction vertices in $\Sigma[G, u]$ are kept. In the second type, additional partial summations are performed, usually involving simple geometrical sums which lead to Dyson-like equations for auxiliary propagators. The Hartree-Fock and second Born approximations (HFA and BA respectively) correspond to the first type while the GW and T-matrix approximations (GWA and TMA respectively) are of the second type. In the HFA and BA the self energy can be obtained directly from the Green's function, whereas in the case of GWA or TMA the Dyson equations for the auxiliary propagators (W in case of GWA and the T-matrix in case of TMA) must be solved simultaneously with the Kadanoff-Baym equations for the Green's function.

The rather simple models that we use do not do justice to all the MBA:s that we consider. In our models, the time-dependent Hartree-Fock approximation is trivial, but it has played an important role for deepening our understanding of, e.g. absorption spectra of atoms and molecules [48]. The GWA [49] has been extremely successful in describing the quasi-particle bands in sp-bonded materials, in particular it has essentially solved the longstanding problem of obtaining correct band gaps in semiconductors and insulators [50, 51]. In Coulomb systems, expansions in the bare interaction u diverge beyond first order as, e.g. in second Born, and one is more or less forced to expand in the screened interaction W. However, the effects of long-range screening has been encapsulated in the local model interaction of the Hubbard model, and the GWA then becomes less interesting. The TMA [52, 53, 54], on the other hand, was designed to treat systems with short-range interaction and is the most relevant approximation for our models.

3.6.1 Hartree-Fock approximation

The simplest MBA is the Hartree approximation where the self energy consists only of the direct first-order term; the first diagram in Fig. 3.2. The Hartree-Fock approximation also incorporates the first-order exchange diagram; the second diagram in Fig. 3.2. Including the exchange term, among other things,

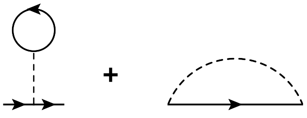

Figure 3.2: Hartree-Fock self energy.

cancels the self interaction in the Hartree approximation. Both these approximations have self energies which are local in time and do not involve any correlations.

3.6.2 Second Born approximation

The simplest MBA which incorporates correlation effects is the direct Born, where the self energy contains, in addition to the Hartree-Fock terms, also the direct second-order diagram; the third diagram in Fig. 3.3. The second Born approximation also includes the second-order exchange diagram; the fourth diagram in Fig. 3.3.

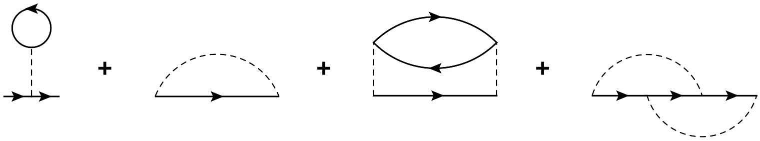

Figure 3.3: Second born self energy.

3.6.3 GW approximation

The GW approximation, see Fig. 3.4, consists in taking all diagrams which include consecutive electron-hole scatterings, the so called bubble diagrams, and adding them up to infinite order [49].

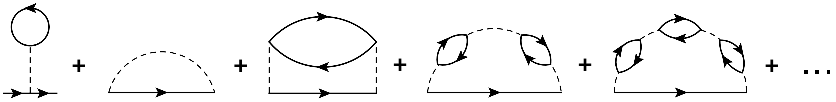

Figure 3.4: GW self energy.

Equivalently the GWA corresponds to keeping the direct first-order term of the expansion of self energy in terms of the screened interaction W. The screened interaction satisfies a corresponding Dyson equation,

$$W(12) = u(12) + \int u(13)\, P(34)\, W(42)\, d34, \tag{3.29}$$

where $u(12) = u(12)\,\delta(z_1 z_2)$ is the bare interaction and the polarisation propagator, P, is given by

$$P(12) = -iG(12)\, G(21)\,. \tag{3.30}$$

The GW self energy finally becomes:

$$\Sigma_{GW}(12) = \Sigma_H + iG(12)\,W(12)\,. \tag{3.31}$$

3.6.4 *T*-matrix approximation

In the T-matrix approximation one builds the T-matrix, T, by adding all electron-electron and hole-hole scatterings [52, 53], the so called the ladder diagrams, see Fig. 3.5.

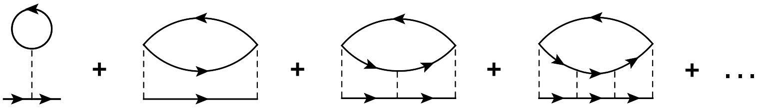

Figure 3.5: T-matrix self energy.

The Dyson equation of the T is,

$$T(12) = \phi(12) - \int \phi(13)\,u(34)\,T(42)\,d34, \tag{3.32}$$

where the so-called irreducible vertex ϕ is defined as

$$\phi(12) = -iG(12)\,G(12)\,. \tag{3.33}$$

The T-matrix self energy becomes:

$$\Sigma_{TM}(12) = \Sigma_{HF} + i\int u(13)\,G(43)\,T(34)\,u(42)\,d34. \tag{3.34}$$

4

Other many-body methods

Many-body perturbation theory is only one among a wide variety of methods to treat systems with interacting particles. In this thesis we will also consider three other methods in order to compare and contrast to many-body perturbation theory. In section 4.1 we will discuss exact diagonalisation, in section 4.2 we will present density functional theory and in section 4.3 we will introduce dynamical mean field theory.

4.1 Exact diagonalisation

Exact diagonalisation or configuration interaction [20] is a numerically exact method where the Hamiltonian is expanded in a given basis and then diagonalised. From the diagonalised Hamiltonian one then obtains the wave function of all the eigenstates, in particular the ground state, which then give access to all observables. The method is exact in the sense that if one used a complete set of basis states it would yield the exact solution. In practice, of course, one has to truncate the basis space and the results are therefore only approximate. The numerical errors are, however, quite controllable and one can get an arbitrarily high accuracy. The time evolution is made with the Lanczos method[1] [55], where the Hamiltonian is represented in a basis in which it is tridiagonal. In this basis it is much easier to diagonalise the Hamiltonian and to make a systematic cutoff of basis states.

The advantages of exact diagonalisation is that it is very general and can deal with any interaction and dimensionality. The main drawback is that one can treat only systems with very few particles.[2] In this thesis we use the exact diagonalisation method to benchmark the approximate results.

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[1] The Lanczos method is only one of many to perform the time evolution, for a detailed review see, e.g. [56].

[2] For the systems we consider we can treat up to 18 sites depending on the filling.

4.2 Density functional theory

Density functional theory (DFT) is one of the most used methodologies in solid state physics and quantum chemistry to study real many-body systems mainly due to its relatively high accuracy and rather simple numerical implementation. The main idea is that one uses the density profile, $n(\mathbf{r})$, as the basic variable to obtain some important properties of a system. This is an enormous simplification since for a spin-less N-particle system, the density depends only on three coordinates while the many-body wave function depends on $3N$.

The modern form of DFT was first formulated by Hohenberg and Kohn in 1964 [57] and shortly afterward generalised to equilibrium systems by Mermin [58] and to spin-polarised systems by von Barth and Hedin [59]. In 1984, Runge and Gross [22] laid the foundation of the extension to time-dependent phenomena and thereby to excited states, the so-called time-dependent density functional theory (TDDFT).

The key quantity in (TD)DFT is the exchange-correlation energy, E_{xc}. This quantity, which is exactly defined, is generally not known and one needs to rely on approximations. Peukert [60] outline possibilities to develop approximations within TDDFT itelself, but generally the approximations in common use have been developed using MBPT or other methods. Fortunately, the simple local density approximation (LDA) [61] works much better than originally expected and other improved approximations have been developed over the years. For a detailed review see, e.g. [62, 63, 64].

4.2.1 Hohenberg-Kohn theorem

In density-functional theory one considers systems with a given interaction $u(\mathbf{r}-\mathbf{r}')$ put in different environments described by different scalar one-body potentials $v(\mathbf{r})$. The ground-state energy E_0 and the corresponding density profile $n(\mathbf{r})$ will then be functionals of $v(\mathbf{r})$, $E_0 \equiv E_0[v]$, etc. The Hohenberg-Kohn theorem [57] states that if the ground-state densities $n_1(\mathbf{r})$ and $n_2(\mathbf{r})$ of two systems (1) and (2) are the same, the corresponding potentials agree up to a constant, $v_1(\mathbf{r}) = v_2(\mathbf{r}) + C$. The mapping $v \to n$ is thus invertible up to a constant, and one can use the density as the fundamental variable. Hohenberg and Kohn defined the basic density functional as the Legendre transform

$$F[n] = E_0[v] - \int \frac{\delta E_0}{\delta v(\mathbf{r})} v(\mathbf{r}) d^3r = E_0[v[n]] - \int n(\mathbf{r}) v(\mathbf{r}) d^3r. \qquad (4.1)$$

Here we have used that, from first order perturbation theory, $\delta E_0/\delta v(\mathbf{r}) = n(\mathbf{r})$. It should be noted that different densities in $F[n]$ corresponds to different systems and not to different densities that a given system might have.

Hohenberg and Kohn also formulated a variational principle and showed that one can obtain the ground-state energy and density by minimising the functional

$$E_v[n] = F[n] + \int n(\mathbf{r})v(\mathbf{r})d^3r \tag{4.2}$$

with respect to n for a fixed potential v. One can thus obtain the ground-state properties of any system by working solely with the density and functionals of the density without referring to the underlying many-body wave function.

4.2.2 The Kohn-Sham scheme

Up to this point one can say that Hohenberg and Kohn provided a much more rigorous way to use the density as the basic variable than had been possible in earlier works [65, 66, 67]. An important step that carried the new formulation far beyond the earlier theories was the ingenious method by Kohn and Sham [68] that allows for an exact treatment of the kinetic energy[3] via a fictitious independent-electron system. In this way only the relatively small terms from exchange and correlation need to be approximated, and already in the simplest LDA treatment the essentially correct shell structure of atoms emerged, something that earlier theories completely failed to describe.

To derive the Kohn-Sham equations we start by rewriting Eq. 4.1 by separating out the Hartree and the non-interacting terms,

$$F[n] = T_0[n] + E_H[n] + E_{xc}[n]. \tag{4.3}$$

Here T_0 is the kinetic energy functional (or F functional) for independent particles, $E_H[n] = \frac{1}{2}\int u(\mathbf{r}-\mathbf{r}')n(\mathbf{r})n(\mathbf{r}')d^3rd^3r'$ is the Hartree energy, and E_{xc} is the exchange-correlation energy functional, i.e. the remaining part of $F[n]$.

In order to find the minimum energy for a fixed number of particles N we introduce a Lagrange parameter μ and minimise $E_v[n] - \mu N$. This leads to the Euler equation

$$\begin{aligned} \mu = \frac{\delta E_v[n]}{\delta n(\mathbf{r})} &= \frac{\delta T_0[n]}{\delta n(\mathbf{r})} + \frac{\delta E_H[n]}{\delta n(\mathbf{r})} + \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})} + \frac{\delta \int vn}{\delta n(\mathbf{r})} & (4.4) \\ &= \frac{\delta T_0[n]}{\delta n(\mathbf{r})} + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) + v(\mathbf{r}). & (4.5) \end{aligned}$$

If we instead had considered independent particles in a potential $V_{eff}(\mathbf{r})$ we would minimise $T_0 + \int V_{eff}n - \mu N$, which leads to

$$\mu = \frac{\delta T_0[n]}{\delta n(\mathbf{r})} + V_{eff}(\mathbf{r}). \tag{4.6}$$

However, for independent particles we can obtain T_0 directly via the one-particle orbitals φ_i for any V_{eff} without referring to its unknown functional

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[3] Strictly speaking only the independent-electron part is treated exactly.

dependence on n:

$$T_0 = \sum_i^{occ} \langle \varphi_i | \hat{t} | \varphi_i \rangle. \tag{4.7}$$

Here, $\hat{t} = -\frac{1}{2}\nabla^2$, is the single-particle kinetic operator. In this way we obtain T_0 for the density $n[V_{eff}]$. By varying V_{eff} until the $n[V_{eff}]$ agrees with a given prescribed density n we can construct $T_0[n]$.[4] If we now choose $V_{eff} = v + v_H + v_{xc}$ we see that we can minimise $E_v[n] - \mu N$ by solving the one-particle equations

$$\left(\hat{t} + v + v_H + v_{xc}\right) \varphi_i = e_i \varphi_i \tag{4.8}$$

self-consistently, where the density at each iteration is

$$n(\mathbf{r}) = \sum_i^{occ} |\varphi_i(\mathbf{r})|^2. \tag{4.9}$$

It is worth mentioning that the orbitals φ_i and corresponding eigenvalues e_i in general have no clear physical meaning. When self-consistency has been achieved, T_0 has been evaluated exactly and the ground-state energy and density have been obtained. If the exact E_{xc} were known the scheme would be exact, but in practice one has of course to use approximations. However, one is approximating only a relatively small contribution to the density functional $F[n]$.

The above Kohn-Sham one-particle scheme assumes that the interacting density n is also the density of an independent-particle system in some other potential V_{eff}. Such densities are usually referred to as v_0-representable. It is in general very difficult to prove v_0-representability, but a relatively large class of atoms and small molecules have been shown via direct computer experiments to have v_0-representable densities.

4.2.3 Local density approximation

The functional E_{xc} describes in principle the ground-state properties of all systems in nature and is of course only approximately known. The simplest approximation is the local density approximation (LDA) where the system is considered to be locally homogeneous and E_{xc} is approximated by the superposition

$$E_{xc}[n] \approx E_{xc}^{LDA}[n] = \int n(\mathbf{r}) \epsilon_{xc}(n(\mathbf{r})) d^3r. \tag{4.10}$$

---

[4] This is actually the only known procedure for constructing T_0 as functional of n.

Here, $\epsilon_{xc}(n_0)$ is the exchange-correlation energy per particle of the homogeneous system with density n_0 in a constant potential v_0,

$$N\epsilon_{xc}(n_0) = E_{tot} - T_0 - E_H - N\int v_0 d^3r. \tag{4.11}$$

The exchange-correlation potential is then found by taking the functional derivative with respect to the density, which in this case reduces to a derivative with respect to the density at point $\mathbf{r}$,

$$v_{xc}^{LDA}(\mathbf{r}) = \left(\frac{d(n\epsilon_{xc}(n))}{dn}\right)_{n=n(\mathbf{r})}. \tag{4.12}$$

The LDA evidently becomes exact in the limit of slowly varying densities, provided that the data for the underlying homogeneous system are known. In our applications to the 3D Hubbard model, these data were obtained from dynamical mean field theory [69].

4.2.4 Time-dependent density functional theory

The time-dependent density functional theory (TDDFT) is the extension of the ground-state DFT to treat excited states and systems out of equilibrium [70]. Similar to ground state DFT, TDDFT is based on a uniqueness theorem which was first proved by Runge and Gross [22] and has since then been given various alternative proofs [71, 72].

The uniqueness theorem concerns systems which are in a given initial state Ψ, which is not necessarily a ground-state, and evolve under a time-dependent one-body external potential, $v(\mathbf{r}, t)$. The theorem then states that if two systems (1) and (2) have the same initial state Ψ, and a later time have density profiles $n_1(\mathbf{r}, t)$ and $n_2(\mathbf{r}, t)$ which coincides, then the two corresponding external potentials must be the same up to a time-dependent constant, i.e. $v_1(\mathbf{r}, t) = v_2(\mathbf{r}, t) + C(t)$. In other words, this theorem establishes an invertible mapping between the time-dependent potentials and the corresponding time-dependent densities.

In analogy to ground state DFT we can now construct a density functional $F[n]$ and an action functional,

$$E_v[n] = F[n] + \int n(\mathbf{r}, t)v(\mathbf{r}, t)d^3r dt. \tag{4.13}$$

The time-dependent densities are then found as stationary trajectories of this action functional. The fact that the functional is only stationary in TDDFT rather than minimal as in ground state DFT makes the time-dependent theory considerably more complicated.

The corresponding exchange-correlation potential is now much more complex object as it incorporates memory effects by depending on the densities at all points in space at all previous times. The simplest approximation in TDDFT is the adiabatic local density approximation (ALDA), where the v_{xc} is taken to be the ground-state one for a given instantaneous density, i.e. $v_{xc}[\mathbf{r}, t; n] = v_{xc}^{LDA}(n(\mathbf{r}, t))$. It is the ALDA which will be used in this thesis.

4.2.5 Density functional theory in lattice models

In these thesis we have applied DFT and TDDFT to discrete Hubbard lattice models outlined in section 2. The hopping then plays the role of the single-particle kinetic energy $-\frac{\nabla^2}{2}$, the local occupancies $\hat{n}_R = \sum_\sigma a^\dagger_{R\sigma} a_{R\sigma}$ the role of the density $\hat{n}(\mathbf{r})$, and the on-site energy parameter w_R the role of the local potential $v(\mathbf{r})$.

As far as the ground-state theory is concerned, the basic Hohenberg-Kohn and Kohn-Sham theorems go through essentially unchanged [73], and local-density functionals (i.e. exchange-correlation energies for homogeneous Hubbard models) have been obtained and parametrised for the 1D Hubbard model [74, 75], and more recently for the 3D Hubbard model [69].

A TDDFT approach to the real-time dynamics of the Hubbard model out of equilibrium was initially considered in [76]. In this work, the exact many-body non-equilibrium dynamics of small 1D Hubbard chains of different lengths and particle densities was performed, and from it, via a reverse-engineering procedure, the exact, time-dependent exchange-correlation potential was obtained, by propagating the time-dependent Kohn-Sham equations. In [76], exact results for the density and the exchange-correlation potential were compared to those from an approximate v_{xc} obtained within the ALDA, and an analysis of non-local adiabatic effects in v_{xc} was carried out. In addition, an inequality was provided as a necessary condition for v_0-representability.

There are various works in which lattice TDDFT has been used very successfully [77, 78, 69]. However, it has recently been found that the Runge-Gross uniqueness proof along the lines of the continuous case does not hold [79, 80]. This observation corroborates the fact that, for lattice Hamiltonians, one can actually find examples which contradict the uniqueness of the correspondence between densities and potentials. If one adopts the bond current as the basic variable, a one-to-one mapping can be established [79] betweeen current densities and Peierls phases [81, 82] of the bond-hopping terms. Thus, care must be exerted in using lattice TDDFT when dealing with issues for which the uniqueness of the density-potential mapping is relevant. In the works of this thesis, the v_0-representability has been demonstrated, but the exchange-correlation potentials may not be unique. For further discussion see, e.g. paper III.

4.3 Dynamical mean field theory

Dynamical mean field theory (DMFT) is a non-perturbative approximation for homogeneous lattice models [84]. This approach becomes exact in the infinite dimension limit [21] and being non-perturbative, it implies that one can, in practice, treat highly correlated systems not accessible to MBPT.

The essence of equilibrium DMFT is that one neglects the momentum dependence of the self energy which results in a frequency-dependent self energy which is local in space. The problem can not be solved directly but one can use a similar trick as in DFT: use an auxiliary system where one knows how to proceed. In DMFT one maps [85] the original lattice into an other system which automatically has a local, frequency-dependent self energy, namely a single impurity embedded in a non-interacting bath,[5] the so-called Anderson impurity model (AIM) [86],

$$H_{AIM} = \sum_{\sigma} \epsilon_0 n_{0\sigma} + U n_{0\uparrow} n_{0\downarrow} + \sum_{\nu\sigma} \epsilon_\nu n_{\nu\sigma} + \sum_{\nu\sigma} \left[V_\nu c^\dagger_{0,\sigma} a_{\nu,\sigma} + V^\dagger_\nu a^\dagger_{\nu,\sigma} c_{0,\sigma} \right]. \tag{4.14}$$

Here c and $c^\dagger$ refer to the impurity, a and $a^\dagger$ refer to the bath and the index ν runs over all bath sites. The ϵ_0 is the impurity on-site energy and U is the interaction strength which is the same as in the original lattice. The ϵ_ν are the on-site energies of the bath and V_ν are the hopping strengths between the bath and the impurity. Both ϵ_ν and V_ν are effective parameters which are determined from the original lattice.

The on-site Green's function of the homogeneous lattice has the form

$$G_{latt}(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{\rho_0(\omega')}{\omega - \omega' - \Sigma_{latt}(\omega')}, \tag{4.15}$$

where ω is a frequency, ρ_0 is the density of states of the non-interacting system and Σ_{latt} is the lattice self energy taken to be momentum independent.

The impurity Green's function is

$$G_{imp}(\omega) = \frac{1}{\omega - \epsilon_0 - \Delta(\omega) - \Sigma_{imp}(\omega)}, \tag{4.16}$$

where

$$\Delta(\omega) = \sum_{\nu} \frac{|V_\nu|^2}{\omega - \epsilon_\nu}, \tag{4.17}$$

---

[5] The choice of mapping the lattice onto a single interacting impurity is arbitrary. The main advantage of this particular mapping is that one can use all the machinery developed to treat the famous Anderson model.

is the embedding self energy of the bath and usually referred to as hybridisation function.

The mapping between the original lattice and the Anderson model is done self-consistently by requiring that the space-local part of the Green's function of the impurity model and that of the original lattice to be the same for the same self energy:

$$G_{latt} = G_{imp}, \tag{4.18}$$

$$\Sigma_{latt} = \Sigma_{imp}. \tag{4.19}$$

There are many different ways to handle the self consistency cycle[6] but they all based on a variation of the effective parameters of the bath.

When self-consistency is reached, we obtain the exchange-correlation potential from Eq. 4.11 and differentiating the E_{xc}^{DMFT} with respect to the density.

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[6] Examples of solvers are exact diagonalisation, quantum Montecarlo, numerical renormalisation group and density matrix renormalisation group.

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Part B

The papers

Summary of the papers

The aim of this thesis is to shed light on the possibilities and limitations of time-dependent many-body perturbation theory. The strategy for this assessment is to compare the MBPT results with two other methods, namely exact diagonalisation and TDDFT, for simple Hubbard clusters. The conclusions of this study can be separated into two different classes.

The first class deals with the varying performance of the approximations depending on the interaction, the filling and the strength and adiabaticity of the external field. These aspects can be summarised in that:

I The TMA is, among the tested MBA:s, the one which stands out the most as its performance in the low density regime is very good, also for quite strong interactions.

II Compared to the TDDFT approach, the MBA:s fail in describing the strong interaction regime but they are, in particular the TMA, better in treating non-adiabatic fields. This can be attributed to the fact that the MBA:s are perturbative in character but do incorporate memory effects.

The second class of conclusions account for genuinely unphysical properties of the perturbative MBA:s. These features can be summarised in that:

III The MBPT may not handle the phase space correctly. In particular the KBE+MBPT give rise to a damped evolution in finite systems. In other words, the finite phase space of the exact solution, which results in an undamped motion, is misrepresented by an infinite one within MBPT.

IV There exists multiple steady and quasi steady states in the KBE+MBPT evolution. That is, when the system evolves under a perturbation it reaches a steady state which depends on how the external field is switched on. In an isolated system the steady states are real. For weakly contacted systems, these steady states are still reminiscent as long-lived metastable states.

V The positiveness condition of correlation functions may be violated. In particular, among the examined MBA:s, positiveness is only guaranteed in the TMA.

Paper I

In paper I we treat short Hubbard chains out of equilibrium with KBE+MBPT, within the HFA, the BA, the GWA and the TMA, and compare these results with those from the exact solution. We find that among the different approximations, the TMA yields the most accurate results, especially at low filling. We also present the unphysical treatment of the phase space of the MBPT. In the ground state this manifests itself as an infinite number of poles of the spectral function (where the exact one has only a finite number) and in the time dynamics it leads to a correlation-induced damping (not present in the exact dynamics) and a broadened spectral function (whereas the exact one remains discrete). We attribute this incorrect handling of the phase space to the implicit inclusion of diagrams of all orders in a system which can accommodate only a finite number of particles. Moreover we show that the steady state reached is not unique but depends on the history of the external field.

For this paper I have produced the codes for the KBE+MBPT evolution, participated actively in the discussion and taken an important part in making the article.

Paper II

In paper II we give a detailed description of the methodology we use for the KBE+MBPT approach, both for treating the ground state and the time dynamics for clusters, isolated and coupled to semi-infinite non-interacting leads. We study the spin-dependent treatment of GWA [1, 2] to decrease the self interaction [3, 4] and see that even if it does improve the results, the GWA is still much inferior to the TMA or the BA. We extract the corresponding TDDFT exchange-correlation potentials of the different approximations via reverse engineering [5] and compare them to the exact one. Similarly to the comparison of the time-dependent densities we see that the TMA exchange-correlation potential is superior to the other approximations. We examine the role of self-consistency in the ground-state spectral function and we observe the well known fact that the spectral properties in general are worsened by self-consistency [6, 7, 8]. We discuss the aspects of the correlation-induced damping for finite and extended systems, where we find that the damping is present in both cases and that it can completely dominate the time dynamics. We examine the history dependence of the steady state where we see that there exists multiple steady states when evolving a finite system while the extended system may present multiple long-lived metastable states.

For this paper I have produced the codes for the KBE+MBPT evolution, participated actively in the discussion and taken an important part in making the article.

Paper III

In paper III, which is an invited paper on a topical issue on TDDFT, we give a review of two aspects of TDDFT from the perspective of lattice model systems: the linear response approach and the adiabatic local density approximation. We present results for the density response function of the 3D homogeneous Hubbard model, and point out a drawback of the linear response scheme based on the linearised Sham-Schlüter equation. Finally we study a small cubic cluster with one interacting impurity under the influence of time-dependent fields by comparing the TDDFT+DMFT to the exact and KBE+MBPT densities. In particular we contrast the non-perturbative nature of TDDFT+DMFT to the history dependence of the KBE+MBPT. We conclude that the TDDFT+DMFT method is much more suited to describe strongly correlated systems while the KBE+MBPT approach is better in treating non adiabatic fields.

In this paper I performed the comparison of KBE+MBPT and TDDFT+DMFT. I produced the codes for the KBE+MBPT evolution, participated actively in the discussion and took a part in making the article.

Paper IV

In paper IV we propose a method of obtaining certain two-body correlations, in particular the double occupancy, from the KBE [9]. We assess the performance of the different approximations by comparing the approximate double occupancies with the exact ones and find that the TMA is very good in the low density regime. We show that the double occupancy may violate the positiveness condition [10] within the BA and the GWA while we prove that it is manifestly positive in the TMA. As an application we study the transmission of the local entanglement entropy [11, 12, 13, 14, 15, 16, 17, 18, 19, 20], calculated within an adiabatic formulation, through an interacting impurity contacted to two semi-infinite leads. We observe that the transmission of entanglement is suppressed by interactions and can be manipulated by a current.

For this paper I have produced the codes for the KBE+MBPT evolution, participated actively in the discussion and taken an important part in making the article.

Note on the numerical implementation

The numerical implementation of the KBE+MBPT evolution which is used in all the four articles is based on three codes that I have written from scratch. The first and second codes are devoted to the determination of the ground-state properties for clusters, isolated and coupled to semi-infinite leads. The third code performs the time evolution with the input from the two first codes.

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