Mean-field theory for the conserved charges in Richardson-Gaudin models

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Voorwoord

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Toelating tot bruikleen

Gemiddeld-veld theorie voor de behouden ladingen in Richardson-Gaudin modellen

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Samenvatting

In deze masterthesis worden twee benaderingstechnieken in de veeldeeltjesfysica bestudeerd en toegepast op de behouden ladingen van de BCS Hamiltoniaan. Deze Hamiltoniaan beschrijft attractieve paarinteracties in een fermionisch gas en is genoemd naar John Bardeen, Leon Neil Cooper and John Robert Schrieffer. In eerste instantie wordt de befaamde BCS-benadering toegepast op deze operatoren. Gaandeweg zal in deze thesis duidelijk worden dat deze techniek tekort schiet om alle behouden ladingen van het paringssysteem accuraat te behandelen door de aanwezigheid van repulsieve interacties. Bijgevolg wordt een extensie op de BCS-benadering geïntroduceerd die steunt op een equations-of-motion principe, gebaseerd op de bekende bewegingsvergelijking van Heisenberg in de kwantummechanica. Deze techniek blijkt een significante verbetering te zijn op conventionele BCS-theorie. Als laatste wordt een poging ondernomen om deze techniek toe te passen op het Heisenberg model, dat een keten van fermionische spins met dichtste-nabuur interactie beschrijft.

I. Introductie

De eigentoestanden van een Hamiltoniaan vinden kan een complex probleem zijn in de kwantumveeldeeltjesfysica. De computationele tijd voor het diagonaliseren van een Hamiltoniaan schaalt met de derde macht van de dimensie van zijn Hilbert ruimte, die op zijn beurt exponentieel schaalt met het aantal deeltjes in het systeem. Voor een aanzienlijk aantal deeltjes wordt dit een zeer inefficiënte methode. Bovendien heeft men vaak enkel interesse voor de grondtoestand en eerste geëxciteerde toestanden van een systeem en is de berekening van hoger gelegen toestanden overbodig. In deze thesis worden benaderingstechnieken toegepast op de behouden ladingen van de BCS Hamiltoniaan. Deze Hamiltoniaan beschrijft het fenomeen van Cooper-paring: fermionen oefenen een attractieve kracht uit op elkaar en groeperen zichzelf in spinloze quasideeltjes, Cooper paren genoemd. Deze quasi-bosonen zijn niet onderhevig aan het Pauli-principe en kunnen allen condenseren in de grondtoestand. In metalen geeft deze Cooper-condensatie aanleiding tot het exotische fenomeen van supergeleiding. Ook in atoomkernen blijkt er een sterke voorkeur te zijn voor Cooper-paring tussen nucleonen [1].

II. Integreerbaarheid

De BCS Hamiltoniaan kan gezien worden als een ***integreerbaar systeem*** [2]. Het concept van integreerbaarheid kan als volgt gedefinieerd worden: een Hamiltoniaan is integreerbaar als deze geschreven kan worden als een lineaire combinatie van n onderling commuterende operatoren, met n het aantal vrijheidsgraden van het systeem. Deze operatoren worden de ***behouden ladingen*** van het systeem genoemd. Door hun onderlinge commutatie delen ze een gemeenschappelijke basis van eigenvectoren en deze basis wordt ook gedeeld door de resulterende Hamiltoniaan. Iedere lineaire combinatie van deze ladingen definieert dan een integreerbaar systeem. De verzameling van alle integreerbare Hamiltonianen, voortgebracht door de behouden ladingen van de BCS Hamiltoniaan, worden *Richardson-Gaudin modellen* genoemd [2].

III. BCS theorie

In 1957 publiceerden John Bardeen, Leon Neil Cooper and John Robert Schrieffer een baanbrekende paper die een theoretische verklaring gaf voor supergeleiding in metalen [3]. In deze Nobelprijs-winnende paper werd de BCS Hamiltoniaan op een benaderende manier opgelost om zo de condensatie van Cooper-paren in de grondtoestand aan te tonen. Hun wiskundige aanpak steunde op het definiëren van een grondtoestand met variationele parameters. Op die manier werd het probleem gereduceerd tot een set van niet-lineaire vergelijkingen met als onbekenden de parameters van de golffunctie, de ***BCS-vergelijkingen*** genoemd. Deze ansatz voor de grondtoestand breekt de $U(1)$-symmetrie van deeltjesbehoud

in de Hamiltoniaan. Echter, BCS toonden aan dat deze fout verwaarloosbaar werd bij een groot aantal deeltjes. In deze thesis wordt de wiskundige machinerie van de BCS-theorie toegepast op de behouden ladingen. De gemodifieerde BCS-vergelijkingen worden afgeleid en er wordt aangetoond dat deze set vergelijkingen equivalent is voor iedere behouden lading in een paringssysteem. Dit betekent dat de behouden lading eenzelfde variationele golffunctie gemeenschappelijk hebben. Vervolgens wordt geïllustreerd dat deze eigenschap typisch blijkt te zijn voor de behouden ladingen en niet veralgemeend kan worden naar arbitraire commuterende operatoren. De gemeenschappelijke golffunctie voor het beschrijven van de grondtoestand van de behouden ladingen blijkt niet voor elke behouden lading accuraat te zijn. Dit kan gestaafd worden met volgende redenering: de behouden ladingen delen een gemeenschappelijke basis. Echter, de eigenvector die de grondtoestand van een bepaalde behouden lading beschrijft, is in het algemeen niet de eigenvector die de grondtoestand van de overige behouden ladingen beschrijft, maar eerder een geëxciteerde toestand. Hetzelfde fenomeen komt voor in de BCS-golffunctie: de variationele golffunctie die de grondtoestand van behouden lading 1 accuraat beschrijft, zal een geëxciteerde toestand van behouden lading 2 beschrijven, wat logischerwijze niet wenselijk is. Vervolgens wordt aangetoond dat het succes of falen van de BCS-beschrijving afhangt van het type behouden ladingen: deze operatoren kunnen op zichzelf geïnterpreteerd worden als paarsystemen waarvan de tekens van de paartermen kunnen verschillen. *Attractieve* en *repulsieve* interacties kunnen geïdentificeerd worden en de BCS-benadering blijkt te falen bij deze repulsieve interacties.

IV. Voorbij de BCS theorie

In een poging om deze repulsieve interacties te kunnen beschrijven wordt een ***equations-of-motion*** methode ontwikkeld in navolging van [4] en [5]. Deze methode is gebaseerd op het berekenen van de commutatierelaties van de Hamiltoniaan met de quasispin-operatoren. Deze vergelijkingen op operator-niveau kunnen dan geëvalueerd worden met een representatie van eigenkets en omgezet worden naar matrixvergelijkingen. Op die manier wordt het veeldeeltjesprobleem omgezet naar een set van niet-lineaire vergelijken waarbij de onbekende matrixelementen dienen bepaald te worden. De benadering zit hem nu in het feit dat de Hilbert ruimte van het probleem artificieel verkleind kan worden door een kleinere representatie van eigenkets te kiezen. Op die manier reduceert het aantal onbekende matrixelementen en niet-lineaire vergelijkingen. Er wordt aangetoond dat een volledige truncatie van de Hilbertruimte tot dimensie 1 aanleiding geeft tot de BCS-vergelijkingen in een zekere simplificatielimiet. Verder wordt geïllustreerd dat deze methode in staat is om de grondtoestand van repulsieve behouden ladingen accuraat te beschrijven en dus een aanzienlijk voordeel biedt ten opzichte van conventionele BCS theorie. In het laatste hoofdstuk wordt een poging gewaagd om met deze benaderingstechniek het Heisenberg model te beschrijven maar dit blijkt geen goede resultaten op te leveren. Er wordt een vermoeden naar voor geschoven dat het falen van deze methode te wijten is aan het onvermijdelijk breken van translationele invariantie die vervat zit in de Hamiltoniaan van het Heisenberg model.

V. Conclusie

In deze thesis worden de mathematische aspecten van BCS-theorie in detail besproken en deze worden toegepast op de behouden ladingen van de BCS Hamiltoniaan. De limieten van deze benaderingstechniek worden blootgelegd bij het toepassen op repulsieve behouden ladingen. De equations-of-motion techniek blijkt een gepaste benaderingstechniek te zijn om deze repulsieve interacties te kunnen beschrijven.

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Abstract

In this master dissertation two approximative solution schemes in quantum many-body pairing systems are discussed in detail: the famous BCS theory and a solution scheme that is based on the reduction of the dimension of the Hilbert space in an equations-of motion approach. The first approximation is named after their creators John Bardeen, Leon Neil Cooper and John Robert Schrieffer. The last solution scheme is seen to offer a distinct improvement compared to BCS theory and it is shown how both schemes are connected in a simplification limit. The schemes will be applied to the *constants of motions* or *conserved charges* of the BCS pairing Hamiltonian. These are a set of operators that commute internally and the BCS pairing Hamiltonian can be written as a linear combination of these conserved charges. A system that can be described with such a set of commuting operators is called *an integrable system*. The existence of conserved charges in a quantum pairing system offers a connection between R.W. Richardson's exact solution scheme of the BCS pairing Hamiltonian and a family of exactly-solvable spin models known as *Gaudin magnets*. An approximate study of the BCS conserved charges can be interesting because of the different physical interpretation of the conserved charges regarding attractive, mixed or repulsive pairing.

In the first chapter of this thesis, an introduction to the pairing problem is given together with a detailed study of the mathematical aspects of the BCS solution scheme. Bardeen, Cooper and Schrieffer received the 1972 Nobel Prize in Physics for this theory, originally meant to explain superconductivity in metals. In the second chapter, the pairing Hamiltonian is presented as an integrable system and the conserved charges are introduced, together with an exact solution scheme by means of a Bethe ansatz. In chapter 3, the BCS theory is applied to the conserved charges and the shortcomings of this scheme are discussed. In chapter 4 an improvement on BCS theory is presented following the footsteps of Alexander Volya, Vladimir Zelevinsky and Shen Yong Ho. In the last chapter, an attempt is made to apply this method to the Heisenberg spin chain model.

Keywords: BCS pairing Hamiltonian, integrable systems, Large Finite Quantum Many-Body Systems

Contents

List of abbreviations

BCS	Bardeen-Cooper-Schrieffer
COM	Constant of motion/conserved charge
RG	Richardson-Gaudin
irrep	Irreducible representation
UPF	Uncorrelated pair filling/Fermi sea
NR	Newton-Raphson
RPA	Random phase approximation
EOM	Equations of motion (approach)
SEOM	Symmetrized equations of motion
DMRG	Density matrix renormalization group method
MG	Majumdar-Ghosh

Chapter 1

The Pairing Hamiltonian and BCS theory

1.1 Fermion pairing: an introduction

The coupling of fermions into spin-zero states, also called Cooper pairs, plays a fundamental role in nuclear and condensed matter physics. The pairing mechanism lies at the base of superconductivity and superfluidity and a lot of experimental data illustrates the tendency of nucleons to pair. Consider for example the nucleus $^{210}_{84}\mathrm{Po}_{126}$. This nucleus contains 2 protons outside of the doubly closed shell[1]. When looking at the energy spectrum, one notices a preference for a $J^p = 0^+$-state as can be seen in Figure 1.1, thus illustrating the preference for Cooper pairing. If these valence protons wouldn't couple, the ground state would consist of a multiplet of states with various total spin possibilities [1]. At the base of these phenomena must lie an attractive force between the particles. In nuclear

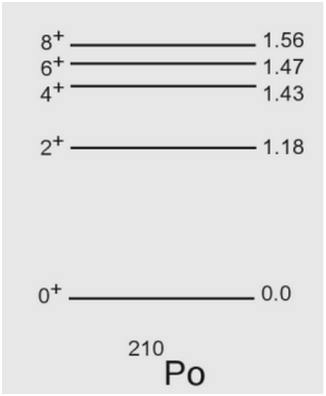


Figure 1.1: Schematic representation of the low-lying levels of ^{210}Po. The spin-parities (J^p) are given together with the level energies in MeV. Figure is taken from [1].

systems, this short-range interaction is created as a residual effect of the strong force. In superconductivity, this attractive interaction is not so obvious, as the Coulomb force between two electrons is repulsive. This apparent contradiction tortured the theoretical minds for almost 50 years after the experimental discovery of superconductivity. The answer came in 1957 when John Bardeen, Leon Neil Cooper and John Robert Schrieffer (BCS) proposed the following mechanism of attraction between electrons: an electron creates a disturbance of the positive lattice through the Coulomb force. The

[1] ^{208}Pb with its 82 protons and 126 neutrons is a so-called doubly magic nucleus.

local displacement of these ions is 'felt' by another electron, consequently creating an indirect (attractive) link between the 2 electrons. Mathematically this mechanism can be modelled as an effective electron-electron interaction mediated by the quanta of these lattice vibrations: the phonon. This interaction is referred to as the *Fröhlich interaction* [2]. The electrons are assumed to have opposite momentum vectors with the same magnitude. Later in this section, it will become clear why this assumption leads to spin-zero pairing. In their Nobel prize-winning paper [3], they showed that this interaction is indeed attractive at energies smaller than the characteristic phonon frequency ω_D. In this way, the attractive interaction can compete and in some cases overcome the Coulomb repulsion. A year before the BCS paper, Cooper already showed that an arbitrary weak net attractive force already gives rise to pairing so the only requirement for pairing is that the effective phonon interaction exceeds the Coulomb repulsion [4]. Because these Cooper pairs behave like bosons, they don't have to obey the Pauli principle and a condensation of a large fraction of the pairs into the same (ground)state is possible at low temperature. This can give rise to peculiar behaviour, as these bosons behave in a fully coherent manner. Indeed, a macroscopic boson condensate does not allow individual particles to change their direction suddenly due to impurities of the lattice or boundaries. This basically explains the zero resistance of a superconducting material: the boson condensate prevents individual particles from scattering and thus preventing any form of dissipation during electric flow.

As already stated, the massive condensation of these Cooper pairs into the ground state can only happen when the temperature is very low. This feature is due to one of the most fundamental concepts of quantum theory: the *De Broglie wavelength* of particles, which scales with the temperature as [5]

$$\lambda_{db} \propto T^{-\frac{1}{2}}. \tag{1.1}$$

At high temperature, the particles behave as classical billiard balls due to the fact that their wave length is much smaller than the average spacing between the particles and their wave character becomes rather unimportant. When the temperature decreases, the wave character becomes more and more important. At a certain temperature, called the *critical temperature* T_c, the De Broglie wavelength has become comparable to the average spacing between the bosons. Below that temperature, the system has more and more difficulty to scatter pairs in excited levels just by using the kinetic energy due to the temperature. Hence, the Cooper pairs start condensing into the ground state. At a temperature very close to zero, the De Broglie wavelength has become so large that the condensate can be described by the wave function of a single boson and all Cooper pairs are fully condensed. A graphical representation of this mechanism is given in Figure 1.2. A visualization of the condensation process can be seen in Figure 1.3. The Cooper pairs condense in a ground state that lies significantly lower than the Fermi surface. A superconducting Fermi gas can always be associated with a gap opening around the Fermi surface, denoted with the *Gap parameter* Δ. Because of the gap in the energy spectrum, excitations of these Cooper pairs can only occur with an energy of at least twice that gap. Thermally excited phonons with energy comparable to 2Δ will scatter the Cooper pair to states above the gap. The electrons from the scattered pair will no longer have equal and opposite momentum, so that eventually the Cooper pair is broken. The idea of Cooper pairing originally arose in the light of superconductive metals but can be extended towards nuclei as stated in the beginning with a brief discussion of the ${}^{210}_{84}\mathrm{Po}_{126}$-nucleus. Shortly after the BCS paper A. Bohr, R. Mottelson and D. Pines suggested a resemblance between the excitation spectra of nuclei and a superconducting metallic state [8]. With some simple arguments, they showed that (Cooper) pairing appears to be an important feature in nuclei. Their reasoning was as follows: In first order, a nucleus can be interpreted as a non-interacting gas of nucleons moving inside a nuclear potential well. This approximation is often referred to as *the Fermi gas model* and is discussed in detail in [7]. In [8], it was stated that the

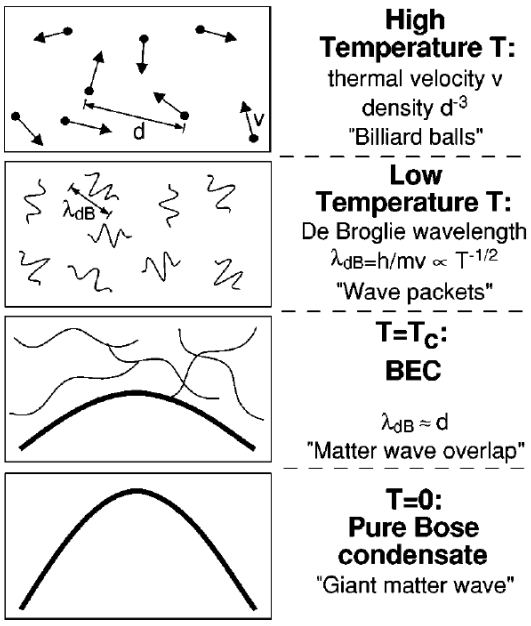


Figure 1.2: Depiction of different temperature regions in a boson gas and the forming of a Bose-Einstein condensate (BEC) at the critical temperature $T = T_c$. The figure is taken from [6]

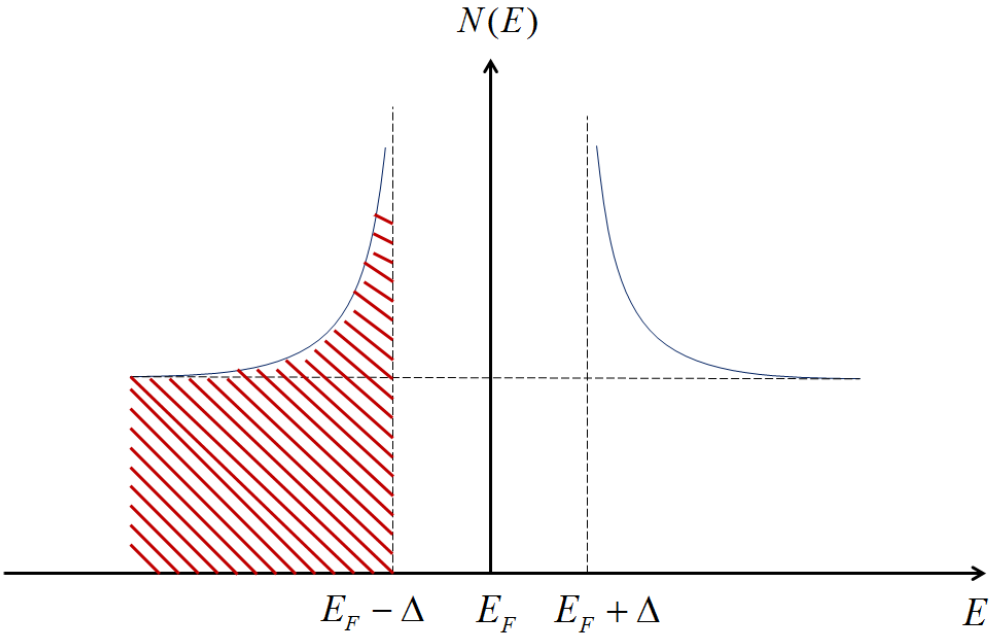


Figure 1.3: Schematic representation of the gap opening 2Δ around the Fermi energy (E_F) in a superconducting or superfluid Fermi gas with a temperature below T_c. The shaded area represents the occupied states. On the y-axis the electron density is given.

single-particle energy spacing δ in a nucleus spectrum is given by

$$\delta = \frac{50}{A}\text{MeV}, \tag{1.2}$$

with A the nucleon number. If nuclei could indeed be accurately described by independent particle motion of the nucleons, one would expect the excitations in the spectrum to have a magnitude of order δ. However, empirical data suggested an excitation of about 1 MeV for heavy even-even nuclei, which is a lot larger than suggested. The data is summarized in Figure 1.4. Such an energy gap

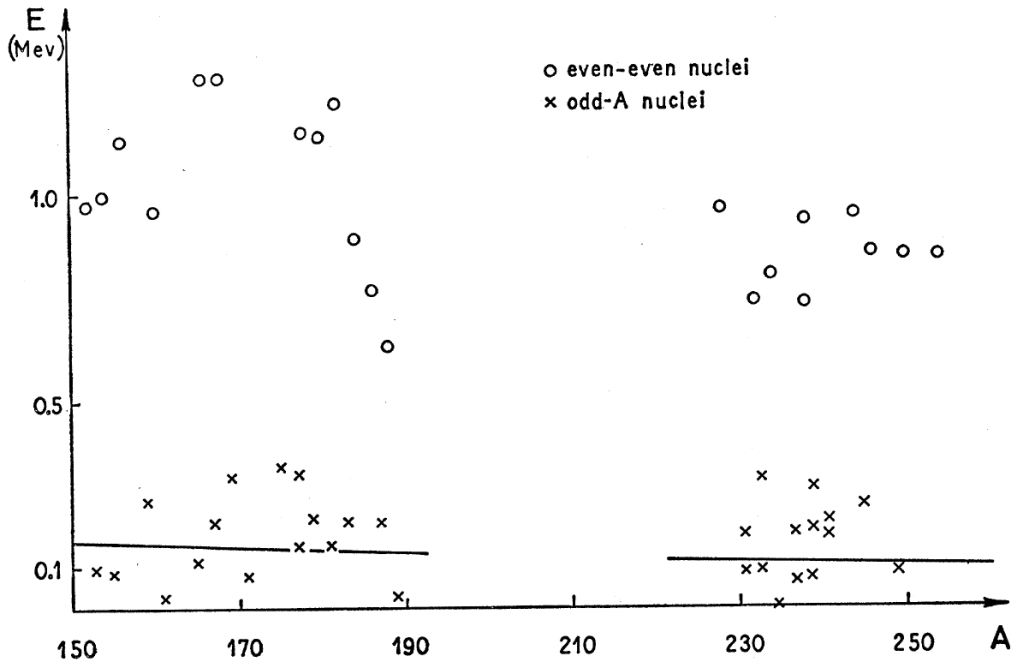


Figure 1.4: Energies of the first excited states in deformed nuclei. It was established that these nuclei have a non-spherical equilibrium shape. Similar spectra are also observed in spherical nuclei. The solid line represents the quantity $\delta/2$. The figure is taken from [8].

opening between the single-particle levels indicates a departure from the free Fermi gas model, due to the residual attracting forces acting between the nucleons. To lowest order, this can be approximated by two-particle interactions, giving rise to the pairing effect. To this point, it is clear that nucleons tend to pair together, but these Cooper pairs dont necessarily have to condense into the absolute ground state. After all, there is no prior knowledge of the nuclear temperature and its disordering feature can throw a spanner in the works. If there is no condensation of Cooper pairs, these bosons behave as individual particles and the excitation of 2 particles remaining as a pair would still have an energy spacing of about δ. These low-lying excitation bands are not observed and strongly indicate the collective feature of these bosons.

The presumption of a superfluid-like nucleus is also able to explain the famous *odd-even effect*. Experiment has established an empirical relation between the nuclear mass M_A of an odd nucleus with atomic number A and its two neighbouring even-even nuclei [9]:

$$M_A = \frac{1}{2}\left(M_{A-1} + M_{A+1}\right) + \Delta/c^2, \tag{1.3}$$

with Δ a certain empirical parameter. After applying the mathematical machinery of BCS theory on nuclei, it turns out that Δ corresponds to a pairing gap related with Cooper pairing, just like in the case of a superconductor. Nowadays, nucleon pairing is considered to be widespread in nature and can, for example, be found in neutron stars where a large portion of the crust and inner part is in a

superfluid state [10].

After this brief motivation of the importance of pairing in nature, it is now time to introduce the mathematical concepts related to the pairing problem. Mathematically, the angular momentum-coupling of two particles to a singlet state can be written down by means of a linear combination of direct products of spin states weighted with the appropriate Clebsch-Gordan coefficients:

$$|J=0,M=0\rangle = \sum_m \frac{(-1)^{j-m}}{\sqrt{2j+1}} \; |jm\rangle \otimes |j,-m\rangle \,. \tag{1.4}$$

The symbols j and m respectively denote the principal and magnetic quantum number of the spin state. The time reversal operator can now be introduced as

$$\mathcal{T} =: Ke^{-i\pi S_y/\bar{h}}, \tag{1.5}$$

where K is the complex conjugation operator and the second factor denotes a rotation of π around the y-axis [11]. In this thesis the time reverse of a spin state will always be denoted with the bar notation $|j\bar{m}\rangle$. It can now be proven that this operator sends the wave function $\psi(t,\vec{x}) \to \psi(-t,\vec{x})$, hence justifying the name 'time reversal' operator. After Fourier transforming the wave function to the momentum space, this corresponds to $a_{\mathbf{p}} \to a_{\mathbf{-p}}$. With the choice of the right phase convention of the spherical harmonics, as discussed in [12], it can be shown that the time reversal of a $|jm\rangle$-state ultimately can be written as:

$$|j\bar{m}\rangle = (-1)^{j+m} \, |j,-m\rangle \,. \tag{1.6}$$

Note that for fermions, with this convention, $|j\bar{\bar{m}}\rangle = -\,|jm\rangle$. Consequently, the Cooper pair (1.4) can be written as a sum of direct products of states with their time reversed state, up to a normalisation factor. Because of the effect of time-reversal in momentum space, it is now clear why the fermions of a Cooper pair have opposite momentum vectors. A classical reasoning can now be given to understand why there is a preference for $J=0$ states in systems with attractive forces [12]: if 2 fermions are in a $J=0$ state, a spherical density distribution is created where the particles can come close together, which is preferable if there's an attractive force between them. Indeed, if 2 particles travel in time-reversed orbits, they encounter each other twice in every orbit. Consequently, they frequently scatter in new time-reversed orbits, creating a spherical density distribution.

Employing the second-quantization formalism, as discussed in detail in [13], the pairing problem can be modelled as the following Hamiltonian, often called the ***BCS pairing Hamiltonian***:

$$\hat{H} = \sum_{jm} \epsilon_j a^\dagger_{jm} a_{jm} + \frac{1}{4} \sum_{jj'mm'} V_{jj'} (-)^{j+j'+m+m'} a^\dagger_{jm} a^\dagger_{j-m} a_{j'm'} a_{j'-m'}, \tag{1.7}$$

with a_{jm} and $a^\dagger_{jm}$ respectively the fermion annihilation and creation operators of a $|jm\rangle$-level with the standard anticommutation relations

$$\{a_{jm}, a^\dagger_{j'm'}\} = \delta_{jj'}\delta_{mm'}. \tag{1.8}$$

The symbols ϵ_j denote the single-particle energies and the first term simply counts the number of fermions in each level, weighted with its energy value. The second term denotes the Cooper pairing as one can recognize the Clebsch-Gordan coefficient of (1.4). The symmetric matrix $V_{jj'}$ is referred to as the interaction matrix[2]. The quantum numbers $|jm\rangle$ can be denoted with a single Greek letter $|\mu\rangle$ to

[2]The symmetry of the interaction matrix ensures hermiticity of the Hamiltonian.

ease notation. In this way, the second-quantization operators become $a^\dagger_{jm} \equiv a^\dagger_\mu$. With this notation, the Hamiltonian can be written more formally as

$$H = \sum_\nu \epsilon_\nu a^\dagger_\nu a_\nu - \sum_{\mu,\nu>0} G_{\mu\nu} a^\dagger_\mu a^\dagger_{\bar{\mu}} a_{\bar{\nu}} a_\nu. \tag{1.9}$$

Here, the interaction matrix is generalized so that the matrix elements have the possibility to also depend on the magnetic quantum numbers. In most cases, however, they are not. The same holds for the single-particle energies. The time-reversed state notation (1.6) is used and the notation $\mu, \nu > 0$ indicates that the sum only goes over the magnetic quantum numbers that are positive, thus incorporating the factor 1/4. This comes down to summing once over each time reversed pair. This Hamiltonian can be rewritten in terms of generalized pair operators S, $S^\dagger$ and S^0, which will be done in section 2.1. $S^\dagger_j$ simply creates a Cooper pair in the j'th energy level, up to a normalisation constant. If all matrix elements $G_{\mu\nu} > 0$, one can now easily see that it is energetically advantageous to make the number of pairs very large. The ground state will then consist of a condensate of these pairs:

$$|GS\rangle \propto (S^\dagger)^{N/2} |\theta\rangle , \tag{1.10}$$

with N the number of particles and $|\theta\rangle$ the vacuum state. It is easy to show that the particle-number operator[3] commutes with the pairing Hamiltonian so that particle number is a conserved quantity of the eigenstates. However, when a macroscopic occupation occurs in the ground state due to condensation of a large number of particles, it makes sense to give up particle number conservation and work in the grand canonical ensemble [13]. Indeed, it will turn out that a variational ground-state ansatz that breaks particle-number symmetry will offer a great approximation to the ground state and this ansatz becomes exact in the limit $N \to \infty$. This is in a nutshell how BCS theory works, which will be discussed in detail in the next section. The theory will be formulated more in the light of nuclear systems, though it was first created as part of a (successful) attempt to explain superconductivity in metals.

1.2 BCS theory

1.2.1 General considerations

In 1957, Bardeen, Cooper and Schrieffer solved the pairing problem in an approximate manner, consequently proving the existence of a superconducting state, lying lower in energy than the Fermi sea [3]. They proposed the following variational ansatz for an eigenstate which will be referred to as the BCS vacuum, denoted by $|\tilde{0}\rangle$:

$$|\tilde{0}\rangle =: \prod_{\nu>0} \left(u_\nu + v_\nu a^\dagger_\nu a^\dagger_{\tilde{\nu}} \right) |\theta\rangle , \tag{1.11}$$

with the real parameters u and v yet to be determined. One can easily see that this ansatz consists of a superposition of states of different particle number. With the help of the Pauli principle and the Taylor expansion of e^x, this ansatz can also be written in the following form:

$$|\tilde{0}\rangle \propto \exp\left(\sum_{\nu>0} \frac{v_\nu}{u_\nu} a^\dagger_\nu a^\dagger_{\bar{\nu}} \right) |\theta\rangle . \tag{1.12}$$

The convenience of this ansatz will become clear if the parameters are defined as coefficients of a unitary transformation on the creation/annihilation operators. This is referred to as a ***Bogoliubov***

[3]This operator will be formally introduced in the next section.

transformation:

$$\begin{aligned} a_\mu &= u_\mu c_\mu + v_\mu c_{\bar{\mu}}^\dagger \\ a_\mu^\dagger &= u_\mu c_\mu^\dagger + v_\mu c_{\bar{\mu}} \\ a_{\bar{\mu}} &= -v_\mu c_\mu^\dagger + u_\mu c_{\bar{\mu}} \\ a_{\bar{\mu}}^\dagger &= -v_\mu c_\mu + u_\mu c_{\bar{\mu}}^\dagger. \end{aligned} \tag{1.13}$$

The unitarity of the transformation results in the identity $|u_\mu|^2 + |v_\mu|^2 = 1$ and the fact that these parameters are always smaller than 1. In this way, new fermion operators are created and these will be referred to as *quasiparticle operators*. It is left to the reader to check that these operators indeed satisfy the fermion anticommutation relations (1.8). In (1.13), the property $a_{\bar{\mu}} = -a_\mu$ is used as already stated in the introduction. The BCS vacuum now has the interesting property that the quasiparticle annihilation operator destroys it:

$$c_\mu \left|\tilde{0}\right\rangle = 0, \tag{1.14}$$

hence verifying the interpretation of $|\tilde{0}\rangle$ as a vacuum state for the quasiparticles. Above identity can be proven by making use of the Baker-Campbell-Hausdorff identity [1].

The BCS Hamiltonian can be written in terms of these quasiparticle operators and the u, v parameters by performing the unitary transformation. Next, the Wick theorem can be applied to the Hamiltonian with respect to the BCS vacuum. The Wick theorem, given without proof, can be formulated as follows [13]:

Theorem 1. *(Wick) A product of a number of particle operators can be written as the sum of all normal ordered products, formed by applying every possible contraction on all possible pairs of operators:*

$$\begin{aligned} abc...yz =& N[abc...yz] + N[\overbrace{ab}^{\square}c...yz] + N[\overbrace{abc}^{\square}...yz] + ... + N[\overbrace{ab}^{\square}c...\overbrace{yz}^{\square}] + ... \\ &= N[abc...yz] + N[\textit{sum over all possible contractions}]. \end{aligned} \tag{1.15}$$

The *normal ordering* of a product of operators with respect to a vacuum $|\tilde{0}\rangle$ is defined as the ordering where all creation operators are to the left of the annihilation operators, so that $\langle\tilde{0}| N[abc...yz] |\tilde{0}\rangle = 0$. One has to bear in mind that normal ordering results in possible sign changes because of the anticommutation properties of fermions. The *contraction* of operators is nothing more than the evaluation of these operators with respect to the vacuum state: $\overbrace{ab}^{\square} =: \langle\tilde{0}| ab |\tilde{0}\rangle$.

After some calculus, the Hamiltonian (1.7) takes the following form

$$\begin{aligned} H &= U_0 + H_{11} + H_{20} + V_{\text{res}} \\ U_0 &= \sum_{\nu>0} \left[2\epsilon_\nu v_\nu^2 - G_{\nu\nu} v_\nu^4\right] - \sum_{\mu,\nu>0} G_{\mu\nu} u_\nu v_\nu u_\mu v_\mu \\ H_{11} &\propto c^\dagger c \\ H_{20} &\propto c^\dagger c^\dagger + cc \\ V_{\text{res}} \equiv H_{22} &\propto c^\dagger c^\dagger c^\dagger c^\dagger + c^\dagger c^\dagger c^\dagger c + c^\dagger c^\dagger cc + h.c.\,. \end{aligned} \tag{1.16}$$

At this point, the exact expression of the terms besides the fully contracted U_0-term are not important yet. U_0 can now be minimized with respect to the parameters. This can be done with the constraint

that the average particle number of the BCS vacuum equals the real particle number, denoted by $\bar{n}$: $\langle\tilde{0}|\,\hat{n}\,|\tilde{0}\rangle = \bar{n}$ with the *number operator* defined as

$$\hat{n} = \sum_{\mu} a_{\mu}^{\dagger} a_{\mu}. \tag{1.17}$$

A Lagrange multiplier λ now has to be introduced and the altered Hamiltonian $\mathcal{H} =: H - \lambda(\hat{n} - \bar{n})$ can be minimized. This corresponds to shifting all single-particle energies $\epsilon_\nu \to \epsilon_\nu - \lambda$ that occur in the Bogoliubov-rotated Hamiltonian (1.16). After the determination of the Bogoliubov parameters, one has to remember to add the term $\lambda\bar{n}$ to the ground-state expression U_0. The number constraint in the variational problem means that the altered Hamiltonian has to be minimal for the correct average particle number i.e. the derivative with respect to n has to vanish for $n = \bar{n}$. This gives rise to the interpretation of the Lagrange multiplier as a chemical potential:

$$\lambda = \frac{\partial}{\partial n} \langle\tilde{0}|\, H\, |\tilde{0}\rangle_{n=\bar{n}}\,. \tag{1.18}$$

Differentiating the ground state energy with respect to v_ν and taking into account the unitarity condition

$$|u_\nu|^2 + |v_\nu|^2 = 1 \Rightarrow \frac{du_\nu}{dv_\nu} = \frac{d\sqrt{1-v_\nu^2}}{dv_\nu} = -\frac{v_\nu}{u_\nu}, \tag{1.19}$$

this eventually leads to the famous ***BCS equations*** [3]:

$$2(\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda)u_\nu v_\nu = \Delta_\nu(u_\nu^2 - v_\nu^2), \qquad \forall\nu, \tag{1.20}$$

with the *gap parameters* defined as

$$\Delta_\nu =: \sum_{\mu>0} G_{\mu\nu}u_\mu v_\mu. \tag{1.21}$$

In general, these non-linear equations have no analytic solution and have to be solved in a numerical and iterative way with, for example, the *Newton-Raphson method (NR)*. This standard method for solving non-linear equations is briefly discussed in Appendix A. The solving process has to be done together with the extra number equation fixing the chemical potential: $\langle\tilde{0}|\,\hat{n}\,|\tilde{0}\rangle = \bar{n}$. With the help of (1.13), the expression of the number operator (1.17) and the property of quasiparticle annihilation operators (1.14) one can obtain for this expression:

$$2\sum_{\nu>0} v_\nu^2 = \bar{n}. \tag{1.22}$$

By now it should be clear why these transformation parameters are often referred to as *occupation amplitudes*: The square of these amplitudes v_μ^2 equals the probability of occupation of the quantum state $|\mu\rangle$. This is a consequence of the following equality:

$$\langle\tilde{0}|\, a_\mu^{\dagger} a_\mu\, |\tilde{0}\rangle = v_\mu^2, \tag{1.23}$$

which is again obtained after rotating to the quasiparticle basis with (1.13) and using the property (1.14). One can now check that the following iterative expressions obey (1.20) provided that the gap parameters are positive quantities:

$$\begin{aligned} u_\nu^2 &= \frac{1}{2}\left[1 + \frac{\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda}{[(\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda)^2 + \Delta_\nu^2]^{1/2}}\right] \\ v_\nu^2 &= \frac{1}{2}\left[1 - \frac{\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda}{[(\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda)^2 + \Delta_\nu^2]^{1/2}}\right]. \end{aligned} \tag{1.24}$$

Since the interaction matrix was defined positive and the u, v-parameters can also assumed to be positive quantities, the gap parameters are indeed always positive. A detailed discussion of the sign of the parameters will be given in section 3.4. Also, the following useful relationship can be easily checked:

$$u_\nu^2 v_\nu^2 = \frac{\Delta_\nu^2}{4\left[(\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda)^2 + \Delta_\nu^2\right]}. \tag{1.25}$$

Inserting this equation in (1.21) results in the famous *Gap equations*:

$$\Delta_\mu = \sum_{\nu>0} G_{\mu\nu} \frac{\Delta_\nu}{2\left[(\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda)^2 + \Delta_\nu^2\right]^{\frac{1}{2}}}, \qquad \forall \mu. \tag{1.26}$$

With the help of these expressions, the other terms of the Hamiltonian can now be written in terms of Δ, ϵ, G. After some calculus, the single-quasiparticle term can be calculated to be:

$$H_{11} = \sum_{\nu>0} \left[(\epsilon_\nu - G_{\nu\nu}v_\nu^2 - \lambda)^2 + \Delta_\nu^2\right]^{1/2} (c_\nu^\dagger c_\nu + c_{\bar{\nu}}^\dagger c_{\bar{\nu}}). \tag{1.27}$$

When calculating the H_{20} term, it quickly becomes visible that the BCS equations (1.20) appear in its coefficient so this term always vanishes when working in the minimized ground state. This can also be proven formally by making use of the Thouless theorem, here given without proof [14]:

Theorem 2. *(Thouless) Suppose that $|\tilde{0}\rangle$ is a general (quasi)particle vacuum. This means that there exists a set of annihilation operators c_ν that destroy the vacuum:*

$$c_\nu |\tilde{0}\rangle = 0, \qquad \forall\ \nu. \tag{1.28}$$

Then any other quasiparticle vacuum $|\tilde{0}\rangle'$, not orthogonal to $|\tilde{0}\rangle$ can be expressed as

$$\begin{aligned} |\tilde{0}\rangle' &= \exp\left[\frac{1}{2}\sum_{\mu\nu} C_{\mu\nu} c_\mu^\dagger c_\nu^\dagger\right] |\tilde{0}\rangle \\ &= \left[1 + \frac{1}{2}\sum_{\mu\nu} C_{\mu\nu} c_\mu^\dagger c_\nu^\dagger + ...\right] |\tilde{0}\rangle\,, \end{aligned} \tag{1.29}$$

where the coefficient matrix C is uniquely determined.

If we now define $|\tilde{0}\rangle'$ as a small deformation (or variation) of $|\tilde{0}\rangle$, i.e. $|\tilde{0}\rangle' =: (1+\delta)|\tilde{0}\rangle$, we get in first order

$$\delta |\tilde{0}\rangle = \frac{1}{2}\sum_{\mu\nu} C_{\mu\nu} c_\mu^\dagger c_\nu^\dagger |\tilde{0}\rangle\,. \tag{1.30}$$

We can now vary the expectation value of the Bogoliubov-transformed Hamiltonian and demand that this expression equals zero. This is equivalent with variating the ground state energy with respect to the amplitude parameters.

$$\delta \langle\tilde{0}| H |\tilde{0}\rangle \propto \langle\tilde{0}| c_\mu c_\nu H |\tilde{0}\rangle + \langle\tilde{0}| H c_\mu^\dagger c_\nu^\dagger |\tilde{0}\rangle = 0. \tag{1.31}$$

Because the Hamiltonian is a Hermitian operator, this results in

$$\langle\tilde{0}| c_\mu c_\nu H |\tilde{0}\rangle = 0, \qquad \forall \mu, \nu. \tag{1.32}$$

This can only be true if the coefficient of $(H_{02}+H_{20})$ is identically zero. This means that minimizing the ground state energy with respect to the amplitudes always results in the vanishing of the $(H_{02}+H_{20})$-term.
Quasiparticle excitations can now be described by states $c_\mu^\dagger |\tilde{0}\rangle$. In addition to the ground state energy an extra term contributes to the total energy:

$$E_{11}^\mu = \left[(\epsilon_\mu - G_{\mu\mu}v_\mu^2 - \lambda)^2 + \Delta_\mu^2\right]^{1/2}. \tag{1.33}$$

This can be used to model an odd-particle system with 1 orbital blocked by a particle (or equivalently a quasiparticle) that doesn't participate in the pairing process. This is called a *seniority-1* state[4]. The odd-even effect in nucleons (1.3) can be explained by means of quasiparticle excitations as shown in [9]. The derivation of this will not be done in this thesis as it is very well described in chapter 13 of [9]. When investigating pair excitations of an even-particle system, states with 2 quasiparticle excitations have to be considered on top of the BCS vacuum. As a consequence, additional corrections will have to be taken into account from the residual interaction term H_{22}. The derivation of this term will not be given here as the exact form of H_{22} is not relevant for this thesis.

The BCS equations always contain the trivial solution

$$\Delta_\nu = 0, \qquad \forall\nu. \tag{1.34}$$

This corresponds to $u_\nu, v_\nu = 0, 1$ which is equivalent to the normal non-interacting Fermion filling of the levels, i.e. a sharp Fermi distribution. Therefore, the gap parameters take on the role of order parameters, signalling a superconducting solution when a gap $\Delta_\nu \neq 0$. Indeed, when a non-trivial solution $\{v\}$ exist, this state lies lower in energy than the Fermi sea, thus favouring the condensation of fermions into Cooper pairs. An intuitive physical interpretation can now be given for the gap parameter:

Gap parameter

The gap parameters not only describes the strength of a pair, but also the strength of the whole condensate. When exciting a pair, this corresponds to the excitation of 2 quasiparticles. This results in an excitation energy of 2 single-quasiparticle energy corrections (1.33) and an extra energy contribution of the residual term:

$$E_{\text{pair}} = E_{11}^\mu + E_{11}^\nu + E_{22}^{\mu\nu} \geq 2\Delta_{\text{smallest}}. \tag{1.35}$$

The value $2\Delta_{\text{smallest}}$ is precisely the gap opening around the Fermi surface that is so typical for superconductivity. The reader is referred back to Figure 1.3 where the gap opening is illustrated. In the figure, a unique gap parameter is depicted that is not level-dependent. This is the case if the interaction matrix is set to a constant. Then the gap equations (1.26) reduce to

$$\frac{1}{G} = \sum_{\nu>0} \frac{1}{2\left[(\epsilon_\nu - Gv_\nu^2 - \lambda)^2 + \Delta^2\right]^{\frac{1}{2}}}. \tag{1.36}$$

Temperature dependence

So far, temperature dependence has been neglected and it was implicitly assumed that $T = 0\,K$. If a temperature dependence is introduced and a constant interaction matrix is considered, a very famous

[4]The concept of seniority will be formally introduced as a quantum number in section 2.1.

result of conventional superconductivity in metals is obtained, relating the critical temperature T_c to the characteristic Debeye frequency ω_D, introduced in section 1.1:

$$kT_c \approx 1.14\hbar\omega_D e^{-\frac{1}{N(0)G}}, \tag{1.37}$$

with $\hbar$ the reduced Planck constant and $N(0)$ the electron density on the Fermi level. This means that the critical temperature for a conventional superconductor can be estimated by means of a few material-dependent parameters. A derivation of this formula is given in Appendix B.

Particle-number fluctuation

The error made in the BCS approximation is the spread in particle number in the BCS vacuum, which can be quantified by deriving an expression for the spread $(\Delta n)^2$ [9]:

$$(\Delta n)^2 =: \langle\tilde{0}| (\hat{n} - \bar{n})^2 |\tilde{0}\rangle . \tag{1.38}$$

Using the fact that

$$\hat{n} |\tilde{0}\rangle = \sum_\alpha a_\alpha^\dagger a_\alpha |\tilde{0}\rangle = \left[\sum_{\mu>0} v_\mu^2 (c_\mu c_\mu^\dagger + c_{\bar{\mu}} c_{\bar{\mu}}^\dagger) + u_\mu v_\mu (c_\mu^\dagger c_{\bar{\mu}}^\dagger - c_{\bar{\mu}}^\dagger c_\mu^\dagger)\right] |\tilde{0}\rangle , \tag{1.39}$$

we obtain after some calculation

$$(\Delta n)^2 = 4 \sum_{\mu>0} u_\mu^2 v_\mu^2 \langle\tilde{0}| c_{\bar{\mu}} c_\mu c_\mu^\dagger c_{\bar{\mu}}^\dagger |\tilde{0}\rangle . \tag{1.40}$$

Since the quasiparticle operators are normalized, the last factor is simply unity. It's not difficult to see that this expression scales linearly with the number of particles and not with a higher exponent: due to the unitarity condition on the coefficients we get

$$(\Delta n)^2 = 4 \sum_{\mu>0} u_\mu^2 v_\mu^2 = 4 \sum_{\mu>0} (1 - v_\mu^2) v_\mu^2 = 4 \sum_{\mu>0} v_\mu^2 - 4 \sum_{\mu>0} v_\mu^4 \propto n. \tag{1.41}$$

For the last proportionality, we made use of (1.22) and the fact that $v^4 < v^2$ since the amplitudes v are considered to be smaller than unity. As a result, the relative error $\frac{(\Delta n)^2}{n^2}$ scales as $\frac{1}{n}$ so the BCS approximation becomes exact in the limit where the number of particles becomes very large.

1.2.2 Dependence on the magnetic quantum number

So far, all the quantities involved in the pairing system received a magnetic quantum-number dependence through the use of the Greek symbol notation $|\mu\rangle$ instead of $|jm\rangle$. However, in a lot of situations the single-particle energies and interaction matrix elements are independent of the magnetic quantum number. In that case, the $2j + 1$ quantum states of the energy level with angular momentum j are degenerate. Because of this, it is obvious that the occupation probabilities in a j-level will be equal for every quantum state. As a result, the amplitudes will only depend on the principal quantum number, i.e. $v_\mu \equiv v_j$. So in practice, it suffices to define the Bogoliubov transformation as follows:

$$\begin{aligned} a_{im} &= u_i c_{im} + v_i c_{i\bar{m}}^\dagger \\ a_{im}^\dagger &= u_i c_{im}^\dagger + v_i c_{i\bar{m}} \\ a_{i\bar{m}} &= -v_i c_{im}^\dagger + u_i c_{i\bar{m}} \\ a_{i\bar{m}}^\dagger &= -v_i c_{im} + u_i c_{i\bar{m}}^\dagger . \end{aligned} \tag{1.42}$$

As a consequence, the gap parameter of the j'th energy level takes the form of

$$\Delta_j = \sum_k \Omega_k G_{kj} u_k v_k, \tag{1.43}$$

with $\Omega_k = k + 1/2$, the pair degeneracy of the j'th level. This symbol denotes the number of time-reversed pair orbitals in an energy level, or equivalently, the maximum number of pairs that can occupy the energy level. In literature, the degeneracy is often defined as $2k + 1$. Throughout this thesis the definition $\Omega_j = k + 1/2$ will always be used unless explicitly stated otherwise. The number equation now takes the form of

$$2\sum_j \Omega_j v_j^2 = n. \tag{1.44}$$

It is now obvious that v_j^2 represents the fractional occupation of the j'th energy level. In Figure 1.5 a schematic representation of the occupation probabilities of a 6-level model with degeneracies $\Omega = 1$ is shown to give some insight in the behaviour of these occupation probabilities.

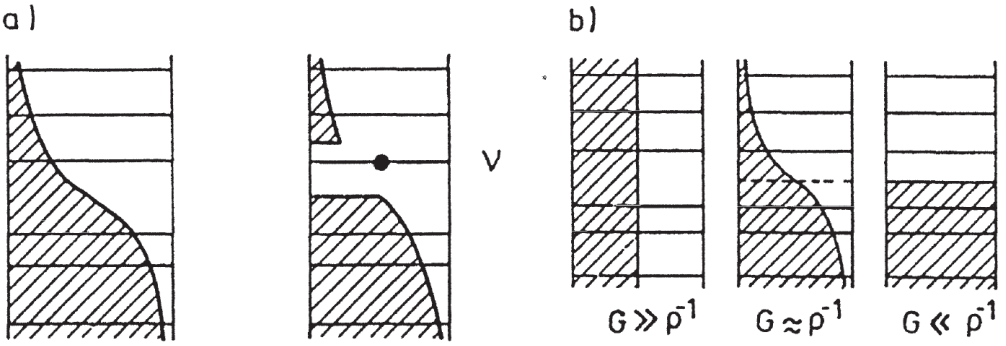


Figure 1.5: Graphical representation of the occupation probabilities of each level in a 6-level model with degeneracies $\Omega = 1$. (horizontal lines). The amount of shaded area on a level/line represents the procentual occupation of that energy level. (a): Probability distribution of the BCS ground state (left-hand side) and of a one-quasiparticle excitation in the orbital indicated by ν (right-hand side). Since no pair can occupy this level any more, the occupation probability predicted by BCS is zero. (b): Probability distribution for different ratios of the pairing strength G to the average distance between the single-particle levels ρ^{-1}. For $G \ll \rho^{-1}$, the pairing interaction is relatively unimportant and the typical fermion filling up to the Fermi level becomes visible. For $G \gg \rho^{-1}$, the single-particle level spacing becomes insignificant and an almost constant occupation for all levels is obtained. The figure is taken from [15].

1.2.3 The Lipkin model

In order to obtain some insight in the behaviour of the BCS approximation, a special case of a 2-level model with constant pairing strength will now be considered where the BCS equations are analytically solvable. The pairing Hamiltonian for 2 levels and a constant interaction matrix takes the following form:

$$H = \epsilon_1 \hat{n}_1 + \epsilon_2 \hat{n}_2 - G \sum_{jj'} \sum_{mm'>0} \left(a^\dagger_{jm} a^\dagger_{j\bar{m}} a_{j'\bar{m}'} a_{j'm'} \right), \tag{1.45}$$

where the summation indices j, j' take on the values $1, 2$. Indices m (m') represent the sum over all positive magnetic quantum numbers of energy level j (j'). The constant interaction strength G

is considered positive. We will consider 2 shells with angular momentum l, energy values $\pm\frac{1}{2}\epsilon$ and degeneracies $\Omega_1 = \Omega_2 = l + \frac{1}{2}$. The Lipkin model [9] is now defined as the system where the number of particles equals $n = 2\Omega$. Thus, in the non-interacting particle system, the lowest lying shell is completely filled. To organize the thoughts, a graphical representation of a possible quantum-state filling is of the Lipkin model with $\Omega = 4$ is given in Figure 1.6.

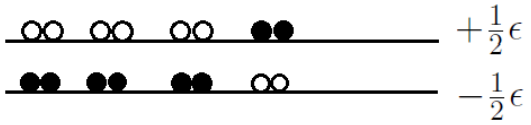


Figure 1.6: Schematic representation of the Lipkin model with $\Omega = 4$. 4 pairs are distributed along the orbitals of the 2 levels. This configuration is one of many possible ways the particles can be distributed over the orbitals. All possible configurations, accompanied with the right weight factors, result in a probability distribution described by v_1^2 and v_2^2.

The particle-number constraint (1.22) now results in

$$v_1^2 + v_2^2 = 1. \tag{1.46}$$

Together with the unitarity conditions $u_i^2 + v_i^2 = 1$ for $i = 1, 2$, this results in the following symmetry:

$$v_1^2 = u_2^2, \qquad v_2^2 = u_1^2. \tag{1.47}$$

Assuming the coefficients to be real and positive[5], we get

$$v_1 = u_2, \qquad v_2 = u_1. \tag{1.48}$$

This symmetry simplifies matters, as the equations are now easily solved. After some calculation, the solutions are given by [9]

$$\begin{aligned} \lambda &= -\frac{3}{4}G \\ v_1^2 &= \frac{1}{2}\left[1 + \frac{1}{x}\right] \\ \Delta &= \Omega G\sqrt{1 - \frac{1}{x^2}} \\ x &= \frac{4\Omega - 1}{2}\frac{G}{\epsilon}. \end{aligned} \tag{1.49}$$

Due to the requirement that the expression under the root in the gap expression has to be positive, it can be seen that a non-trivial BCS solution only exists for an interaction strength above the critical value

$$G_{cr} = \frac{2\epsilon}{4\Omega - 1}, \tag{1.50}$$

denoting a *BCS phase transition* with the gap as order parameter. The gap parameter in function of the variable x is shown in Figure 1.7. It is important to note that this phase transition, i.e.

[5]This will be discussed in detail in section 3.5.

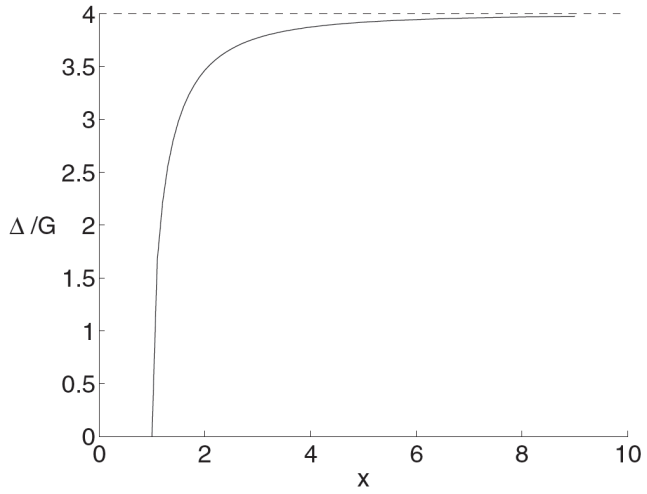
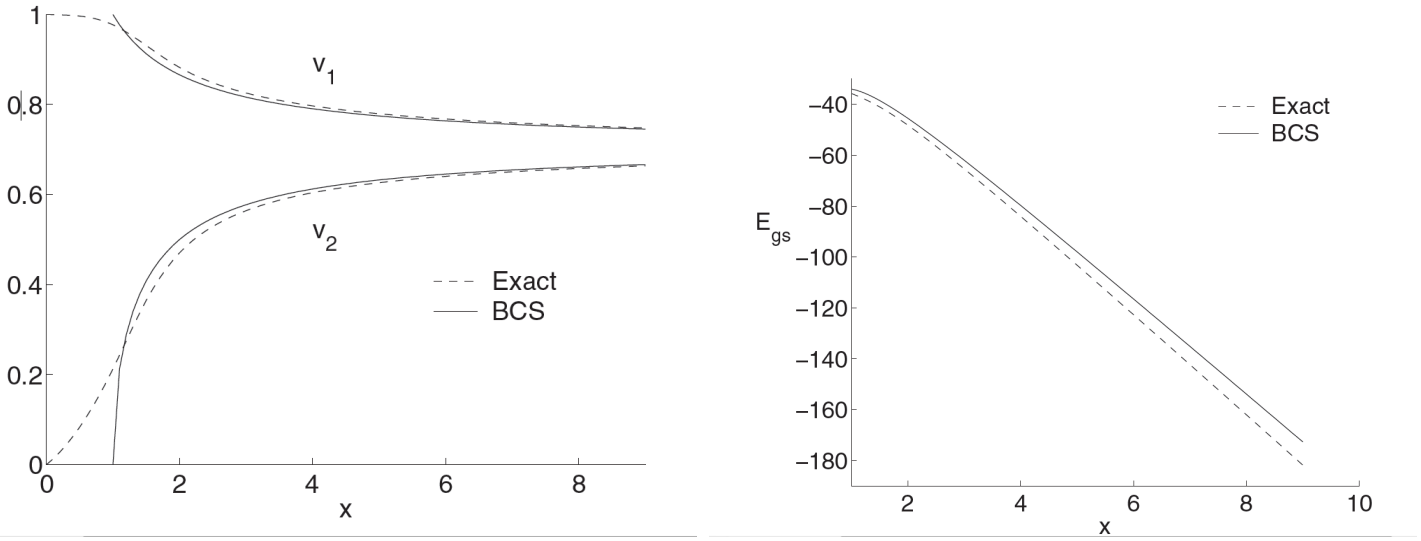


Figure 1.7: The BCS gap parameter is shown in function of x defined as $x =: \frac{4\Omega-1}{2}\frac{G}{\epsilon}$. A critical value of the interaction strength is observed. The figure is taken from [9].

the sudden transition from the Fermi sea to a boson condensate for non-zero values of G, does not occur in the exact case. This can be attributed to *finite size effect*: the small number of particles results in a relatively large error of the BCS approximation, which becomes visible through the sudden phase transition. Although a critical interaction strength is observed, the occupation amplitudes and ground state energy approximate the exact values obtained by direct diagonalization very well, as seen in Figure 1.8.



(a) Occupation amplitudes.

(b) Ground-state Energy.

Figure 1.8: Comparison between the BCS solution and the exact diagonalisation solution of the Lipkin model with $j = 7/2$. The occupation amplitudes and ground-state energy are given in function of the variable x. The figure is taken from [9].

Chapter 2

Integrability of the pairing Hamiltonian and exact solution scheme

While the BCS approximation can be very accurate for large many-body systems, it can lead to significant errors regarding smaller systems because of the occurrence of particle-number fluctuations. In an aluminium superconductor for example, which has a critical temperature of $T_c = 1.20\,K$, the average electron density is about $2.11 \times 10^{20}\,\text{electrons}/cm^3$ [16]. For a macroscopic piece of superconducting aluminium, the relative error caused by particle-number fluctuation, which scales as $\frac{1}{N}$, is negligible. With nuclei however, it's a whole different ball game as the largest nuclei contain less than 300 nucleons[1]. For these smaller many-body systems, a more accurate solution scheme can be required. Of course, one can always rely on exact diagonalization of the Hamiltonian matrix. However, the computational time for diagonalizing a matrix scales with the third power of the dimension of the Hilbert space, which in turn scales exponentially with system size. It is obvious that for larger nuclei the diagonalization procedure becomes very time-consuming. Fortunately, there exists an exact solution scheme discovered independently by R.W. Richardson and M. Gaudin [18, 19, 20] of which the computational time scales linearly with the number of pairs in the system. In this chapter, this exact solution scheme will be discussed in detail. However, the scope of applicability is limited for larger systems, as this exact solution scheme is prone to singularities and can become computationally very demanding. Before discussing the exact solution scheme, the notion of *integrability* of a Hamiltonian will be introduced in subsection 2.1.2. Basically, this means that such a Hamiltonian can be written as a linear combination of internally commuting operators. Since these operators commute with each other and with the resulting Hamiltonian, they share a common basis of eigenvectors. Therefore, finding the eigenvectors of one operator completely solves the full Hamiltonian.

[1] Currently, the nucleus with the highest atomic number and atomic mass of all the elements discovered so far is one with 294 nucleons of which 118 protons. The temporary IUPAC name given for this element is *Ununoctium* [17].

2.1 Integrability of the pairing Hamiltonian

2.1.1 The quasispin formalism

As already stated in section 1.1, operators that create and annihilate Cooper pairs can be defined in the following way [21]:

$$\begin{aligned} S_j^\dagger &=: \frac{1}{2}(a_j^\dagger \odot a_j^\dagger) =: \frac{1}{2}\sum_m a_{jm}^\dagger a_{j\bar{m}}^\dagger = \sum_{m>0} a_{jm}^\dagger a_{j\bar{m}}^\dagger \\ S_j &=: \left(S_j^\dagger\right)^\dagger = -\sum_{m>0} a_{jm} a_{j\bar{m}} \\ S_j^0 &=: \frac{1}{2}\hat{n_j} - \frac{1}{2}\Omega_j, \end{aligned} \tag{2.1}$$

with $\Omega_j = j + 1/2$ and the number operator $\hat{n_j}$ is again defined as follows:

$$\hat{n_j} = \sum_m a_{jm}^\dagger a_{jm} = \sum_{m>0} (a_{jm}^\dagger a_{jm} + a_{j\bar{m}}^\dagger a_{j\bar{m}}). \tag{2.2}$$

A plus sign appears in (2.2) because the time-reversal bars are responsible for a factor $(-1)^{2(j+m)}$ which is always positive for fermions. With these operators, the BCS pairing Hamiltonian can be written in the following way:

$$\hat{H} = \sum_j \epsilon_j (2S_j^0 + \Omega_j) + g \sum_{jj'} S_j^\dagger S_{j'}. \tag{2.3}$$

Note that in order to coincide with the normal attractive pairing case, the interaction strength g has to be taken negative now (compare with (1.9). Throughout this thesis, g is assumed to be negative, unless explicitly stated otherwise. The operators in (2.1) are called *quasispin operators* and they close under the following commutation relations, forming an $su(2)$ algebra:

$$[S_j^0, S_{j'}^\dagger] = S_j^\dagger \delta_{jj'}, \qquad [S_j^0, S_{j'}] = -S_j \delta_{jj'}, \qquad [S_j^\dagger, S_{j'}] = 2S_j^0 \delta_{jj'}. \tag{2.4}$$

These are the same commutation relations as the angular momentum algebra [22]. In total analogy with angular momentum, quasispin states $|d_i, \mu_i\rangle$ can be constructed which obey the following relations :

$$\begin{aligned} S_i^\dagger |d_i, \mu_i\rangle &= \sqrt{(d_i - \mu_i)(d_i + \mu_i + 1)}\, |d_i, \mu_i + 1\rangle \\ S_i |d_i, \mu_i\rangle &= \sqrt{(d_i + \mu_i)(d_i - \mu_i + 1)}\, |d_i, \mu_i - 1\rangle \\ S_i^0 |d_i, \mu_i\rangle &= \mu_i |d_i, \mu_i\rangle . \end{aligned} \tag{2.5}$$

The 'magnetic' quantum number μ_i ranges from $-d_i$ to $+d_i$ and the lowest weight state of these S_i^0 eigenstates is thus denoted as $|d_i, -d_i\rangle$. From (2.5) it can be seen that, for the i'th level, the S_i operator destroys the lowest weight so this state can be interpreted as the absence of pairs. Taking into account the definition of the S^0 operator, the quantum numbers d_i and μ_i have to correspond to

$$\begin{aligned} d_i &= \frac{1}{2}\Omega_i - \frac{1}{2}v_i \\ \mu_i &= \frac{1}{2}n_i - \frac{1}{2}\Omega_i, \qquad \Omega_i = i + 1/2, \end{aligned} \tag{2.6}$$

with n_i the total number of fermions in the level i. The symbol v_i is referred to as the *seniority* of the i'th energy level and corresponds to the number of particles in a level that are unpaired: they don't participate in the pairing with other particles and therefore reduce the number of possible pairs in that level. When a level j has a degeneracy of $\Omega_j = j + 1/2$, up to Ω_j pairs can occupy this level. If this level contains an unpaired fermion, i.e. $v_j = 1$, only $\Omega_j - 1$ pairs can occupy this level. Therefore, unpaired fermions can prevent a certain orbital from participating in the pair condensation. This is called the *Blocking effect* [1]. A schematic overview of the relation between the concept of seniority and the quantum numbers d, μ is given in Figure 2.1.

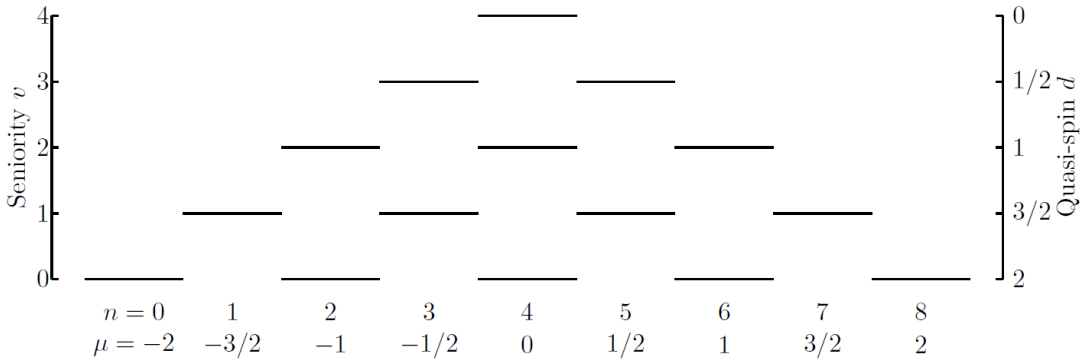


Figure 2.1: Schematic representation of the quantum numbers of an energy level with angular momentum $j = 7/2$ and degeneracy $\Omega_j = (j + 1/2) = 4$. The connection between the seniority v, the number of fermions n and the quantum numbers d and μ, given by (2.6) is shown. Increasing the seniority reduces the number of possible pairs in the level. When $v = 4$, the only possible set of quantum numbers is $|d, \mu\rangle = |0, 0\rangle$: no pairs can occupy this energy level. This figure is based on a similar scheme in [1].

The pair vacuum $|\theta\rangle$ can now be constructed as the direct product of the lowest quasispin-weights of each energy level:

$$|\theta\rangle =: |d_1, -d_1\rangle \otimes ... \otimes |d_i, -d_i\rangle ... \tag{2.7}$$

The wave function of N pairs condensing in the k'th level of an $m-$level system is given by

$$\begin{aligned} |(0_1, ..., N_k, ..., 0_m)_{\text{norm}}\rangle &= |d_1, -d_1\rangle \otimes ... \otimes |d_k, -d_k + N\rangle \otimes ... \otimes |d_m, -d_m\rangle \\ &= \prod_{j=0}^{N-1} \frac{(S_k^\dagger)^N}{\sqrt{(2d_k - j)(j+1)}} |\theta\rangle \,. \end{aligned} \tag{2.8}$$

The normalization conditions are obtained by making use of (2.5).

An important concept of an algebra is the quadratic Casimir operator. For the quasispin $su(2)$-algebra, this operator takes the form of

$$\mathscr{C}_2[su(2)_i] = \frac{1}{2}(S_i^\dagger S_i + S_i S_i^\dagger) + (S_i^0)^2. \tag{2.9}$$

This operator equals a constant value that is dependent only on the irreducible representation (irrep) that is used. For a more detailed discussion on Casimir operators, the reader is referred to Appendix

C. Using the irrep with the *uncorrelated pair filling (UPF)* as basis vectors[2], this constant can be obtained by evaluating the Casimir operator with respect to the vacuum. The Casimir expression becomes:

$$\langle\theta|\,\mathscr{C}_2[su(2)_i]\,|\theta\rangle = d_i(d_i+1). \tag{2.10}$$

2.1.2 Definition of integrability

Definition 1. A Hamiltonian is said to be ***integrable*** if it can be written as a linear combination of n commuting operators with n corresponding to the number of degrees of freedom. In a system with m single-particle energy levels, the number of degrees of freedom will be defined as m [20].

We consider the following set of m operators as an ansatz for an integrable system of m energy levels:

$$R_i = S_i^0 + g\sum_{k\neq i}^{m}\left[\frac{1}{2}X_{ik}(S_i^\dagger S_k + S_k^\dagger S_i) + Z_{ik}S_i^0 S_k^0\right] \qquad \forall i = 1,...,m, \tag{2.11}$$

with X, Z, for now, arbitrary matrices with dimension $m\times m$ and an interaction strength g. These operators will be referred to as ***constants of motion (COM)*** or ***conserved charges***. Demanding these set of operators to commute results in identities involving the X, Z coefficients. After some tedious algebraic work [23, 24], the following integrability conditions, also called the ***Gaudin equations***, are obtained:

$$X_{ij} = -X_{ji}, \qquad Z_{ij} = -Z_{ij}, \qquad X_{ij}X_{jk} - X_{ik}(Z_{ij}+Z_{jk}) = 0. \tag{2.12}$$

If the X, Z-matrix elements obey above conditions, the operators commute and any linear combination of the conserved charges is said to be an integrable Hamiltonian. It will turn out that the BCS pairing Hamiltonian (1.7) is an integrable system and with a specific implementation of X, Z it can be written as a weighted sum of the conserved charges (2.11). Since $[H, R_i] = 0$, it is clear why the operators are called conserved charges: the eigenvalues of these operators are conserved quantities of the system.

If two operators commute, they share a common basis of eigenvectors [25] so it suffices to find the eigenspectrum of one constant of motion only. This will be done by means of a Bethe Ansatz, which will be discussed in detail in the following subsection. It's easy to see that the constants of motion commute with the S^0 operator and consequently the number operator. This means that the eigenstates have a definite particle number and thus a definite pair number. From now on, let's denote the number of pairs with N and the number of energy levels with m.

2.1.3 Exact solution by means of a Bethe Ansatz

This ansatz for the wave function was introduced by Hans Bethe in 1931 to find the exact eigenspectrum of the one-dimensional antiferromagnetic Heisenberg model [26]. The Heisenberg model will be briefly touched upon in the last chapter of this thesis. In its simplest form, it consists of constructing a wave function ansatz with parameters that have to be determined by means of (non-linear) coupled equations. The Bethe Ansatz for the pairing problem takes the following form:

$$|\psi\rangle = \prod_{\alpha=1}^{N} S_\alpha^\dagger\,|\theta\rangle\,, \tag{2.13}$$

[2]By *uncorrelated pair filling*, we mean a direct product of the quasispin pair operators on top of the vacuum, i.e. filling the levels with pairs without scattering between the levels. If only the lowest energy levels were filled, this would resemble the Fermi sea in a quasispin formalism.

with N the total number of fermion pairs. Here a new generalized pair creation operator was used which is defined as follows:

$$S_\alpha^\dagger =: \sum_{i=1}^{m} X_{i\alpha} S_i^\dagger. \tag{2.14}$$

A new index α is introduced in the X-matrix. This can be interpreted as new elements added to the matrix. As already stated, the index $\alpha \in \{1, ...N\}$. When the matrices will be parametrized[3], i.e. $X_{ij} = f_x(\eta_i, \eta_j)$, these new indices will result in extra parameters E_α so that $X_{i\alpha} = f_x(\eta_i, E_\alpha)$. These parameters, called *rapidities*, are the unknowns of the Bethe Ansatz and it will turn out that they have to obey a set of non-linear equations, called the *Richardson-Gaudin equations* [18, 19].

Just like in the quasispin case, additional generalized pair operators can be defined in analogous way:

$$S_\alpha =: (S_\alpha^\dagger)^\dagger, \qquad S_\alpha^0 =: \sum_{i=1}^{m} Z_{i\alpha} S_i^0. \tag{2.15}$$

The reader can check that these generalized Gaudin operators also close under a so-called ***Gaudin-algebra*** [27]:

$$\begin{aligned} [S_\alpha^\dagger, S_\beta] &= 2X_{\alpha\beta}(S_\alpha^0 - S_\beta^0) \\ [S_\alpha^0, S_\beta^\dagger] &= X_{\alpha\beta} S_\alpha^\dagger - Z_{\alpha\beta} S_\beta^\dagger. \end{aligned} \tag{2.16}$$

The newly introduced matrices with fully Greek indices are defined with the help of the integrability conditions

$$Z_{i\alpha} X_{i\beta} = X_{\alpha\beta} X_{i\alpha} - Z_{\alpha\beta} X_{i\beta}. \tag{2.17}$$

In the parametrization scheme, they correspond to $X_{\alpha\beta} = f_x(E_\alpha, E_\beta)$ and $Z_{\alpha\beta} = f_z(E_\alpha, E_\beta)$. Now, in order to see if the Bethe Ansatz is indeed a valid candidate for an eigenstate, one has to try to pull the constant of motion through the ansatz and see if there is indeed a chance of the ansatz being an eigenstate of the COM. Therefore, commutation relations of the Gaudin operators and the COM are needed. The necessary commutators can be calculated to be

$$\begin{aligned} [R_i, S_\alpha^\dagger] =& X_{i\alpha} S_i^\dagger (1 - g S_\alpha^0) - g Z_{\alpha i} S_\alpha^\dagger S_i^0 \\ [[R_i, S_\alpha^\dagger], S_\beta^\dagger] =& -g S_i^\dagger Z_{\alpha\beta} (X_{i\beta} S_\alpha^\dagger - X_{i\alpha} S_\beta^\dagger). \end{aligned} \tag{2.18}$$

After some algebraic work, it turns out that the Bethe Ansatz is indeed an eigenstate of R_i with eigenvalues

$$r_i = d_i(-1 + g \sum_{k \neq i}^{m} Z_{ik} d_k + g \sum_{\beta=1}^{N} Z_{\beta i}), \tag{2.19}$$

provided the following set of equations are fulfilled:

$$1 + g d_\alpha - g \sum_{\beta \neq \alpha}^{N} Z_{\beta\alpha} = 0, \qquad \alpha = 1, ...N. \tag{2.20}$$

with a generalization of the quasispin principal quantum number d_α defined as

$$d_\alpha =: \sum_{i=1}^{m} Z_{i\alpha} d_i. \tag{2.21}$$

[3]The parametrization of the matrices will be further discussed in subsection 2.1.4.

The above set of N non-linear equations, called ***Richardson Gaudin (RG) equations***, determine the rapidities E_α and consequently the wave function and eigenvalues. As already mentioned above, the internal commutation of the conserved charges results in a common basis of eigenvectors. This can be seen explicitly by looking at the RG equations. These equations are only dependent on the integrable system energies and degeneracies and not on the type of conserved charge.

The advantage of the RG method is that the number of equations to be solved scales with the number of pairs in the system. This is a major advantage opposed to exact diagonalization: the computational time for diagonalizing an $A \times A$-matrix scales with A^3 and the matrix dimension scales exponentially with the number of particles. However, there is a drawback to this method, which will briefly be discussed in section 2.3.

2.1.4 The rational model

The following parametrization of the X, Z-matrices can be considered, obeying the integrability conditions (2.12):

$$X_{ij} = Z_{ij} = \frac{1}{\epsilon_i - \epsilon_j}, \tag{2.22}$$

and the 'rapidity-extended' matrices with Greek indices can be written down in the same way. Then it is easy to show that (2.11) can be written as

$$R_i = S_i^0 + g \sum_{k \neq i}^{m} \frac{\vec{S}_i \cdot \vec{S}_k}{\epsilon_i - \epsilon_k}. \tag{2.23}$$

This Hamiltonian resembles a spin chain with a principle position i interacting with all other positions k[4]. The first single particle term S_i^0 can be interpreted as a magnetic field with strength $B = 1$ applied over the spin position i. A graphical representation of this can be seen in Figure 2.2. The rational model is part of a wider range of parametrizations. Together they are called *Generalized Gaudin models* or *Gaudin magnet systems* [20]. In this thesis only the rational model will be considered. Another parametrization is the *hyperbolic parametrization* which can be used to construct the $p_x + ip_y$ pairing Hamiltonian that describes p-wave pairing in a two-dimensional system [28]. The X- and Z-matrices then take the following form:

$$X_{ij} = g\frac{\epsilon_i \epsilon_j}{\epsilon_i^2 - \epsilon_j^2}, \qquad Z_{ij} = \frac{g}{2}\frac{\epsilon_i^2 + \epsilon_j^2}{\epsilon_i^2 - \epsilon_j^2}, \tag{2.24}$$

which also obey the integrability conditions (2.12).

Let's sum up all these COM and see what Hamiltonian is constructed. It turns out that the weighted sum can be written as [29]

$$\sum_{i=1}^{m} 2\epsilon_i R_i = \sum_{i=1}^{m} \epsilon_i \hat{n}_i + g \sum_{i,k=1}^{m} S_i^\dagger S_k - g \sum_{i=1}^{m} \mathscr{C}_2[su(2)_i] + g \left(\sum_{i=1}^{m} S_i^0 \right) \left(\sum_{i=1}^{m} S_i^0 - 1 \right), \tag{2.25}$$

Because S^0 commutes with the Hamiltonian, its eigenstates will have a definite particle number and will also be eigenstates of the S^0 operator. This means that the last term in (2.25) can simply be replaced by its eigenvalue

$$-g \left(N - \sum_{i=1}^{m} d_i \right) \left(N - \sum_{i=1}^{m} d_i - 1 \right). \tag{2.26}$$

[4] In this thesis, these positions will be referred to as the non-principal positions.

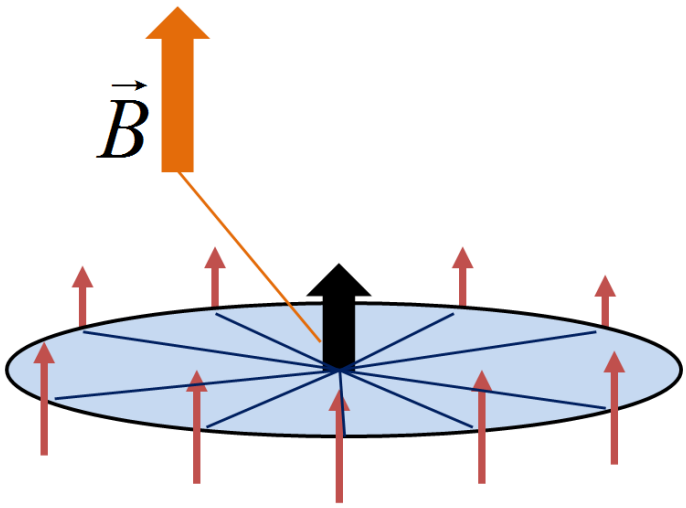


Figure 2.2: Graphical representation of a conserved charge in the rational model. A central, or principal spin interacts with a range of other spins that don't interact with each other. A magnetic field $\vec{B}$ is applied on the principal spin.

Recalling the Casimir operator also being a constant, it can be seen that the weighted sum over the conserved charges equals the pairing Hamiltonian up to a few constants. The weights ϵ_j who also appear in the parametrization of the X-and Z-matrices resemble the single-particle energies of the BCS pairing system.

In analogy with the constants of motions, the same Bethe Ansatz $|\psi\rangle = \prod_{\alpha=1}^{N} S_\alpha^\dagger |\theta\rangle$ can be pulled through the Hamiltonian to compute the eigenvalues and RG equations. As already mentioned above, these RG equations will have to be the same as the pairing Hamiltonian shares the same eigenvectors. After some algebra, the RG equations are indeed obtained:

$$1 + 2g \sum_{j=1}^{m} \frac{d_j}{2\epsilon_j - E_\alpha} + 2g \sum_{\beta \neq \alpha}^{N} \frac{1}{E_\alpha - E_\beta} = 0, \qquad \forall \alpha. \tag{2.27}$$

The eigenvalues turn out to be

$$E = \sum_{\alpha=1}^{N} E_\alpha + \sum_{j=1}^{m} \epsilon_j v_j. \tag{2.28}$$

Note that a rescaling was performed on the rapidities such that $X_{\alpha j} = \frac{1}{E_\alpha/2 - \epsilon_j}$ instead of $X_{\alpha j} = \frac{1}{x_\alpha - \epsilon_j}$ as this is often done. By looking at (2.28), it is now intuitively clear why the rapidities E_α are also called *pair energies*. The total energy seems to be built out of the sum of these 'energies' corresponding to the pairs and the unpaired fermions resulting from the seniority contribute as single-particle energy additions. It has to be noted that the interpretation of the rapidities being pair 'energies' has to be taken with a grain of salt. It turns out that these values can become complex. Moreover, because the total energy E is a real quantity, the rapidities E_α have to come in complex conjugate pairs. The existence of complex conjugate pairs can be checked explicitly by writing out the RG equations in a real and complex part. Alternatively, it can be proved that the rapidities are always the roots of a polynomial with real coefficients, resulting in real or complex conjugate pair solutions [30]. For a small interaction strength g this polynomial turns out to be the generalized Laguerre polynomial. A derivation of this can be found in the Appendix D.

2.1.5 Numerical example of the RG equations

It was already stated that these rapidities can come in complex conjugate pairs. As an example, the RG equations are numerically solved with a PYTHON routine for a 6-level model with degeneracy $\Omega = 1$ for each level. Four pairs are considered, resulting in the existence of sets of 4 rapidities. The real and imaginary part of the rapidities are shown in Figure 2.3. It can be readily seen that the rapidities organize themselves in complex conjugate pairs when the interaction parameter g is turned on. The _textitpython routine starts solving these equations by starting from $g = 0$ and then gradually turning on the parameter g. Starting from $g = 0$, where the UPF diagonalizes the Hamiltonian, an initial uncorrelated 'Fermi' distribution of the pairs over the energy levels has to be inserted. When turning on g, the solution evolves continuously, starting from this initial distribution in $g = 0$. For every initial UPF distribution a solution of rapidities exists. More information about this mechanism is given in Appendix D. There it is discussed that for very small g, the rapidities converge to the single-particle energies if pairs occupy those levels in the initial UPF distribution. A method is also discussed to determine which initial UPF distribution gives rise to the ground state of a certain conserved charge, based on Laguerre polynomials. In Figure 2.3, the rapidities converge to the values $3, 4, 5$ and 6, which are the energies corresponding to the occupied levels of the chosen initial distribution. If a set of rapidities is found, the eigenvalue energy of a certain conserved charge or the BCS Hamiltonian corresponding to this set of rapidities can be found by respectively inserting the solution in (2.19) and (2.28).

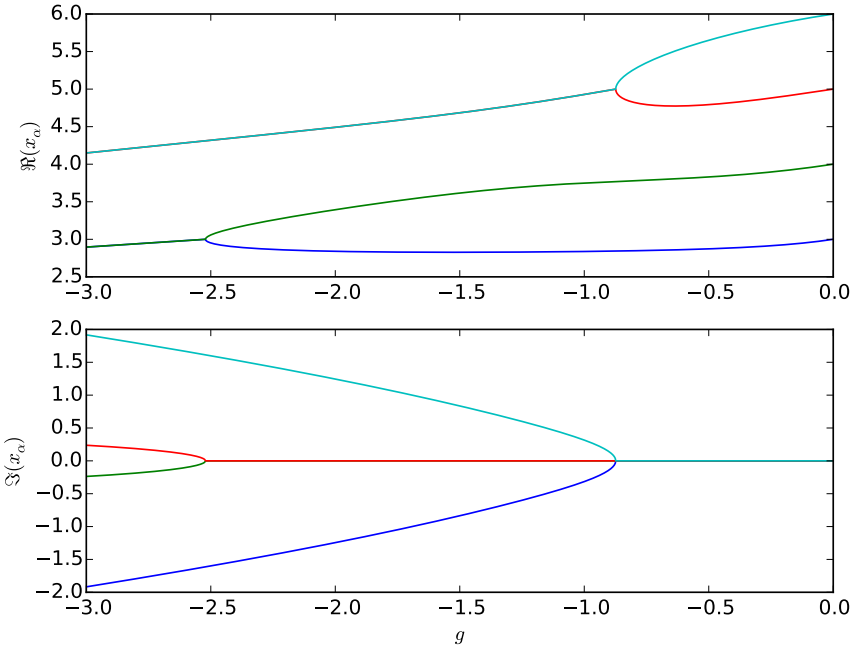


Figure 2.3: Real and imaginary part of a set of rapidity functions of a 6-level model with single-particle energies $\{6.0, 5.0, 4.0, 3.0, 2.0, 1.0\}$ and degeneracies $\Omega = 1$.

2.1.6 Discussion of the different types of conserved charges

The conserved charges in the rational model are the building blocks for the BCS pairing Hamiltonian (1.7) and there are as many conserved charges as there are energy levels in the pairing system. These conserved charges can also be interpreted as a type of pairing Hamiltonian: the term containing the X-matrix resembles a pairing part and the term containing the Z-matrix acts as an extra single-particle term. Because of the antisymmetry condition $X_{ij} = -X_{ji}$, the pairing parts of the conserved charges in a pairing system will be attributed with a different sign opposed to the other conserved charges. But what does this mean physically? Let's consider a conserved charge with principal level i and with all X positive (and $g < 0$). Throughout the thesis such conserved charge will be called a *fully attractive COM*. If $g = 0$ the lowest-energy configuration is the Fermi sea where the levels $k \neq i$ are filled first, resulting in an energy of 0. As already mentioned, in the quasispin formalism, the Fermi sea or UPF can be written as a direct product of the quasispin pair operators. If g is turned on, it's easily seen that it can become energetically advantageous to scatter pairs into the i-level because there is an attractive force between pairs of level i and levels $k \neq i$. A 'superconducting' solution exists that lies underneath the Fermi sea. Now, what happens when all X become negative, resulting in *repulsive pairing*? Intuitively one can think that it is now energetically disadvantageous to scatter pairs into the i'th level so the Fermi-sea filling is still the ground state of the system. Quantum mechanically this is not true as will be shown now with a simple non-diagonal pairing system with 2 particles written in the quasispin formalism:

$$\mathcal{H} = (S_i^0 + d_i) + G_{ik}\left[S_i^\dagger S_k + S_k^\dagger S_i\right], \tag{2.29}$$

with $G_{ik} > 0$, so we are dealing with repulsive pairing. This system has 2 energy levels i, k with degeneracies equal to 1 so that $d_i = d_k = 1/2$. The Hamiltonian can now be diagonalized in the normalized basis set:

$$\begin{aligned} |1\rangle &= S_i^\dagger |\theta\rangle \\ |2\rangle &= S_k^\dagger |\theta\rangle . \end{aligned} \tag{2.30}$$

It turns out that the lowest eigenvalue equals -0.61803 for $G_{ik} = 1$, which is lower than the Fermi-sea filling of zero energy. The eigenstate corresponding to this value is

$$|\psi\rangle = -0.53\,|1\rangle + 0.85\,|2\rangle . \tag{2.31}$$

This means that the possibility of a quantum-mechanical phase factor can lead to a scattered state that is lower lying than the Fermi sea. A more intricate example of repulsive pairing is discussed in [31]. The result of this can be seen in Figure 2.4, where a 2-level Hamiltonian of type (2.29) is solved with 10 particles and the angular momentum of the 2 shells are $j = 41/2$. It can be seen that for every value of G_{ik}, the ground state lies below the Fermi sea of zero energy.

Above system was a non-diagonal pairing system. Let's see what happens when the diagonal term is inserted. Then the Hamiltonian becomes:

$$\mathcal{H} = (S_i^0 + d_i) + \sum_{jj'}^{i,k} G_{jj'}\left[S_j^\dagger S_{j'}\right], \tag{2.32}$$

with $G_{ii} = G_{kk} = G_{ik} = G$. This system was also solved with 10 particles and angular momentum $j = 41/2$ of the shells in [31]. The result can be found in Figure 2.5. It can be seen that no superconducting solution exists underneath the Fermi sea of zero energy when the interaction strength is positive.

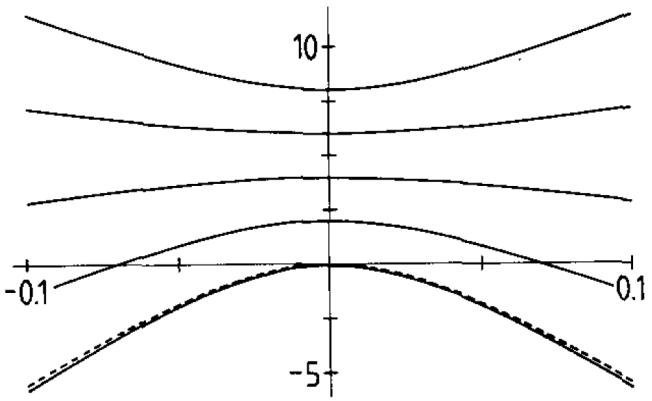


Figure 2.4: Energy spectrum of 10 particles with seniority 0 subject to the Hamiltonian force (2.29) with shells of angular momentum $j = 41/2$. The y-axis denotes the energy. The x-axis denotes G_{ik} in arbitrary units. The energy and strength quantities are given in units of the single-particle energy of the i-shell, which is unity. Figure taken from [31].

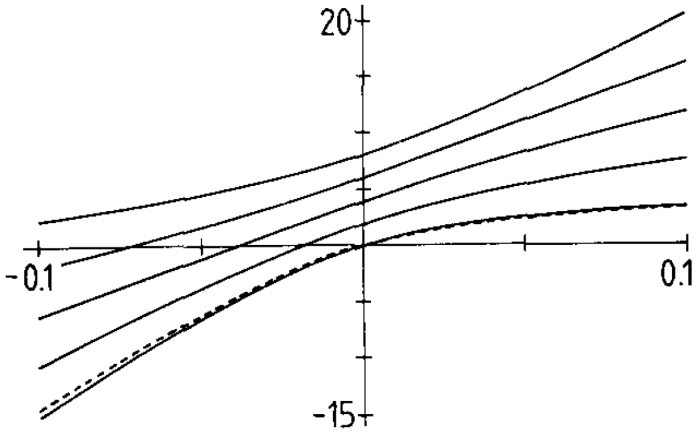


Figure 2.5: Energy spectrum of the Hamiltonian (2.32) with exactly the same conditions as in Figure 2.4. Figure taken from [31].

2.2 Thermodynamical limit and BCS theory

Both Richardson and Gaudin showed that the RG equations approach the BCS equations in the right thermodynamical limit by using an electrostatic analogy for the pairing system. A review of this is given in [20] and [32]. The RG equations for a system of M levels with degeneracies $\Omega_j = 1$ and N pairs are ($g < 0$)

$$\frac{1}{g} = \sum_{j=1}^{M} \frac{-1}{\epsilon_j - E_\alpha} - \sum_{\beta \neq \alpha}^{N} \frac{2}{E_\alpha - E_\beta}, \qquad \forall \alpha. \tag{2.33}$$

Let's model a 2D plane as a complex plane where a set of M charges with $q = -1/2$ are fixed at positions ϵ_j on the real positive axis. Also present is an external uniform electric field, with strength $-1/2g$ pointing along the real axis. We can now address the problem of finding the equilibrium positions of N charges with $q = 1$ in this plane. The equilibrium positions will be denoted by E_μ. The charges are subject to their mutual repulsion, the interaction with the fixed charges and with the

uniform field. The electrical potential of the system can now be written down easily. In addition, it has to be noted that the Coulomb potential in 2 dimensions is proportional to the logarithm of the spatial coordinate [33]. The 2D potential is given by $W + W^*$ with W equal to

$$W = \frac{1}{2}\sum_{i,\mu}\log(\epsilon_i - E_\mu) - \sum_{\mu>\nu}\log(E_\nu - E_\mu) - \frac{1}{4}\sum_{i>j}\log(\epsilon_i - \epsilon_j) - \frac{1}{2g}\left(\sum_\mu E_\mu - \frac{1}{2}\sum_i \epsilon_i\right). \quad (2.34)$$

Minimizing the potential energy by differentiating it with respect to E_μ remarkably leaves us with the Richardson-Gaudin equations! Looking at the electrostatic analogy, it can now be intuitively seen that the rapidities come in complex conjugate pairs: the real axis is a symmetry axis of the system so that for every solution its complex conjugate is also a solution.

Now, the following limit is considered

- $M \to \infty$
- $\rho =: N/M$ remains fixed
- The single-particle energies ϵ (or equivalently the position of the fixed charges) are fixed within an interval Ω on the real axis.

In this continuum limit discrete sums turn into integrals. We have, for example, that a discrete sum over the energy levels $\sum_{j=1}^{M}(= M)$ can be identified with the integral $\int_\Omega \rho(\epsilon)d\epsilon$, where $\rho(\epsilon)$ equals a negative charge density. Consequently the total charge of these fixed charges in the interval Ω is given by $\int_\Omega \rho(\epsilon)d\epsilon = M/2$. Now the assumption is made that the rapidities of the ground state organize themselves into a single symmetric arc for a given g. An example of this can be seen in Figure 2.6, where the rapidities of a 2-level model are shown. The arc-forming is a computational observation and is yet to be proved theoretically. It can be shown that the equation of the arcs in 2.6 are given

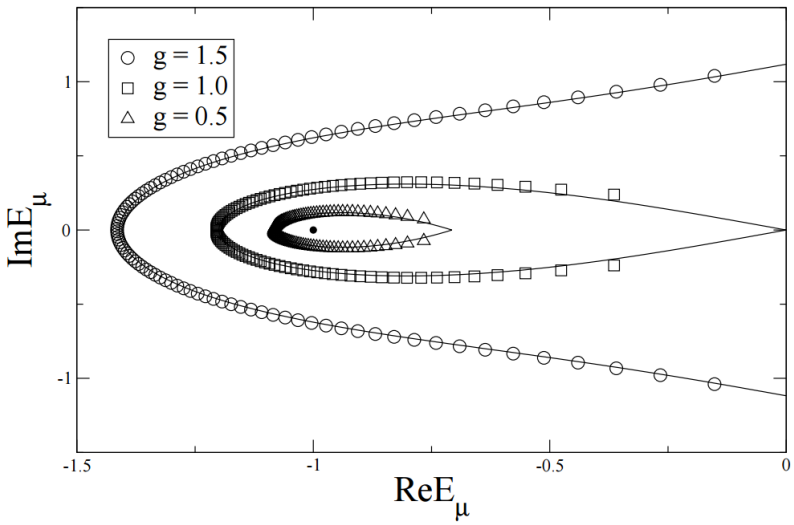


Figure 2.6: Plot of the rapidities of a 2-level pairing system with energies $\pm\epsilon$. The system contains 100 pairs and the level degeneracies are $\Omega = 100$ for interaction strengths $g = 0.5, 1, 1.5$. The figure is taken from [32] where the positive interaction strength convention is applied. The energies are in units of ϵ.

by [32]

$$x^2 + y^2 + g^2 = \frac{2xg}{\tanh(2x/g)}. \tag{2.35}$$

This arc ends at the position of the last pair of rapidities and the endpoints can be parametrized as $2\lambda \pm 2i\Delta$. This parametrization can be done, not only for the 2-level model discussed in Figure 2.6, but also for a system in the thermodynamical limit where the number of energy levels goes to infinity. Both Richardson and Gaudin proved that these parameters λ and Δ are indeed respectively the BCS potential and gap parameter in the thermodynamical limit by making use of techniques of complex analysis. They showed, among other things, that the RG equations in the thermodynamical limit reduce to the BCS gap equation

$$\int_\Omega \frac{\rho(\epsilon)d\epsilon}{\sqrt{\left(\frac{\epsilon}{2} - \lambda\right)^2 + \Delta^2}} = \frac{1}{G}, \tag{2.36}$$

which is the continuum limit of the gap equation with a level-independent gap (1.36).

It was already discussed in the first chapter that the particle-number error for the BCS approximation disappears as $N \to \infty$. However, when $N \to \infty$ and the number of energy levels remains finite, a superconducting solution doesn't always exist. This can be seen by looking at Figure 2.6. The assumption is made that, when $N \to \infty$, the last pair of rapidities will organize themselves towards $\mathbb{R}(E_\mu) \to 0$ and the arc is filled up continuously with rapidity pairs. When $g > \epsilon$ the arc is open at $\mathbb{R}(E_\mu) = 0$ thus signalling a non-zero gap Δ. For $g \leq \epsilon$ the arc closes at $\mathbb{R}(E_\mu) = 0$. This results in no gap. It is further shown in [32] that this case indeed resembles the Fermi sea.

2.3 Importance of approximate methods

The computational time for diagonalizing an $A \times A$-matrix usually scales with A^3. For large many-body systems this can become computationally very challenging since A scales exponentially with system size. As already discussed above, exact solutions of the pairing Hamiltonian are found in terms of a set of non-linear equations: the Richardson-Gaudin equations. Solving these equations, unfortunately, can be a burdensome task because of the occurrence of singularities: it turns out that the equations are infected by singular points where the rapidities can become degenerate and make the RG equations singular (see the second and last term of (2.27)). It has been shown that these singular points arise when multiple rapidities converge towards one of the single-particle levels [34, 35]. In this way, the divergences of the second and third term can cancel each other exactly. This is logical as the right hand side of (2.27) equals zero and therefore is always finite. However, it is obvious that standard numerical solver techniques like the NR method can't handle these singularities and the complications arising from solving these equations can limit the computational gain over diagonalization. This means that investigating approximative schemes can still be very useful to this day to investigate the general behaviour of these systems. It has to be noted that a lot of effort is made to develop numerical recipes to get around those singularities. In [36] for example, a method is developed based on a pseudodeformation of the quasispin algebra. In [37], a method is developed based on a new set of eigenvalue-based variables, building further on the work of [38] and [39].

In the remainder of this master dissertation, the conserved charges in the rational model will be solved in an approximative manner. Investigating the conserved charges can be interesting for 2 reasons:

- Because the conserved charges all commute they share the same eigenbasis. It will be interesting to investigate whether an approximation scheme conserves this feature.

- The conserved charges all have different physical interpretations because of the sign of the X-coefficients as discussed in subsection 2.1.6. It will be interesting how the approximation scheme handles Hamiltonians with repulsive pairing parts.

Two approximation schemes will be considered: standard BCS theory and a particle-conserving extension to BCS theory following the work of [40] and [41]. The particle-conserving approach will then be tested on the Heisenberg spin chain, describing nearest-neighbour interaction.

Chapter 3

BCS theory of the conserved charges

In this chapter, the BCS theory for the constants of motion of the pairing Hamiltonian in the rational model

$$R_i = S_i^0 + g\sum_{k\neq i}^{m}\left[\frac{1}{2}X_{ik}(S_i^\dagger S_k + S_k^\dagger S_i) + Z_{ik}S_i^0 S_k^0\right], \qquad \forall i = 1, ..., m, \tag{3.1}$$

will be derived and discussed intensively. In section 3.1 the derivation will be done in an analogous manner to standard BCS theory in section 1.2. In section 3.3 the numerical approach used to solve the modified BCS equations will be discussed. In section 3.4 it is investigated if there is a link between the solutions of the different conserved charges of a pairing system, keeping in mind that they share the same set of eigenvectors in the exact solution case. Throughout this chapter, the operator $2R_i$ will be treated to avoid numerous $\frac{1}{2}$-factors.

3.1 Derivation of the BCS theory

3.1.1 The BCS equations

The conserved charges consist of a pairing part with a specific implementation of the interaction matrix $G_{\mu\nu}$ and a single-particle energy correction containing the Z-coefficient. The pairing part can be written as

$$(2R_i)_{\text{pair}} \propto g\sum_{k,j} G_{jk}S_k^\dagger S_j \tag{3.2}$$

with G_{kl} obeying the following conditions:

- $G_{aa} = 0,\ \forall a$
- if $l = i$: $G_{ki} = X_{ik}$
- if $k = i$: $G_{il} = X_{il}$
- Always one index has to be i, otherwise the coefficient equals zero.

For the single-particle energy correction of the BCS ground state expression, the following term (denoted with the symbol Z) has to be rotated with a Bogoliubov transformation and fully contracted by evaluating this term with respect to the BCS vacuum (1.11):

$$Z = \frac{g}{2}\sum_{k\neq i} Z_{ik}(\sum_m a_{im}^\dagger a_{im} - \Omega_i)(\sum_{m'} a_{km'}^\dagger a_{km'} - \Omega_k). \tag{3.3}$$

Because of the fact that the interaction matrix and single-particle energies[1] are independent of the magnetic quantum number, the rotation (1.42) can be used. After some basic calculations, making use of (1.13), this results in the following contraction term:

$$(Z)_{contr} = \frac{g}{2}\sum_{k\neq i} Z_{ik}\Omega_i\Omega_k \left\{1 + 4v_i^2v_k^2 - 2(v_i^2 + v_k^2\right\}. \tag{3.4}$$

After altering the Hamiltonian with the chemical potential term, i.e. $2R_i \to 2R_i - \lambda(\hat{n} - n)$ and the usage of some basic algebra, the fully contracted Hamiltonian thus becomes:

$$\begin{aligned} U_0 =&(2-2\lambda)\Omega_i v_i^2 - 2\lambda\sum_{k\neq i}\Omega_k v_k^2 \\ &+ 2g\sum_{k\neq i}\Omega_i\Omega_k X_{ik}u_iv_iu_kv_k \\ &+ \frac{g}{2}\sum_{k\neq i} Z_{ik}\Omega_i\Omega_k \left\{1 + 4v_i^2v_k^2 - 2(v_i^2 + v_k^2\right\} \\ &- \Omega_i + \lambda n, \end{aligned} \tag{3.5}$$

with n the number of fermions in the system. Differentiating this expression with respect to v_j and making use of (1.19), the modified BCS equations are obtained:

$$\begin{aligned} &- gX_{ik}\Omega_i u_i v_i(u_k^2 - v_k^2) = u_kv_k\left\{gZ_{ik}\Omega_i\left[2v_i^2 - 1\right] - 2\lambda\right\}, \qquad \forall k \neq i \\ &- g\left[\sum_{k\neq i}\Omega_k X_{ik}u_kv_k\right](u_i^2 - v_i^2) = u_iv_i\left\{\sum_{k\neq i} gZ_{ik}\Omega_k[2v_k^2 - 1] + 2 - 2\lambda\right\}. \end{aligned} \tag{3.6}$$

The system gaps can now be introduced as

$$\begin{aligned} \Delta_i &=: -g\sum_{k\neq i}\Omega_k X_{ik}u_kv_k \\ \Delta_k &=: -gX_{ik}\Omega_i u_iv_i, \qquad \forall k \neq i. \end{aligned} \tag{3.7}$$

If the system gaps are positive the amplitudes can be written as

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left[1 + \frac{gZ_{ik}\frac{\Omega_i}{2}\left[2v_i^2 - 1\right] - \lambda}{\left[(gZ_{ik}\frac{\Omega_i}{2}\left[2v_i^2 - 1\right] - \lambda)^2 + (\Delta_k)^2\right]^{1/2}}\right] \\ u_i^2 &= \frac{1}{2}\left[1 + \frac{\sum_{k\neq i} gZ_{ik}\frac{\Omega_k}{2}\left[2v_k^2 - 1\right] + 1 - \lambda}{\left[(\sum_{k\neq i} gZ_{ik}\frac{\Omega_k}{2}\left[2v_k^2 - 1\right] + 1 - \lambda)^2 + (\Delta_i)^2\right]^{1/2}}\right]. \end{aligned} \tag{3.8}$$

When one of the gaps become negative, the sign of the second term in the amplitude expression has to be inverted. It is now easily seen that these expressions coincide with the normal pairing BCS

[1]It has to be noted that the real *single-particle energies* of the conserved charges are respectively 1 for the principal level and 0 for the non-principal level as they appear as coefficients of the isolated counting operator terms of the levels. They should not be confused with the ϵ-parameters. These are the single-particle energies of the BCS pairing system, but are just parameters of the X-and Z-matrices in the conserved charges. However, in this thesis the term single-particle energies will also be used for the parametrization of the matrices. The difference will be clear from the context.

expressions (1.24) apart from a single-particle energy correction containing the Z-matrix. Again, the BCS equations (3.6) have to be solved together with the number equation that fixes the chemical potential:

$$2\sum_j \Omega_j v_j^2 = n, \tag{3.9}$$

3.1.2 Quasiparticle excitation energy

Using, for example,

$$N[\sum_m a_{im}^\dagger a_{im}] = \sum_{m>0}(u_i^2 - v_i^2)(c_{im}^\dagger c_{im} + c_{\bar{im}}^\dagger c_{\bar{im}}), \tag{3.10}$$

the quasiparticle energy can be calculated to be

$$\begin{aligned} H_{11} =&(1-\lambda)\sum_{m>0}(u_i^2 - v_i^2)(c_{im}^\dagger c_{im} + c_{\bar{im}}^\dagger c_{\bar{im}}) \\ &- \lambda \sum_{\substack{k\neq i \\ m'>0}}(u_k^2 - v_k^2)(c_{km'}^\dagger c_{km'} + c_{\bar{km'}}^\dagger c_{\bar{km'}}) \\ &- 2g \sum_{\substack{k\neq i \\ m>0 \\ m'>0}} X_{ik}u_k v_k u_i v_i (c_{im}^\dagger c_{im} + c_{\bar{im}}^\dagger c_{\bar{im}} + c_{km'}^\dagger c_{km'} + c_{\bar{km'}}^\dagger c_{\bar{km'}}) \\ &+ \frac{g}{2}\sum_{k\neq i} Z_{ik}\Bigg\{\Omega_k(2v_k^2-1)(u_i^2-v_i^2)\sum_{m>0}(c_{im}^\dagger c_{im} + c_{\bar{im}}^\dagger c_{\bar{im}}) \\ &+ \Omega_i(2v_i^2-1)(u_k^2-v_k^2)\sum_{m'>0}(c_{km'}^\dagger c_{km'} + c_{\bar{km'}}^\dagger c_{\bar{km'}})\Bigg\}. \end{aligned} \tag{3.11}$$

Setting all elements $Z_{ik} = 0$ provides a check for the calculations as then the conserved charges reduce to a normal pairing Hamiltonian. Only considering, for example, the $|im\rangle$-level, H_{11} becomes:

$$H_{11}^{im} = \left[(1-\lambda)(u_i^2 - v_i^2) + 2\Delta_i u_i v_i\right](c_{im}^\dagger c_{im} + c_{\bar{im}}^\dagger c_{\bar{im}}). \tag{3.12}$$

With the help of (3.8) and some rearranging the following result is obtained, in accordance with (1.33):

$$E_{11}^{im} = ((1-\lambda)^2 + \Delta_i^2)^{1/2}. \tag{3.13}$$

It can be easily showed that the $H_{22}-$part contains only terms of the form

$$c_{im}^\dagger c_{\bar{im}}^\dagger c_{km'} c_{\bar{km'}} + c.c., \qquad k \neq i, \tag{3.14}$$

because the interaction matrix is not diagonal. This means that quasiparticle excitations on top of the BCS-vacuum will have no energy contribution of the H_{22} term. If we consider quasiparticle excitations, we only have to take into account the quasiparticle energies of the H_{11}-term.

3.2 The Lipkin model of the conserved charges

3.2.1 Attractive conserved charge

As in the normal pairing case, a Lipkin model of the conserved charges (with $g < 0$) can be considered with 2 levels, denoted with 1 and 2. The degeneracies Ω are chosen to be 1 for both levels and the

number of particles $n = 2\Omega$ equals 2. Level 1 is considered to be the principal level. This model corresponds to one pair in a two-level system. The energies and the X-matrix can be set to

$$\begin{aligned} \epsilon_1 &= \epsilon/2 \\ \epsilon_2 &= -\epsilon/2 \\ \Rightarrow X_{12} &= Z_{12} = 1/\epsilon. \end{aligned} \tag{3.15}$$

The positive value of the X-matrix element gives rise to an attractive conserved charge. The COM then becomes

$$2R_1 = 2S_1^0 + \frac{g}{\epsilon}\left[(S_1^\dagger S_2 + S_2^\dagger S_1) + 2S_1^0 S_2^0\right]. \tag{3.16}$$

Exact RG solution For one pair, the RG equations (2.27) reduce to a single equation which is analytically solvable. The single rapidity x_α will be designated by x ($\alpha = 1$). The problem boils down to solving the following equation to find x:

$$\begin{aligned} &1 + g(Z_{1x}d_1 + Z_{2x}d_2) = 0 \\ \Rightarrow &1 + g\left(\frac{1}{\frac{\epsilon}{2} - x} + \frac{1}{-\frac{\epsilon}{2} - x}\right) = 0 \end{aligned} \tag{3.17}$$

The solution is given by

$$x^\pm = \frac{g \pm \sqrt{g^2 + \epsilon^2}}{2}, \tag{3.18}$$

and the energy eigenvalues are given by

$$2r_1^\pm = -1 + \frac{g}{2\epsilon} + \frac{2g}{2x^\pm - \epsilon}. \tag{3.19}$$

The average number of particles of the Bethe eigenstate[2] $|\psi\rangle = S_x^\dagger |\theta\rangle$ in an energy level j is given by the following expression

$$v_j^2 = \frac{\langle 0| S_x \hat{n}_j S_x^\dagger |0\rangle}{\langle 0| S_x S_x^\dagger |0\rangle}, \tag{3.20}$$

and after some algebraic work the following result is obtained for the average number of particles in both energy levels:

$$v_j^2 = \frac{2|X_{jx^\pm}|^2}{|X_{1x^\pm}|^2 + |X_{2x^\pm}|^2}, \qquad j = 1, 2, \tag{3.21}$$

with the X-matrices given by

$$X_{1x^\pm} = \frac{1}{\frac{\epsilon}{2} - x^\pm}, \qquad X_{2x^\pm} = \frac{1}{-\frac{\epsilon}{2} - x^\pm}. \tag{3.22}$$

The ground state is the state where the principal level has an occupation of ≤ 0.5 per particle because it lies the highest in energy. Therefore, the ground state is characterized by the minus sign in (3.18). Of course this very simple model can also be exactly solved by diagonalizing a 2×2-matrix.

[2]With $S_x^\dagger$, the generalized Gaudin creation operator (2.14) is meant.

The BCS solution The BCS equations (3.6) reduce to

$$\begin{aligned} -2\frac{g}{\epsilon}u_1v_1(u_2^2-v_2^2) &= -2u_2v_2\left\{\frac{g}{\epsilon}\left[1-2v_1^2\right]+2\lambda\right\} \\ -2\frac{g}{\epsilon}u_2v_2(u_1^2-v_1^2) &= -2u_1v_1\left\{\frac{g}{\epsilon}[1-2v_2^2]-(2-2\lambda)\right\}. \end{aligned} \tag{3.23}$$

The number constraint condition becomes

$$\langle\tilde{0}|\,\hat{n}\,|\tilde{0}\rangle = 2\sum_{\mu>0}v_\mu^2 = 2\Omega(v_1^2+v_2^2)\equiv 2, \tag{3.24}$$

which reduces to $v_1^2+v_2^2=1$ if $\Omega=1$. Because of the unitarity condition $u_j^2+v_j^2$ for $j=1,2$ we have the following identity, just like in subsection 1.2.3:

$$\begin{aligned} v_1 &= u_2 \\ v_2 &= u_1, \end{aligned} \tag{3.25}$$

which makes the BCS equations easy to solve. After some algebraic work, it can be found that

$$\begin{aligned} \lambda &= \frac{1}{2} \\ v_1^2 &= \frac{1}{2}\left[1+\frac{\epsilon}{2g}\right] = u_2^2 \\ u_1^2 &= \frac{1}{2}\left[1-\frac{\epsilon}{2g}\right] = v_2^2. \end{aligned} \tag{3.26}$$

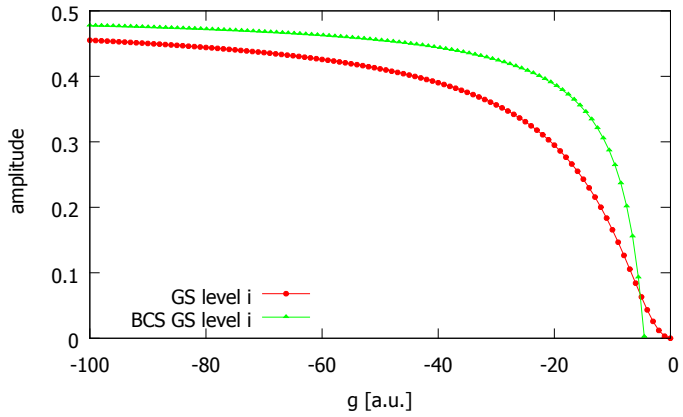
v_1^2 and v_2^2 represent respectively the occupation probability of the principal level 1 and the non-principal level 2. To compare this quantity with the quantity in (3.21) this result has to be multiplied with the degeneracy of the level. In this way v_j^2 can be interpreted as the expected number of particles in the level. Just like in the case of subsection 1.2.3, a critical interaction strength exists as the occupation probabilities are physical quantities that can't become negative:

$$g_{cr} = -\frac{\epsilon}{2}. \tag{3.27}$$

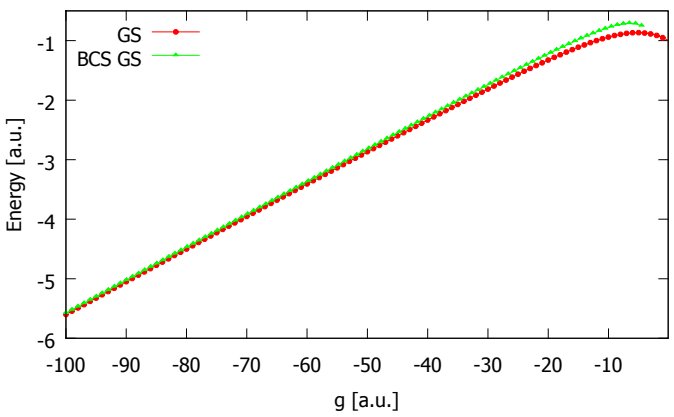
Above this negative value, no BCS solution exists except for the trivial one. The above BCS solution can be easily generalized to arbitrary degeneracy Ω by making the substitution $g\to g\Omega$ in the expression for the occupation amplitude. Note that for $n>2$ the RG equations aren't analytically solvable any more, but the BCS equations still are.
The reader can see in Figure 3.1 that the ground-state energy and occupation amplitude of the principal level are in good agreement with the exact solution. The BCS ground state always lies above the exact ground state which is in agreement with the variational principle. A look can be taken at the particle-number error made in the BCS approximation for arbitrary degeneracy Ω in the Lipkin model:

$$(\Delta_n)^2 = 4(u_i^2v_i^2+u_k^2v_k^2) = 2\left[1-\left(\frac{\epsilon}{2\Omega g}\right)^2\right]. \tag{3.28}$$

The relative error $\frac{(\Delta_n)^2}{n^2}$ indeed disappears when $n\to\infty$, which means that $\Omega\to\infty$ in the Lipkin model. As a last remark, it can be noted that the critical interaction strength $g_{cr}=\frac{-\epsilon}{2\Omega}$ disappears when $\Omega\to\infty$. This means that a non-trivial solution exists for every value of g.



(a) Occupation amplitude of the principal level (i).



(b) Ground-state energy.

Figure 3.1: Comparison between the BCS solution and the exact diagonalization solution of the Lipkin model with $\epsilon = 9$. The occupation amplitude of the principal level (denoted with i) and ground-state energy (GS) are given in function of the interaction strength g.

3.2.2 Repulsive conserved charge

In a 2-level system, another conserved charge exists with level 2 as the principal energy level. This conserved charge takes the form of

$$2R_2 = 2S_2^0 - \frac{g}{\epsilon}\left[(S_2^\dagger S_1 + S_1^\dagger S_2) + 2S_2^0 S_1^0\right], \tag{3.29}$$

with now a minus sign in front of the negative g because of the antisymmetry $X_{12} = -X_{21}$. The solution is the same as the first constant of motion except for a sign change in front of the interaction strength. Because of the special normalisation condition of the Lipkin model this results in a switch between the occupation and 'unoccupation' amplitude. The solution can be summarized as follows:

$$\begin{aligned} u_2^2 &= v_1^1 = u_2^1 \\ u_1^2 &= v_2^1 = u_1^1. \end{aligned} \tag{3.30}$$

The upper index refers to the principal level of the conserved charge, the lower index refers to the occupation amplitude of that level. We can see that the amplitude sets are independent of the upper index and therefore the BCS solutions are the same for the 2 conserved charges. This makes sense as the 2 conserved charges share the same eigenvectors because of internal commutation. However, the ground state of one conserved charge isn't necessarily the ground state of another conserved charge (in general it isn't) but rather an excited state. This can be seen by comparing the BCS solution of $2R_2$ with the exact solution, shown in Figure 3.2. The BCS approximation describes the excited state of the system.

3.3 Numerical approach to solving the BCS equations

A PYTHON routine was programmed in order to solve the generalized BCS equations (3.6). These non-linear equations are solved by means of the NR method. As this method demands an initial guess for the amplitudes, this could create some problems because no prior knowledge of the values of these amplitudes is known. Experience has taught that the best way of finding a solution is to start from

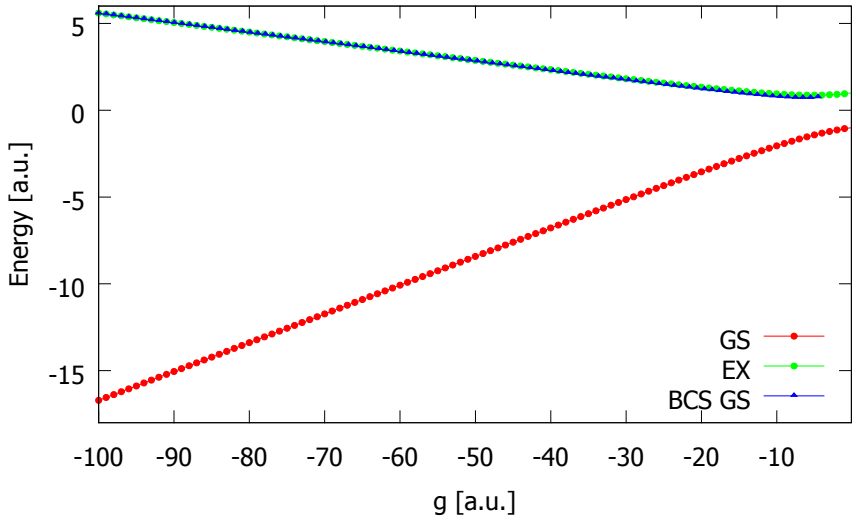


Figure 3.2: Energy spectrum of the repulsive Lipkin model (3.29. The ground state (GS) and the excited state (EX) obtained from diagonalization is given, together with the BCS-approximated energy.

a large value of the interaction strength g. It appears that the outcome of the NR solver is not very sensitive to the initial guess for large g and convergence is easily achieved with a random initial guess. The obtained solution can then be used as an initial guess for a value g' which is a little lower than g. In this way, we can find solutions for lower values of g. It turns out that, in most cases, the limit $g \to 0$ cannot be reached as the NR procedure doesn't always converge for very low g.
A FORTRAN routine was used to study the exact solutions of the conserved charges and compare them with the BCS solutions. This routine relies on exact diagonalization of the Hamiltonian. First, a basis set is constructed by applying $S^\dagger$-operators on top of the vacuum in every way possible. Therefore the basis set consists of a series of vectors that resemble an UPF of the system. Then the Hamiltonian matrix is constructed in this basis set and the matrix is diagonalized with the help of the LAPACK package for FORTRAN 90. All the exact solutions in this thesis are calculated with this routine. It was already stated in the introduction of chapter 2 that an exact diagonalization method is not computationally efficient in many-body physics as the computer time scales A^3 with A the dimension of the Hilbert space. However, in this thesis the number of particles doesn't exceed 44 so the calculations were still manageable with the FORTRAN routine.

3.4 Equivalence of the different conserved charges

It was already discussed that the conserved charges share the same set of eigenvectors. Now the question arises whether this is noticeable in their BCS equations: could the conserved charges share the same solutions to their BCS equations? It was already established for the 2-level Lipkin model that this is the case. Now, it turns out that the equivalence of the BCS solutions for different conserved charges appears to be valid, not only for a 2 level system, but for an m-level system with arbitrary m. This is formulated in the following theorem:

Theorem 3. *(Equivalence theorem) The BCS equations are equivalent for every conserved charge of an integrable m-level pairing system.*

Before proving the theorem, let's organize the thoughts a bit by repeating the modified BCS

equations of 2 conserved charges R_i, R_j of an m-level pairing system. Both sets of equations share the particle-number constraint that fixes the chemical potential.

R_i :

$$\begin{cases} -g\left[\sum_{k\neq i}\Omega_k X_{ik}u_k v_k\right](u_i^2-v_i^2) = u_i v_i\left\{\sum_{k\neq i} gZ_{ik}\Omega_k[2v_k^2-1]+2-2\lambda\right\} \\ -gX_{ik}\Omega_i u_i v_i(u_k^2-v_k^2) = u_k v_k\left\{gZ_{ik}\Omega_i\left[2v_i^2-1\right]-2\lambda\right\}, \qquad \forall k\neq i. \end{cases} \tag{3.31}$$

R_j :

$$\begin{cases} -g\left[\sum_{k'\neq j}\Omega_k X_{jk'}u_{k'} v_{k'}\right](u_j^2-v_j^2) = u_j v_j\left\{\sum_{k'\neq j} gZ_{jk'}\Omega_{k'}[2v_{k'}^2-1]+2-2\lambda\right\} \\ -gX_{jk'}\Omega_j u_j v_j(u_{k'}^2-v_{k'}^2) = u_{k'} v_{k'}\left\{gZ_{jk'}\Omega_j\left[2v_j^2-1\right]-2\lambda\right\}, \qquad \forall k'\neq j. \end{cases} \tag{3.32}$$

Proof. Throughout the proof, there will be referred to, for example, the first equation of R_i, as $(1)^i$. The following proof is valid for an arbitrary number of levels.
In general, all equations $(n)^i$ of R_i, except for the first one, can be written as

$$\frac{-2\lambda_i}{g\Omega_i u_i v_i} = -X_{in}\frac{(u_n^2-v_n^2)}{u_n v_n} + Z_{in}\frac{(u_i^2-v_i^2)}{u_i v_i}, \qquad \forall n\neq i. \tag{3.33}$$

The left hand side of all the equations are equal so we can write the following identity:

$$-X_{ik}\frac{(u_k^2-v_k^2)}{u_k v_k} + Z_{ik}\frac{(u_i^2-v_i^2)}{u_i v_i} = -X_{ij}\frac{(u_j^2-v_j^2)}{u_j v_j} + Z_{ij}\frac{(u_i^2-v_i^2)}{u_i v_i}, \qquad \forall k,j\neq i. \tag{3.34}$$

When collecting the terms with $\frac{u_i^2-v_i^2}{u_i v_i}$ and making use of the integrability condition

$$Z_{ik} - Z_{ij} = \frac{X_{ji}X_{ik}}{X_{jk}}, \tag{3.35}$$

we can rewrite the above identity as

$$-X_{jk}\frac{(u_k^2-v_k^2)}{u_k v_k} + X_{ji}\frac{(u_i^2-v_i^2)}{u_i v_i} = -\frac{X_{ij}X_{jk}}{X_{ik}}\frac{(u_j^2-v_j^2)}{u_j v_j}. \tag{3.36}$$

Then, after again using the integrability condition

$$Z_{jk} - Z_{ji} = -\frac{X_{ij}X_{jk}}{X_{ik}}, \tag{3.37}$$

we arrive at the following identity:

$$-X_{jk}\frac{(u_k^2-v_k^2)}{u_k v_k} + Z_{jk}\frac{(u_j^2-v_j^2)}{u_j v_j} = -X_{ji}\frac{(u_i^2-v_i^2)}{u_i v_i} + Z_{ji}\frac{(u_j^2-v_j^2)}{u_j v_j}. \tag{3.38}$$

We see that $\forall k\neq j$, the right-hand side is only dependent on j (and i) and independent of k. We now define the function λ_j as follows and it will turn out that this definition is equivalent to the chemical potential of the COM with principal level j:

$$\frac{-2\lambda_j}{g\Omega_j u_j v_j} \equiv -X_{ji}\frac{(u_i^2-v_i^2)}{u_i v_i} + Z_{ji}\frac{(u_j^2-v_j^2)}{u_j v_j}, \tag{3.39}$$

so (3.38) becomes

$$-X_{jk}\frac{(u_k^2-v_k^2)}{u_k v_k}+Z_{jk}\frac{(u_j^2-v_j^2)}{u_j v_j}=\frac{-2\lambda_j}{g\Omega_j u_j v_j},\qquad \forall k\neq j. \tag{3.40}$$

These are exactly the BCS equations of the j'th conserved charge (with the exception of the first equation $(1)^j$) and λ_j indeed takes up the role of the chemical potential. It is now easy to see that, with the help of (3.39) and the antisymmetry conditions $X_{ik}=-X_{ki}$ and $Z_{ik}=-Z_{ki}$, $(1)^i$ can be rewritten as just the sum of all chemical potentials

$$\sum_{a=1}^{m}\lambda_a=1. \tag{3.41}$$

In a similar manner, it can be seen that (3.41) is also the first equation of the other conserved charges. □

The proof can be summarized as follows: with the right definition of the variables λ_j with $j\neq i$, we can rewrite $(1)^i$ as the sum of chemical potentials. We then see that this equation is shared by every conserved charge. The other equations can also be derived from the equations of R_i with the help of the integrability conditions. It is important to remark that this equivalence theorem results in the occupation amplitudes of the different conserved charges to be equal but not the chemical potentials. These quantities can be seen as fine-tuning parameters that adjust themselves in such a way that an equivalence in the occupation amplitudes is reached. The restriction of these fine-tuning parameters is that their sum has to equal 1.

It is no coincidence that the sum of the chemical potentials equals 1: summing over all the constants of motions gives us (cf. with (2.25))

$$\sum_j 2R_j=\sum_j 2S_j^0\propto\sum_j\hat{n}_j, \tag{3.42}$$

as all other terms disappear due to antisymmetry of the X- and Z-matrices. As a result, the partial derivative of this sum to the particle number equals 1. Since the chemical potential of an operator $\mathcal{H}$ is defined as $\frac{\partial\mathcal{H}}{\partial n}$ and differentiation is a linear property, the sum of the chemical potentials will indeed be equal to 1.

As already mentioned previously, if the BCS solution of R_i is a good approximation of its exact ground state, it will be a good approximation of an eigenvector for a different conserved charge R_k. However, it won't be the ground state but rather an excited state of this system. Now the question arises whether the BCS solution really is a minimum of the contraction energy in that case. In every standard textbook about BCS theory, it is always assumed that the obtained extremum is a minimum of the contraction energy, though in all these cases a fully attractive pairing Hamiltonian is treated. What happens when a conserved charge is considered with one or more negative X-coefficients? Does a non-trivial minimum still exists or is the non-trivial solution a saddle point or extremum? A first way to check this is by calculating the Bordered Hessian matrix when numerically solving the BCS equations.

In general: We want to minimize a function $f(x_1,...,x_n)$ with a set of k constraints
$C_h=\{\vec{x}\in R^n : h_i(\vec{x})=c_i, i=1,...k\}$ on the variables.

Definition 2. The bordered Hessian matrix is defined as the $(k+n)\times(k+n)$- matrix [42]

$$\mathbf{H}=\begin{pmatrix} 0 & ... & 0 & \frac{\partial h_1}{\partial x_1} & ... & \frac{\partial h_1}{\partial x_n} \\ ... & ... & ... & ... & ... & ... \\ 0 & ... & 0 & \frac{\partial h_k}{\partial x_1} & ... & \frac{\partial h_k}{\partial x_n} \\ \frac{\partial h_1}{\partial x_1} & ... & \frac{\partial h_k}{\partial x_1} & \frac{\partial^2 L}{\partial x_1^2} & ... & \frac{\partial^2 L}{\partial x_n \partial x_1} \\ ... & ... & ... & ... & ... & ... \\ \frac{\partial h_1}{\partial x_n} & ... & \frac{\partial h_k}{\partial x_n} & \frac{\partial^2 L}{\partial x_1 \partial x_n} & ... & \frac{\partial^2 L}{\partial x_n^2} \end{pmatrix}, \tag{3.43}$$

with $L(x_1,...,\mu_1,...\mu_k) =: f(\vec{x}) - \sum_{i=1}^{k} \mu_i(h_i(\vec{x}) - c_i)$ and $\mu_1,...,\mu_k$ Lagrange multipliers.

The nature of an extremum with constraints can be determined by looking at the sign of the principal minors of **H**. This is summarized in the following theorem [42], here given without proof:

Theorem 4. *Suppose that an $x^* = (x_1^*,...,x_n^*)$ and $\mu^* = (\mu_1^*,...\mu_k^*)$ is found such that (x^*,μ^*) is an extremal point of L, then*

- *x^* is a local maximum if the last $n-k$ principal minors alternate in sign where the last minor has the sign $(-1)^n$. The last leading principal minor is simply the determinant of the complete bordered Hessian **H**.*
- *x^* is a local minimum if the last $n-k$ principal minors have the same sign $(-1)^k$.*
- *In all other cases x^* is a saddle point of L.*

A *Leading principal minor of order k* of an $n\times n$-matrix is defined as the determinant of the leading principal submatrix obtained by deleting the last $n-k$ rows and columns of the matrix [43]. The theorem also applies to an unconstrained case. In order to obtain this, k is simply set equal to zero. Applied to our problem, the bordered Hessian matrix to be implemented takes the following form:

$$\mathbf{H}=\begin{pmatrix} 0 & \frac{\partial h}{\partial v_1} & ... & \frac{\partial h}{\partial v_n} \\ \frac{\partial h}{\partial v_1} & \frac{\partial^2 U_0}{\partial v_1^2} & ... & \frac{\partial^2 U_0}{\partial v_n \partial v_1} \\ ... & ... & ... & ... \\ \frac{\partial h}{\partial v_n} & \frac{\partial^2 U_0}{\partial v_1 \partial v_n} & ... & \frac{\partial^2 U_0}{\partial v_n^2} \end{pmatrix}. \tag{3.44}$$

The symbol h stands for the variational constraint $h =: \langle\tilde{0}|\,\hat{n}\,|\tilde{0}\rangle - N = \sum_l 2\Omega_l v_l^2 - N$.
It is numerically checked that for partially or fully repulsive conserved charges the extremum of the energy is respectively a saddle point or a maximum. This can be also seen graphically for a repulsive 2-level model in Figure 3.3. An 'upward going mountain ridge' can be seen. Together with the number constraint (3.9) that produces a curve in the 3-dimensional space, a unique maximum is singled out (which is not shown here). Notice the extrema at the edges: particle-hole solutions are always a trivial solution to the BCS equations. Of course, the nature of the extremum can only be determined in specific numerical cases and a general recipe for the nature of the extremum would be convenient. A paper published in 1962 [44] gives a way out. In this paper, the nature of the extremum is linked to the sign of the quasiparticle excitation energies. The paper reviews a pairing Hamiltonian of the form (1.9) where the signs of the matrix elements $G_{\mu\nu}$ are not specified. If all matrix elements $G_{\mu\nu}$ are positive, the Hamiltonian represents a fully attractive pairing Hamiltonian and vice versa. A general Bogoliubov transformation is performed and the following matrix is defined:

Definition 3. $\mathscr{M}\{E_\mu\} = \|\mathscr{M}_{\mu\nu}\| = \|2E_\mu\delta_{\mu\nu} + V_{\mu\nu}\|$,

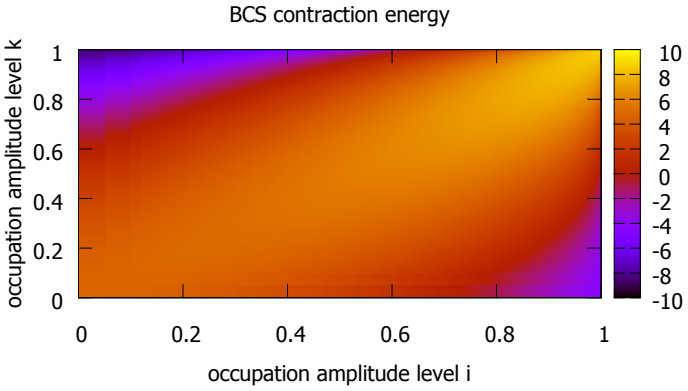


Figure 3.3: Heat map of a conserved charge of a 2-level model. The number of particles was not fixed. The (non)-principal level is denoted with the index i (k). The X- and Z-matrices in the rational model were parametrized with $\epsilon_i = -4.5$ and $\epsilon_k = 4.5$ such that $X_{ik} < 0$ and the conserved charge is repulsive. The interaction strength was set to $g = -30$ and the degeneracy of the levels was set to $\Omega_i = \Omega_k (= j + 1/2) = 2$. The map shows the BCS contraction energy (3.5) without the chemical potential term as a function of the occupation amplitudes v_i and v_k.

with E_μ the quasiparticle excitation energy of quantum state $|\mu\rangle$. Then the following theorem is proven in [44]:

Theorem 5. *If there is a non-trivial solution $\{v^*\}$ to the BCS equations such that $\mathscr{M}\{E_\mu\}$ has only positive diagonal elements, then the extremal value of the contraction energy $U_0(\{v^*\})$ is the absolute minimum of the contraction energy.*

Of course, the proof is carried out with a general pairing Hamiltonian and not with the extra Z-terms of the conserved charge. However, in this thesis, the theorem will be considered valid in the case of the conserved charges and this will be accepted without proof. Redoing the whole proof lies outside the scope of this thesis. When looking at the modified BCS equations for the conserved charges, the Z-component acts as an energy correction on the single-particle energies. With a redefinition of the single-particle levels (that are now dependent on the occupation amplitudes), the 'iterative solutions' (3.8) are exactly the same as in the case of the standard BCS pairing Hamiltonian. When looking at the quasiparticle excitation energies, the same redefinition results in the same form of expression as in the normal pairing case. Therefore it can be expected that the above theorem is still valid for the conserved charges. The conserved charges don't contain a diagonal interaction term V_{mm} so the theorem reduces to the following: if a non-trivial BCS solution is reached and one or more quasiparticle excitation energies of (3.11) are negative, then this extremum is not a global minimum of the contraction energy. Now, when does the excitation energy becomes negative? This brings us to the following statement:

Theorem 6. *The sign of an excitation energy of a certain level depends on the sign of its gap parameter.*

Proof. Let's assume the following:

- A non-trivial BCS solution is found with the amplitudes u, v all positive.

- $X_{ik} < 0$ for a certain non-principal level k. Through (3.7), it can be seen that the gap parameter $\Delta_k < 0$.

It was already discussed in subsection 3.1.1 that the signs in the iterative amplitude expressions (3.8) of an energy level have to be inverted when its gap parameter is negative. Now let's consider the quasiparticle energy for a quantum state in the k'th level for the conserved charge R_i. The excitation energy for this level is given by

$$E_k = \left[-\lambda + \frac{g}{2} Z_{ik} \Omega_i (2v_i^2 - 1)\right] (u_k^2 - v_k^2) + 2\Delta_k u_k v_k, \qquad k \neq i. \tag{3.45}$$

Making use of the fact that Δ_k is negative and inserting the right iterative amplitude expression, we easily obtain

$$E_k = -\left(\left[-\lambda + \frac{g}{2} Z_{ik} \Omega_i (2v_i^2 - 1)\right]^2 + (\Delta_k)\right)^{1/2}. \tag{3.46}$$

□

It can be concluded that a *negative X-coefficient*, creating a negative gap parameter of a non-principal level through (3.7), results in an extremal energy value that is not a minimum. This means that the BCS solution isn't capable of describing the true ground state of a repulsive system and since the particle-hole configurations are always a trivial solution of the BCS equations, this non-trivial solution energy will most likely lie above the Fermi sea energy. The link between a negative gap parameter and the nature of the extremum of the contraction energy is computationally tested extensively with the help of the Bordered Hessian matrix. Therefore it is safe to assume that theorem 5 is indeed valid in the case of the conserved charges.

So far, we have only looked for positive and real values of u, v when trying to solve the BCS equations. However, the occupation amplitudes can be easily generalized to negative or complex values. Now the question arises whether a complex generalization of the Bogoliubov amplitudes will result in the occurrence of a minimum and therefore be a good approximation to the ground state. This will be the subject of the next section.

3.5 Generalization of the Bogoliubov transformation

Because of the form of the BCS ground state (1.11) it can be stated without loss of generality that the u-coefficients are positive and real as discussed in [45]. Indeed, the BCS vacuum can be written solely in terms of the quotients $\frac{v_\nu}{u_\nu}$ so the complex phase of u_ν can be freely chosen. The unitary Bogoliubov transformation can be generalized as follows, with the possibility of v being a complex number:

$$\begin{aligned} a_{im} &= u_i c_{im} + v_i c_{i\bar{m}}^\dagger \\ a_{im}^\dagger &= u_i c_{im}^\dagger + v_i^* c_{i\bar{m}} \\ a_{i\bar{m}} &= -v_i c_{im}^\dagger + u_i c_{i\bar{m}} \\ a_{i\bar{m}}^\dagger &= -v_i^* c_{im} + u_i c_{i\bar{m}}^\dagger, \end{aligned} \tag{3.47}$$

and the real part of the ground-state energy becomes:

$$\begin{aligned} U_0 =&(2-2\lambda)\Omega_i|v_i|^2 - 2\lambda\sum_{k\neq i}\Omega_k|v_k|^2 \\ &+ 2g\sum_{k\neq i}\Omega_i\Omega_k X_{ik}u_i|v_i|u_k|v_k|\cos[\phi_i-\phi_k] \\ &+ \frac{g}{2}\sum_{k\neq i}Z_{ik}\Omega_i\Omega_k\left\{1+4|v_i|^2|v_k|^2-2(|v_i|^2+|v_k|^2\right\} \\ &- \Omega_i + \lambda n \end{aligned} \tag{3.48}$$

where $|v_j|$ and ϕ_j represents respectively the absolute value and phase of the complex amplitude v_j. Differentiating to ϕ_k results in the requirement that

$$\sin[\phi_i-\phi_k]=0, \qquad \forall k\neq i. \tag{3.49}$$

Without loss of generality ϕ_i can now be set equal to zero because there are no further restrictions on the phases, hence ϕ_i is a degree of freedom. In other words, the occupation amplitude of the principal level v_i can always be defined as real and positive. This means that, in order to obey (3.49), v_k will be either positive or negative and real ($\phi_k = 0, \pi$). The following ansatz can now be made: with every negative X_{ik}-coefficient, the cosine in (3.48) is set to -1. Because of the fact that these cosines will also appear in the definition of the gap parameters, this means that the gaps in the BCS equations will always be positive. This can be interpreted as taking the absolute value of X_{ik} in the gap[3] and treating the v-amplitudes as positive. In that case, a global minimum is reached because of Theorem 6 and a superconducting solution is found below the Fermi sea. The solution with the appropriate minus signs added will be referred to as the *Generalized BCS solution*

Let's apply this method to the following example with 2 constants of motion. Throughout this thesis, the single-particle energies and degeneracies will be portrayed in arrays: $\epsilon = \left[\epsilon_i, \epsilon_{k_1}, ...\epsilon_{k_{m-1}}\right]$ and $\Omega = \left[\Omega_i, \Omega_{k_1}, ...\Omega_{k_{m-1}}\right]$. The first element of these arrays denotes the principal level (i) of the COM and the other elements represent the non-principal levels (k_a). In this way, all information of a COM can be summarized in these two arrays. As already discussed, the single-particle energies of the pairing system parametrize the X- and Z-matrices in the rational model as

$$X_{ij} = Z_{ij} = \frac{1}{\epsilon_i - \epsilon_j}. \tag{3.50}$$

When $\epsilon_i < \epsilon_{k_a}$ for a certain non-principal level k_a, a repulsive part occurs because $X_{ik_a} < 0$. In this way, it can be seen in the example below that the first constant of motion (COM 1) is fully attractive and the second constant of motion (COM 2) contains one repulsive part. This is simply done by interchanging the first two energy levels

Example 1

$$\begin{cases} m = 4 \\ \text{COM 1}: \ \epsilon = [4,3,2,1] \\ \text{COM 2}: \ \epsilon = [3,4,2,1] \\ \Omega\,(= j+1/2) = [1,1,1,1] \\ N_{\text{part}} = 4. \end{cases}$$

[3] And only in the gap! In the rational model, we have for the matrices that $Z = X$. These Z-matrices, which appear in the third term of (3.48), are not taken positive because no cosines enter this term.

This system with 4 particles contains 6 eigenstates[4]. In Figure 3.4, the eigenvalues of COM 1 are given together with the BCS solution. It's clear that the BCS solution is in excellent agreement with the exact ground state and also the first excited state is approximated well. This state is constructed by applying 2 quasiparticle creation operators on the BCS vacuum and therefore adding the two lowest H_{11}-terms of (3.11) on top of the ground state. In Figure 3.5, the energy spectrum of COM 2 is given.

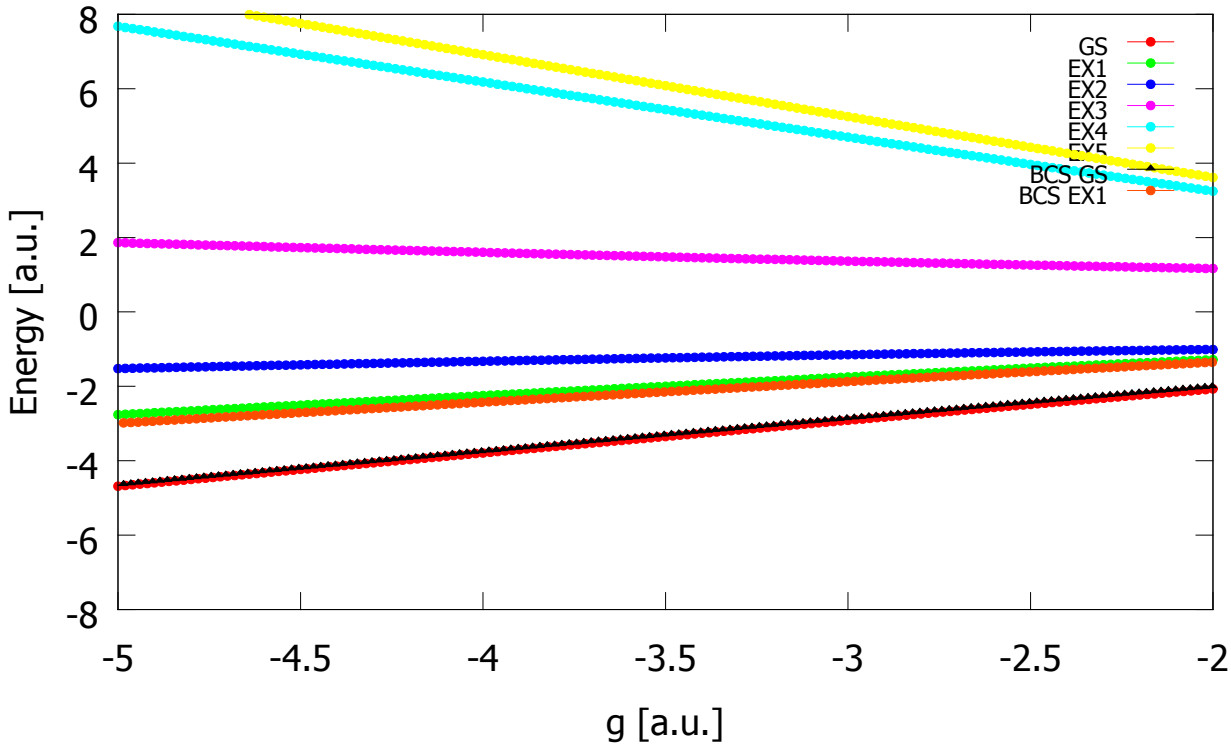


Figure 3.4: Energy spectrum (GS and EX1, EX2,...) of COM 1 together with the BCS approximation of the ground state (BCS GS) and the first excited state (BCS EX1).

Here, the regular BCS solution with strictly positive amplitudes (BCS com)[5] approximates the second excited state very well. This solution is shared with the solution of COM 1 because of theorem 3 and thus produces the same occupation amplitudes as the ground state in COM 1. This is as expected when investigating the exact eigenvectors in the diagonalization procedure: the second excited state of COM 2 and the ground state of COM 1 indeed share the same eigenvector. The generalized BCS solution is constructed by introducing the appropriate minus signs. It can be seen that this solution does not approximate the ground state very well and even appears to lie closer to the first excited state. Hence, this Bogoliubov generalization does not appear to be an accurate approximation to the ground state of the conserved charge. Of course it is not necessarily expected that a BCS-like approximation is accurate for only 4 particles, but the major difference between COM 1 and COM 2 signals a not so promising trend. Let's move on to a larger system with 5 energy levels and 44 particles:

[4]Since each level can contain no more than 1 pair, the dimension of the Hilbert space is simply $\binom{4}{2}$: 2 pairs distributed over 4 orbitals.

[5]The identifier BCS *com* stands for common, as in common solution.

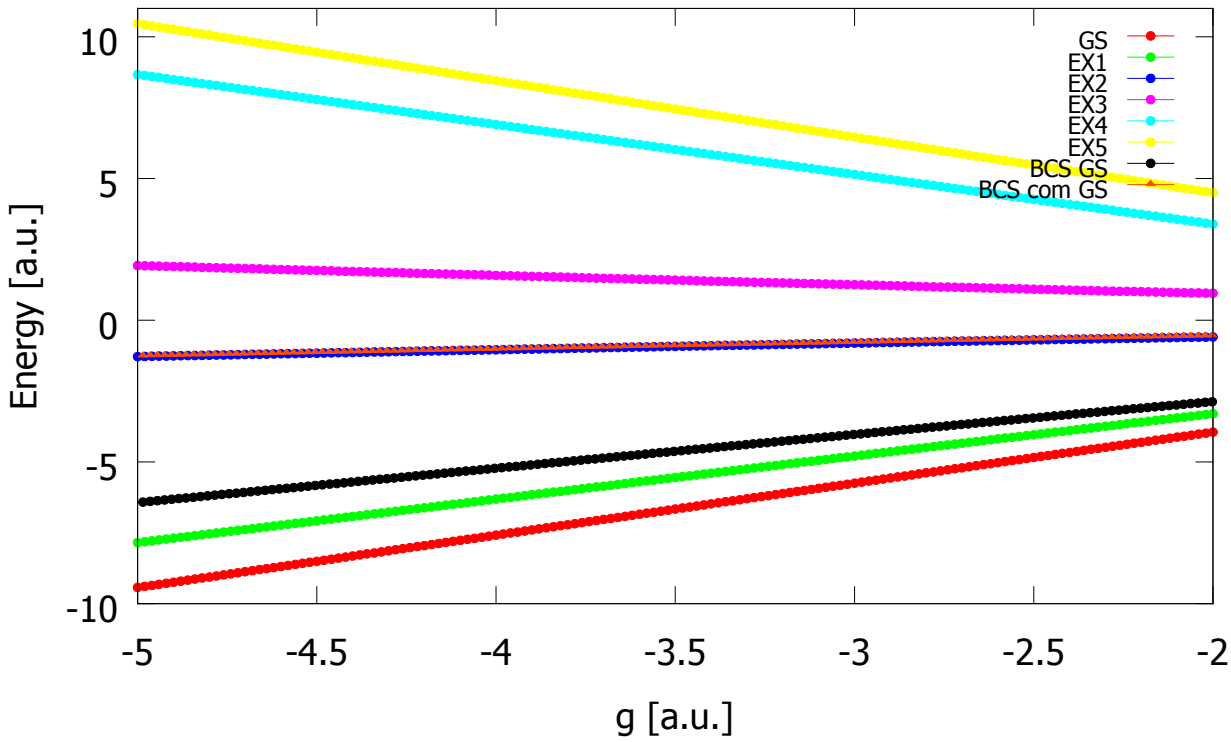
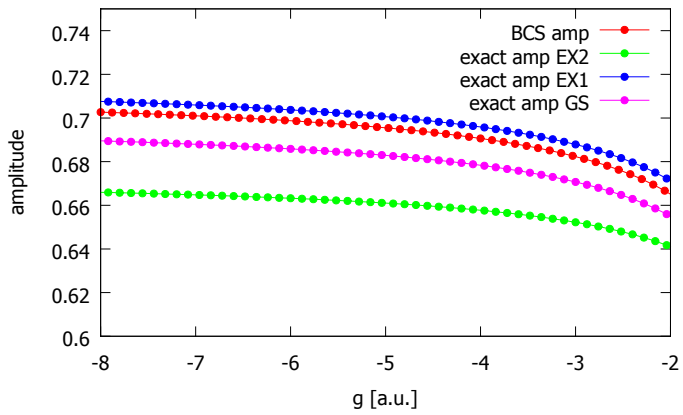


Figure 3.5: Energy spectrum (GS and EX1, EX2,...) of COM 2 together with the BCS approximation. The solution with positive amplitudes that is equivalent with the solution of COM 1 is indicated with (BCS com GS). The generalized solution with the introduction of the appropriate minus signs in the v-amplitudes is indicated with (BCS GS).

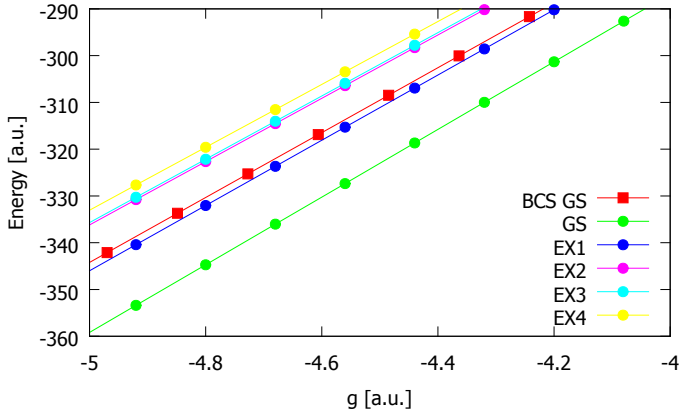
Example 2

$$\begin{cases} m = 5 \\ \epsilon = [4, 5, 3, 2, 1] \\ \Omega = [7, 7, 7, 7, 7] \\ N_{\text{part}} = 44 \end{cases}$$

The low-lying energy spectrum and occupation amplitude of the principal level are shown in Figure 3.6, together with their generalized BCS approximation. The generalized solution predicts the right order of magnitude of the lowest-lying energy states: note that there are 1750 energy states and the highest state lies more than 1500 units above the ground state. However, the ground-state-energy approximation is less accurate in comparison to the BCS approximation of the fully attractive case, which is exact up to 2 decimals and previously discussed examples. In this example the difference to the closest eigenstate is of order 4 units. Although BCS predicts the order of magnitude rather well, there is still a big lack of accuracy in partially repulsive Hamiltonians. It looks like it approximates the first excited state better than the ground state. It is checked that the other conserved charges with repulsive parts all approximate an excited state better than the ground state but the accuracy is never as good as in the fully attractive case. In the next chapter, an attempt will be made to go beyond BCS theory and accurately describe these repulsive interactions.



(a) Exact occupation amplitudes for the ground state and first 2 excited states of the principal level together with the BCS approximation of its ground state.



(b) Exact energy spectrum of the low-lying states (GS, EX1,...) together with the BCS approximation of the ground state (BCS GS).

Figure 3.6: Comparison between the BCS solution and the exact diagonalisation solution of example 2 for various interaction strengths g.

3.6 Properties of the BCS-approximated conserved charges

It was shown that BCS theory is capable of describing the ground state of seniority-0 and seniority-1 states by means of the following approximated Hamiltonian, containing single-quasiparticle excitations:

$$[H]_{BCS} = U_0^i + \sum_\alpha E_\alpha c_\alpha^\dagger c_\alpha. \tag{3.51}$$

For every conserved charge of a pairing system, the above approximation can be written down. In the case of these COM, pair excitations (or equivalently 2 quasiparticle excitations) are also described with (3.51) because of the specific nature of the residual term H_{22} (see (3.14)). Now the question arises whether the BCS-approximated version of these conserved charges still describes an integrable system. In other words, do these BCS-approximated conserved charges still commute with each other?

3.6.1 Integrability of the BCS approximations

Before answering this question, let's introduce a new $su(2)$-algebra which will be indicated by $su(2)^c$. Just as in the case of the regular second-quantization operators , quasispin operators can be defined in terms of the quasiparticle operators. This can be referred to as the *quasiparticle-quasispin algebra*. These $su(2)$-operators will be denoted by the symbol A:

$$A_j^\dagger =: \frac{1}{2}(c_j^\dagger \odot c_j^\dagger), \qquad A_j =: \frac{1}{2}(c_j \odot c_j), \qquad A_j^0 =: \frac{1}{2}\hat{n}_j^c - \frac{1}{4}\Omega_j, \tag{3.52}$$

with $\hat{n}_j^c$ the operator that counts the number of quasiparticles. The dot operator $\odot$ was already defined in (2.1). The operation of the $su(2)^c$-operators on the BCS vacuum is completely analogous to (2.5) with the real vacuum $|\theta\rangle$ replaced by the BCS vacuum. For example:

$$A_k^\dagger |\tilde{0}\rangle = A_k^\dagger |\tilde{d}_i, -\tilde{d}_i\rangle = \sqrt{2\tilde{d}_i}\, |\tilde{d}_i, -\tilde{d}_i + 1\rangle\,, \tag{3.53}$$

so the BCS vacuum can be interpreted as the lowest weight of a quasiparticle pair representation. As a result of the definition of A_j^0 and the fact that the number of quasiparticles equals the number of

actual particles due to unitarity of the Bogoliubov transformation, the symbol $\tilde{d_j}$ equals d_j which is given in (2.6). It can be checked that $su(2)^c$ relates with the regular quasispin $su(2)$-algebra by means of the following transformation:

$$\begin{pmatrix} A_j^\dagger \\ A_j^0 \\ A_j \end{pmatrix} = \begin{pmatrix} (u_j^*)^2 & 2u_j^* v_j^* & -(v_j^*)^2 \\ -u_j^* v_j & |u_j|^2 - |v_j|^2 & -u_j v_j^* \\ -v_j^2 & 2u_j v_j & u_j^2 \end{pmatrix} \begin{pmatrix} S_j^\dagger \\ S_j^0 \\ S_j \end{pmatrix}. \tag{3.54}$$

For generality reasons, the Bogoliubov parameters are assumed to be complex, but it is already shown in section 3.5 that for the conserved charges the parameters are real. This transformation can be interpreted as a rotation of the quasispin operators. It can be verified that this transformation is closed under matrix multiplication, which signals a group structure. If we assign an upper index i or l to the amplitudes indicating 2 different and arbitrary Bogoliubov transformations, the transformation matrix V_a (with a an arbitrary energy level) obeys:

$$\begin{aligned} &V_a^i . V_a^l = V_a^{i+l} \qquad \text{if} \\ &u_a \xrightarrow{i+l} u_a^i u_a^l - v_a^i v_a^l \\ &v_a \xrightarrow{i+l} u_a^i v_a^l + u_a^l v_a^i. \end{aligned} \tag{3.55}$$

The BCS approximation can now be written in terms of these quasispin operators

$$\begin{aligned} [R_i]_{BCS} &= U_0^i + \sum_\alpha E_\alpha^i (c_\alpha^i)^\dagger c_\alpha^i \\ &= U_0^i + \sum_j E_j^i \left(2(A_j^i)^0 + \Omega_j \right), \end{aligned} \tag{3.56}$$

with the upper index of the quasiparticle operators and energies referring to the principal level of the corresponding conserved charge. The commutation of two BCS-approximated conserved charges now takes the following form

$$[R_i, R_l] = 4 \sum_\alpha E_\alpha^i E_\alpha^l [(A_\alpha^i)^0, (A_\alpha^l)^0]. \tag{3.57}$$

The commutator can be calculated by making use of the transformation (3.54) and the quasispin commutation relations. Demanding internal commutation eventually results in the following integrability condition:

$$u_a^i v_a^i [(u_a^l)^2 - (v_a^l)^2] = u_a^l v_a^l [(u_a^i)^2 - (v_a^i)^2], \tag{3.58}$$

which is fulfilled when $\left\{v^i\right\} = \left\{v^l\right\}$. This makes sense because the conserved charges share the same set of equations (theorem 3) and have common solutions. However, the BCS equations have multiple solutions. For example, there are always the trivial particle-hole solutions and multiple generalized solutions with the introduction of minus signs also occur. If the normal solution with positive amplitudes is taken for one conserved charge and the trivial solution for the other conserved charge, the BCS-approximated conserved charges don't commute any more. This is due to the fact that commuting expressions don't always commute order by order in the second-quantization operators: the identity $[R_i, R_l] = 0$ is an absolute identity and independent of the choice of basis. A different linear Bogoliubov transformation can be done on each conserved charge with coefficients $\left\{v^i\right\} \neq \left\{v^l\right\}$ while still maintaining this identity. The conserved charges then take the form of, after applying Wick's theorem, $R_i = U_0^i + \sum_\alpha E_\alpha^i (c^i)_\alpha^\dagger (c^i)_\alpha + V_{res}^i$ where the quasiparticle operators are now equipped with an upper index referring to the type of linear transformation. The V_{res} term is quadrilinear in c-operators and the second term is bilinear. It is now due to the $su(2)$ commutation relations that

the commutation of bilinear terms and quadrilinear terms are not totally independent: relations like $[S^\dagger, S] = 2S^0$ link quadrilinear with bilinear terms.

It can be concluded that the BCS-approximated conserved charges still commute if a mutual solution $\{v\}$ of both sets of BCS equations is used for the Bogoliubov transformations.

3.6.2 Summing the BCS approximations

As already discussed, summing the conserved charges with the right weight factors results in the pairing Hamiltonian up to the Casimir operator and an additional term

$$g\left(\sum_i S_i^0\right)\left(\sum_i S_i^0 - 1\right). \tag{3.59}$$

This term can be interpreted as a constant and replaced by its eigenvalue because the Hamiltonian obeys particle-number symmetry and the exact eigenstates contain a definite number of particles. In the BCS approximation scheme, this reasoning is not valid any more because the BCS vacuum violates particle-number symmetry. As an example, the contraction terms (3.5) of all the conserved charges of a pairing system can be summed with the single-particle energies as weight factors, i.e. $\sum_i \epsilon_i U_0^i$. Again, the upper index on the contraction energy refers to the principal level of the corresponding conserved charge. After some calculus it is quickly seen that the expression of the contraction energy for the normal pairing Hamiltonian (1.16) is not reached. This is as expected because the evaluation of (3.59) with respect to the BCS vacuum does not leave us with a constant that is independent of the u, v-parameters. To calculate this term efficiently, a unitary rotation can be performed on the quasispin operators with (3.54) to arrive in the quasiparticle-quasispin basis. Then (3.59) becomes

$$\begin{aligned}
&\langle\tilde{0}|\, g\left(\sum_i S_i^0\right)\left(\sum_i S_i^0 - 1\right)|\tilde{0}\rangle \\
=&-g\sum_i(1-2v_i^2)\,\langle\tilde{0}|\,A_i^0\,|\tilde{0}\rangle + g\sum_{k,l}(u_k^2-v_k^2)(u_l^2-v_l^2)\,\langle\tilde{0}|\,A_k^0 A_l^0\,|\tilde{0}\rangle + u_k v_k u_l v_l\,\langle\tilde{0}|\,A_k A_l^\dagger\,|\tilde{0}\rangle \\
=&\frac{g}{2}\sum_i \Omega_i(1-2v_i^2) + \frac{1}{4}\sum_{k,l}\Omega_k\Omega_l(u_k^2-v_k^2)(u_l^2-v_l^2) + \sum_k \Omega_k u_k^2 v_k^2.
\end{aligned} \tag{3.60}$$

This result is obtained by making use of (3.52) and (2.5). Adding this expression to the weighted sum of the contraction energies indeed leaves us with the right BCS ground-state energy after some calculus. As a last remark, the reader can note that the Casimir operator has to be invariant under the Bogoliubov transformation because this is just a linear transformation in the used representation:

$$\frac{1}{2}(S_j^\dagger S_j + S_j S_j^\dagger) + (S_j^0)^2 = \frac{1}{2}(A_j^\dagger A_j + A_j A_j^\dagger) + (A_j^0)^2 = d_j(d_j+1). \tag{3.61}$$

3.7 Equivalence theorem revisited

It has to be noted that the equivalence of BCS-like equations of the conserved charges cannot be generalized towards arbitrary commuting operators as a counterexample can be easily found. The following 2 commuting matrices can be considered:

$$A = \begin{pmatrix} 2 & 0 & -\frac{1}{2}\sqrt{2} \\ 0 & 2 & -\frac{1}{2}\sqrt{2} \\ -\frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2} & 2 \end{pmatrix}, B = \begin{pmatrix} \frac{17}{4} & -\frac{3}{4} & -\frac{7}{4}\sqrt{2} \\ -\frac{3}{4} & \frac{17}{4} & -\frac{7}{4}\sqrt{2} \\ -\frac{7}{4}\sqrt{2} & -\frac{7}{4}\sqrt{2} & \frac{7}{2} \end{pmatrix}. \tag{3.62}$$

These matrices originate from 2 different diagonal matrices, with the same orthogonal transformation applied to it. Then, a variational (normalised) wave function is considered with one free parameter a:

$$\psi = \begin{pmatrix} \cos(a) \\ \frac{1}{2}\sin(a)\sqrt{2} \\ \frac{1}{2}\sin(a)\sqrt{2} \end{pmatrix}. \tag{3.63}$$

The purpose is now to evaluate these matrices with respect to this wave function and determine the optimal value of a in order to obtain the minimum 'energy' value as is done in the BCS procedure. The energy expressions become

$$\begin{aligned} \psi^\dagger A\psi &= -\sin a\cos a + \frac{1}{2}\sqrt{2}\cos a^2 - \frac{1}{2}\sqrt{2} \\ \psi^\dagger B\psi &= -\frac{3}{4}\sqrt{2}\cos a\sin a - \frac{7}{2}\sin a\cos a + \frac{7}{4}\sqrt{2}\cos a^2 + \frac{3}{8}\cos a^2 - \frac{7}{4}\sqrt{2} + \frac{31}{8}. \end{aligned} \tag{3.64}$$

Searching for the extremal values of both expressions results in the following solutions for the parameter a:

$$\begin{aligned} a_A &= -0.47766, \quad 2.66393, \quad 1.09314, \quad -2.04845 \\ a_B &= -0.50614, \quad 2.63545, \quad 1.06466, \quad -2.07694. \end{aligned} \tag{3.65}$$

It's clear that no common solution exists in this case. Therefore, the equivalence theorem appears to be invalid in the general case of commuting operators. This can be reasoned in a more general way, as is done below:

Consider 2 square operators/matrices of dimension n that commute: $[H_1, H_2] = 0$. Then these operators are diagonal in the same eigenbasis. Let's assume this eigenbasis is a priori known so that

$$\begin{aligned} H_1 &= \text{diag}(d_1^1, ...d_1^n) \\ H_2 &= \text{diag}(d_2^1, ...d_2^n). \end{aligned} \tag{3.66}$$

The lower index of the diagonal elements refers to the corresponding operator and it is assumed that the set of eigenvalues for the operators are not equal. Then a variational ansatz can be constructed with parameters $a_1, ...a_m$ with $m \neq n$ so that the ansatz can be written as[6]

$$\psi(a_1, ...a_m) = \begin{pmatrix} f_1(a) \\ f_2(a) \\ ... \\ f_n(a) \end{pmatrix}, \tag{3.67}$$

with $f_1, ..., f_n$ arbitrary functions which obey the normalization constraint $f_1(a)^2 + ... + f_n(a)^2 = 1$ for all possible values of a. Evaluating the matrices with respect to the wave function results in the following 'contraction' energies:

$$\begin{aligned} \psi^\dagger H_1\psi &= (f_1)^2 d_1^1 + (f_2)^2 d_1^2 + ... + (f_n)^2 d_1^n \\ \psi^\dagger H_2\psi &= (f_1)^2 d_2^1 + (f_2)^2 d_2^2 + ... + (f_n)^2 d_2^n. \end{aligned} \tag{3.68}$$

Finding the extrema of these expressions results in the following sets of equations:

[6]Remark that if $m = n$ and the functions f_i are chosen well, the exact eigenstates can be reproduced and the problem would be solved exactly. Of course, in that case the equivalence would be trivial because the operators share the same set of eigenstates.

H_1**:**

$$\begin{cases} 2f_1\frac{\partial f_1}{\partial a_1}d_1^1 + 2f_2\frac{\partial f_2}{\partial a_1}d_1^2 + ... + 2f_n\frac{\partial f_n}{\partial a_1}d_1^n = 0 \\ 2f_1\frac{\partial f_1}{\partial a_2}d_1^1 + 2f_2\frac{\partial f_2}{\partial a_2}d_1^2 + ... + 2f_n\frac{\partial f_n}{\partial a_2}d_1^n = 0 \\ ... \\ 2f_1\frac{\partial f_1}{\partial a_n}d_1^1 + 2f_2\frac{\partial f_2}{\partial a_n}d_1^2 + ... + 2f_n\frac{\partial f_n}{\partial a_n}d_1^n = 0 \end{cases} \tag{3.69}$$

H_2**:**

$$\begin{cases} 2f_1\frac{\partial f_1}{\partial a_1}d_2^1 + 2f_2\frac{\partial f_2}{\partial a_1}d_2^2 + ... + 2f_n\frac{\partial f_n}{\partial a_1}d_2^n = 0 \\ 2f_1\frac{\partial f_1}{\partial a_2}d_2^1 + 2f_2\frac{\partial f_2}{\partial a_2}d_2^2 + ... + 2f_n\frac{\partial f_n}{\partial a_2}d_2^n = 0 \\ ... \\ 2f_1\frac{\partial f_1}{\partial a_n}d_2^1 + 2f_2\frac{\partial f_2}{\partial a_n}d_2^2 + ... + 2f_n\frac{\partial f_n}{\partial a_n}d_2^n = 0. \end{cases} \tag{3.70}$$

It is clear that, in general, these equations aren't equivalent as the ansatz functions are chosen arbitrarily. If the functions are chosen in a special manner, the equations of course can become equivalent. For example, if the functions are chosen to obey the following conditions, where $\forall k$, there exists a k' so that

$$\frac{\partial f_i}{\partial a_k}d_2^i = \frac{\partial f_i}{\partial a_{k'}}d_1^i, \qquad \forall i, \tag{3.71}$$

then the equations become equivalent. Of course, more intricate relations can hold so that there could be an equivalence which isn't immediately obvious. Also, in a real situation, the eigenbasis, the diagonal elements and the form of the ansatz functions are not a priori known so it isn't clear if there would be an equivalence.

It can be safely concluded that a generalization of the equivalence theorem for the conserved charges towards arbitrary commuting operators isn't possible.

Chapter 4

Beyond BCS theory: Equations of motion approach

Clearly, standard BCS theory isn't adequate for describing repulsive interactions and the need exists to go beyond BCS theory. This can be done in numerous ways. One can, for example, perform number-projection techniques on BCS theory, because its major drawback is the particle-number violation [46, 47, 48]. One can also take into account the residual interaction term and treat this term with the *random phase approximation* (RPA) [49]. In this thesis, however, a simple and elegant method will be used consisting of the truncation of the Hilbert space of the pairing system. This technique is developed in [40] by Alexander Volya and Vladimir Zelevinsky and will be quickly reviewed in section 4.1. In section 4.2, a small modification will be made by taking into account an additional symmetry of the system: the quasispin algebra.

4.1 The Volya method: A particle number conserving approach

The following pairing Hamiltonian will be considered[1]

$$\mathcal{H} = \sum_{\nu} \epsilon_\nu a_\nu^\dagger a_\nu - \frac{1}{4} \sum_{\nu\nu'} G_{\nu\nu'} p_\nu^\dagger p_{\nu'}, \tag{4.1}$$

with the operators p defined as $p_\nu =: a_\nu a_{\bar{\nu}}$ and, as always, $G_{\nu\nu'}$ a symmetric matrix independent of the magnetic quantum number and thus invariant under time reversal. Now, a ground state with even particle number N will be denoted as $|N\rangle$ and its corresponding energy as $E(N)$. Ground states with odd particle number $N \pm 1$ will be interpreted as seniority-1 states containing an unpaired fermion with quantum number ν and these will be denoted as $|N \pm 1, \nu\rangle$ with energy $E(N \pm 1)$. The 'occupation' amplitudes will now be defined in a somewhat different way as they will be regarded as transition amplitudes:

$$\begin{aligned} v_\nu(N) &=: \langle N-1, \bar{\nu}| \, a_\nu \, |N\rangle \\ u_\nu(N) &=: \langle N+1, \nu| \, a_\nu^\dagger \, |N\rangle \, . \end{aligned} \tag{4.2}$$

It will be assumed that the amplitudes are invariant under time reversal. Right now, these transition amplitudes have nothing to do with the original notion of occupation probabilities of energy levels, but when the approximation scheme will be introduced the equivalence will become clear. In analogy

[1] We will closely follow the notation of [40] here.

with BCS theory, a gap parameter can also be defined as follows:

$$\Delta_\nu(N) = \frac{1}{2} \langle N-2| \sum_{\nu'} G_{\nu\nu'} p_{\nu'} |N\rangle . \tag{4.3}$$

The approximation method is loosely based on the famous Heisenberg equation [13, 41] where the time evolution of an operator is described with respect to a Hamiltonian:

$$i\frac{d}{dt}(\hat{X}) = [\hat{X}, \hat{H}]. \tag{4.4}$$

In a time-independent system like the BCS pairing Hamiltonian, the commutator $[\hat{X}, \hat{H}]$ can now be calculated and consequently a set of equations can be constructed by taking the expectation value of these commutator relations with respect to a representation of eigenstates. These equations will then contain the matrix elements of the operators with respect to the used representation and the energies of the system The following equations of motion will be used:

$$[a_\nu, H] = \epsilon_\nu a_\nu + \frac{1}{2} \sum_{\nu'} G_{\nu\nu'} a^\dagger_{\bar{\nu}} p_{\nu'} \tag{4.5}$$

$$[a^\dagger_\nu, H] = -(\epsilon_\nu - G_{\nu\nu} a^\dagger_\nu) - \frac{1}{2} \sum_{\nu'} G_{\nu\nu'} a_{\bar{\nu}} p^\dagger_{\nu'}. \tag{4.6}$$

Now, the identity operator of the full Hilbert space takes the form of

$$\mathbf{1} = \sum_{N,\alpha_N} |N, \alpha_N\rangle \langle N, \alpha_N| , \tag{4.7}$$

with index N the particle number and index α running over every state with a definite particle number N. This means that $|N, \alpha_N\rangle$ can refer to, not only an excited state of seniority zero, but also a state with general seniority v, i.e. it can contain any number of broken pairs. The approximation scheme now consists of truncating the full Hilbert space to that space spanned by *only ground states of seniority 0 or 1.* So if N is even, the part of the identity operator containing this particle-number sector reduces to

$$\sum_{\alpha_N} |N, \alpha_N\rangle \langle N, \alpha_N| \approx |N\rangle \langle N| . \tag{4.8}$$

If N is odd, this part of the identity operator becomes

$$\sum_{\alpha_N} |N, \alpha_N\rangle \langle N, \alpha_N| \approx \sum_{\nu} |N, \nu\rangle \langle N, \nu| , \tag{4.9}$$

with the sum going over all possible orbitals. With this approximation scheme, the last term of (4.5) can be written as

$$\begin{aligned} &\langle N-1, \bar{\nu}| \frac{1}{2} \sum_{\nu'} G_{\nu\nu'} a^\dagger_{\bar{\nu}} p_{\nu'} |N\rangle \\ &\approx \langle N-1, \bar{\nu}| a^\dagger_{\bar{\nu}} |N-2\rangle \langle N-2| \frac{1}{2} \sum_{\nu'} G_{\nu\nu'} p_{\nu'} |N\rangle \\ &= \Delta_\nu(N) u_\nu(N-2). \end{aligned} \tag{4.10}$$

Now, the equations of motion (4.5) and (4.6) can be evaluated with respect to $|N\rangle , |N-1, \bar{\nu}\rangle$ and $|N-2\rangle$ and the truncated identity operator can be inserted where necessary. It is now assumed

that, even in the truncated scheme, the states $|N\rangle, |N-1,\bar{\nu}\rangle, |N-2\rangle$ are still eigenstates of the Hamiltonian so that $H|N\rangle = E(N)|N\rangle$. A new parametrization of the energy can also be performed by introducing the variables μ and e_ν in the following way:

$$\begin{aligned} E(N-2) &= E(N) - 2\mu(N) \\ E(N-1;\nu) &= E(N) - \mu(N) + e_\nu(N) - \frac{G_{\nu\nu}}{2}. \end{aligned} \tag{4.11}$$

After some basic calculus this eventually leads to the following set of equations

$$\begin{aligned} [e_\nu(N) + \epsilon_\nu - \frac{G_{\nu\nu}}{2} - \mu(N)]v_\nu(N) + \Delta_\nu(N)u_\nu(N-2) = 0 \\ \Delta_\nu(N)v_\nu(N) + [e_\nu - (\epsilon_\nu - \frac{G_{\nu\nu}}{2} - \mu(N))]u_\nu(N-2) = 0, \end{aligned} \tag{4.12}$$

where it was assumed that the gaps are real so that $\Delta^* = \Delta$. It can now be seen that, on the level of the approximation scheme, the transition amplitudes can be interpreted as occupation amplitudes

$$\langle N| a_\nu^\dagger a_\nu |N\rangle \approx \langle N| a_\nu^\dagger |N-1,\bar{\nu}\rangle \langle N-1,\bar{\nu}| a_\nu |N\rangle = |v_\nu(N)|^2, \tag{4.13}$$

by again inserting the truncated identity. By making use of the fermionic anticommutation relations $\{a_\mu, a_\nu^\dagger\} = \delta_{\mu\nu}$ one can obtain the unitarity condition, introduced in the first chapter:

$$|u_\nu(N)|^2 + |v_\nu(N)|^2 = 1. \tag{4.14}$$

After some manipulation of (4.12), the following relation for e_ν can be obtained:

$$e_\nu^2 = (\epsilon_\nu - \frac{G_{\nu\nu}}{2} - \mu(N))^2 + \Delta_\nu(N)^2. \tag{4.15}$$

The reader can already recognize the BCS-like form of the quasiparticle excitation energy in this expression. Making use of (4.12) and summing over the quantum number ν while using (4.13) eventually leads to the following set of equations:

$$\begin{aligned} \Delta_\nu(N) &= \frac{1}{2}\sum_{\nu'} G_{\nu\nu'} \frac{\Delta_{\nu'}(N)v_{\nu'}^2(N)}{e_{\nu'} - (\epsilon_{\nu'} - \frac{G_{\nu'\nu'}}{2} - \mu(N))}, \qquad \forall\nu \\ \Omega - N + 2 &= \sum_\nu \frac{\Delta_\nu^2(N)}{[e_\nu(N) - (\epsilon_\nu - \frac{G_{\nu\nu}}{2} - \mu(N))]^2} v_\nu^2(N), \end{aligned} \tag{4.16}$$

with Ω denoting the number of all single-particle quantum states, i.e. $\Omega =: 2\sum_{\nu>0}$. Assuming the amplitudes $v_\nu(N)$, $\forall\nu$ to be known, (4.16) can now be solved for $\Delta_\nu(N)$ and $\mu(N)$. Then, the amplitudes can be calculated for $N-2$ particles with the following equation (this can be obtained by repeating the calculation that leads to 4.16 but not summing over ν)

$$v_\nu(N-2)^2 = 1 - \frac{\Delta_\nu(N)^2}{[e_\nu(N) - (\epsilon_\nu - \frac{G_{\nu\nu}}{2} - \mu(N))]^2} v_\nu(N)^2, \qquad \forall\nu, \tag{4.17}$$

and repeat the procedure all over again. Therefore, starting with $N = \Omega$, we have that $v_\nu(\Omega) = 1$, $\forall\nu$. Starting from this knowledge we can begin the recursive procedure until the desired particle number is reached. If the values of $\mu(N)$ are known, the system energies can be calculated by means of (4.11). In [40] it is argued that ignoring the N-dependence leads to the standard BCS expressions. It is easily

seen that omittance of particle number dependency, i.e. $v_\nu^2(N) \approx v_\nu^2(N-2) \equiv v_\nu^2$ leads to the standard BCS expressions:

$$v_\nu^2 = \frac{1}{2}\left[1 - \frac{\epsilon_\nu - \frac{G_{\nu\nu}}{2} - \mu(N))}{e_\nu(N)}\right], \qquad \forall\nu. \tag{4.18}$$

It is also illustrated in the paper that this particle-number conserving approach has an improved accuracy with respect to standard BCS theory, as can be seen in Figure 4.1.

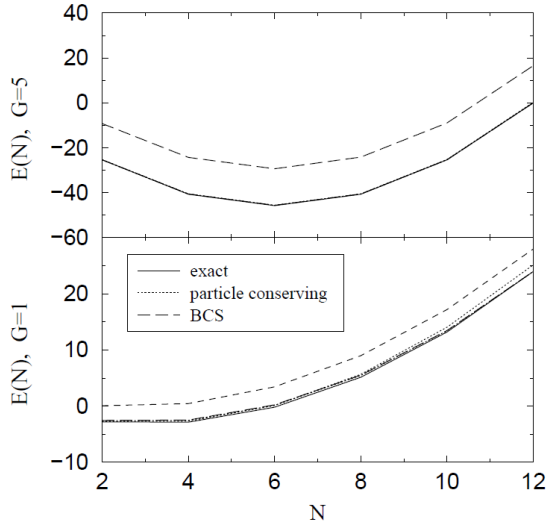


Figure 4.1: Comparison of standard BCS and the particle-conserving method. The system used is an equidistant model of 6 levels with degeneracies $\Omega = 1$ and single-particle energies $0, 1, 2, 3, 4, 5$. The pairing interaction matrix is set to a constant. This model is sometimes referred to as the *Picket-fence model* [50]. The figure is taken from [40].

4.2 Generalization by means of the quasispin algebra: The EOM approach

In this section, the method of Volya will be generalized and applied to the conserved charges (3.1) of the pairing Hamiltonian. The method of Volya can be generalized in the following way

- Instead of the fermion operators, the quasispin operators will be used to construct the equations of motion. This makes sense because the pairing Hamiltonian and its conserved charges can be written solely in terms of these operators. Through the Bethe Ansatz, we also have the knowledge that the eigenvectors are constructed with the $S^\dagger$-operators. Therefore, making use of the quasispin algebra makes more sense than utilizing the fermion operators which describe pair breaking when applied to pairing eigenstates. The use of the quasispin algebra immediately results in knowledge of the Casimir operator which can also be used instead of a set of equations of motion. Moreover, this identity is shared by all conserved charges. This can increase the chances of having an equivalence theorem like in chapter 3.

- The Hilbert space doesn't have to be fully truncated to allow only the ground state per particle-number sector. A bigger dimension of the Hilbert space can be allowed, which means more equations and matrices with dimension bigger than one. On the one hand, this will increase

the computational time. On the other hand, this will allow (low-lying) excited states to be described accurately together with the ground state. Furthermore, this will allow the user to improve the accuracy in a systematic way: if the desired accuracy is not reached, the dimension of the truncated Hilbert space can be increased and the calculations can be redone.

This generalization will be referred to as the ***Equations-of-motion approach (EOM)***. Because of the increased complexity of the approximation scheme (possibility of bigger truncated Hilbert space), a parametrization and manipulation towards a more BCS-like form will not be undertaken. However, it will turn out that neglecting the dependence of particle number in the fully truncated EOM will result in the standard BCS equations.

Making use of the $su(2)$ commutation relations, the following $2m$ equations of motion become[2] ($j \neq i$):

$$[R_i, S_i^\dagger] = S_i^\dagger + g \sum_{k \neq i} \left[-X_{ik} S_k^\dagger S_i^0 + Z_{ik} S_i^\dagger S_k^0 \right] \tag{4.19}$$

$$[R_i, S_j^\dagger] = g \left[-X_{ij} S_i^\dagger S_j^0 + Z_{ij} S_i^0 S_j^\dagger \right] \tag{4.20}$$

$$[R_i, S_i^0] = g \sum_{k \neq i} \left\{ \frac{1}{2} X_{ik} \left[-S_i^\dagger S_k + S_k^\dagger S_i \right] \right\} \tag{4.21}$$

$$[R_i, S_j^0] = \frac{g}{2} X_{ij} \left[S_i^\dagger S_j - S_j^\dagger S_i \right]. \tag{4.22}$$

The reader can quickly see that, when performing the sum over j in the last EOM (4.22), its right-hand side equals the right-hand side of (4.21). When these equations of motion will be evaluated with respect to the Hamiltonian eigenstates, they become matrix equations, just like in section 4.1. It will turn out that the left-hand side of the diagonal terms of (4.21) and (4.22) will both be equal to zero, thus making the two expressions not fully independent. Hence, this approach produces less equations than expected and it will turn out that additional information will be needed. Let's avoid future problems by discarding (4.21) and (4.22) completely and instead use the Casimir identity, as this will provide a sufficient amount of equations. The Casimir operator takes the following form after using the commutation relation $[S^\dagger, S] = 2S^0$:

$$S_l^\dagger S_l - S_l^0 + (S_l^0)^2 = d_l(d_l + 1), \qquad \forall l. \tag{4.23}$$

Let's evaluate these EOM and the Casimir identities with respect to N-particle and $(N-2)-$particle eigenstates where a label α is assigned to. This label can denote the relative position of the excited state: $\alpha = 1$ can be referred to as the ground state, $\alpha = 2$ as the first excited state, etc... It is important to note that this label doesn't describe different seniority states because the seniority is already fixed in the Casimir identities. As already stated above, the identity operator of the full Hilbert space takes the form of (4.7). Equations (4.19) and (4.20) are now evaluated with $\langle N_\alpha | \dots | (N-2)_{\tilde{\beta}} \rangle$ and (4.23) with $\langle N_\alpha | \dots | N_\beta \rangle$. The excitation index of the $(N-2)$-particle sector will always be denoted with a

[2] m is the number of energy levels, as always.

tilde. With the application of the identity operator in the suitable places, the equations become:

$$\begin{aligned}
&(E_\alpha(N) - E_{\tilde{\beta}}(N-2) - 1)(S_i^\dagger)_{\alpha\tilde{\beta}} = g\sum_{k\neq i}\Big[-X_{ik}(S_k^\dagger)_{\alpha\tilde{\gamma}}(S_i^0)_{\tilde{\gamma}\tilde{\beta}}(N-2) + Z_{ik}(S_i^\dagger)_{\alpha\tilde{\gamma}}(S_k^0)_{\tilde{\gamma}\tilde{\beta}}(N-2)\Big] \\
&(E_\alpha(N) - E_{\tilde{\beta}}(N-2))(S_j^\dagger)_{\alpha\tilde{\beta}} = -gX_{ij}(S_i^\dagger)_{\alpha\tilde{\gamma}}(S_j^0)_{\tilde{\gamma}\tilde{\beta}}(N-2) + gZ_{ij}(S_i^0)_{\alpha\gamma}(N)(S_j^\dagger)_{\gamma\tilde{\beta}}, \qquad \forall j \neq i \\
&(S_l^\dagger)_{\alpha\tilde{\gamma}}(S_l)_{\tilde{\gamma}\beta} - (S_l^0)_{\alpha\beta}(N) + (S_l^0)^2_{\alpha\beta}(N) = d_l(d_l+1)\delta_{\alpha\beta}, \qquad l = 1,2,...,m.
\end{aligned} \tag{4.24}$$

Einstein summation over the double γ- and $\tilde{\gamma}$-indices is always implied. The following definitions were introduced in the above set of equations:

$$\begin{aligned}
&(S_j^\dagger)_{\alpha\tilde{\beta}} \equiv \langle N_\alpha|\, S_j^\dagger\, |(N-2)_{\tilde{\beta}}\rangle \\
&(S_j^0)_{\alpha\beta}(N) \equiv \langle N_\alpha|\, S_j^0\, |N_\beta\rangle \\
&(S_j)_{\tilde{\alpha}\beta} \equiv \langle (N-2)_{\tilde{\alpha}}|\, S_j\, |N_\beta\rangle = \left[\left(S_j^\dagger\right)_{\beta\tilde{\alpha}}\right]^\dagger.
\end{aligned} \tag{4.25}$$

The correct number of particles can now be imposed through the S^0-operator, which is proportional to the number operator. This results in the following set of equations:

$$\sum_l \left(S_l^0\right)_{\alpha\alpha}(N) = \frac{N}{2} - \frac{1}{2}\sum_l \Omega_l, \qquad \forall\alpha, \tag{4.26}$$

with as always $\Omega_j = j + 1/2$. Instead of using the entire Hilbert space, its dimension can now be truncated to obtain a smaller subspace. Let's denote the dimension of the truncated Hilbert space of N particles as ζ and $\tilde{\zeta}$ for the $(N-2)$-particle space.

The equations (4.24) and (4.26) together account for $m\zeta\tilde{\zeta} + m\zeta^2 + \zeta$ equations and the unknown variables are the matrices $E_\alpha(N)$, $(S_j^\dagger)_{\alpha\tilde{\beta}}$, $(S_j^0)_{\alpha\beta}(N)$, which form an equal amount of unknowns. The quantities with an $(N-2)$-dependency are assumed to be known just like in the Volya method. We can for example start with the vacuum $(N-2) = 0$ where the quantities $S^0(0)$ and $E(0)$ are known. With this knowledge, we can solve the equations for the N-dependence and work our way up to the desired particle number. For ease of notation, a particle-number dependence of the $S^\dagger$-operators in (4.24) was omitted. However, it is important to remark that such a particle-number index is implicitly assumed when starting the recursive procedure by increasing the particle number

The S^0-operators in (4.24) have both N- and $(N-2)$-dependence. However, the reader can notice that on the operator level, i.e. (4.19)-(4.22), the factors on the right-hand side can be swapped because of the fact that $i \neq k, j$. This has the consequence that the equations of motion on matrix level, i.e. (4.24), can be made more symmetrical: we can for example choose to only have an $(N-2)$-dependence of the S^0-matrices in the first two sets of equations of (4.24). Throughout this thesis we will refer to the EOM with only one kind of S^0-operator in the first 2 sets of (4.24) as the ***symmetrized EOM (SEOM)***.

Reality of the quasispin matrices

The quasispin matrices can always be assumed real since they are real in the exact (non-truncated) case. Indeed, in [38] it is proved that the matrix elements in the exact case can always be written as

the determinant of a real matrix. This matrix contains functions $\Lambda^x(\epsilon_i)$ with x denoting the set of rapidities of the Bethe Ansatz. Despite the fact that the rapidites can become complex, Λ is always real because

$$\Lambda^x(\epsilon_i) = \sum_\alpha \frac{1}{\epsilon_i - x_\alpha}, \tag{4.27}$$

and the rapidities always come in complex conjugate pairs. Also, since the conserved charges are Hermitian operators, its eigenvalues are real and linear combinations of eigenstates with degenerate eigenvalues can always chosen to be real.

4.3 Numerical approach to solving the EOM

A PYTHON routine was programmed to solve the EOM for arbitrary truncation. Starting from the vacuum state, a (truncated) basis set is first created with UPF vectors with particle number $N = 2$, $N = 4$, etc... This basis set serves as an initial guess for very small g as these basis vectors are eigenstates for $g = 0$. Therefore, the starting point of the routine is at very small g. For a certain g, the unknowns are solved for every particle number and these solutions are then used as an initial guess for the next g. For the solving process, the routine make use of the `fsolve` method from the NUMPY-package [51], based on the NR-method. However, these equations are non-linear and capable of having multiple solutions. Indeed, besides the imposed equations (4.24) and (4.26) there are many more equations the exact solution (without truncation) has to obey. The equations (4.21) and (4.22) that were omitted for example, or the matrix form of the quasispin algebra commutation relations. Together, all these equations constitute one unique solution that coincides with exact diagonalization[3]. Omitting certain equations opens up the possibility of multiple solutions, with many of them maybe not physical, for example the occurrence of a negative occupation amplitude. One always has to check whether the obtained solutions are physical in nature. Also, because of the possibility of multiple solutions, the output can be sensitive to the initial guess. If the wrong initial guess is chosen, the possibility can occur that the solution does not include the ground state in the truncation scheme. To know which basis vector can give rise to the ground state, one can consider a perturbation expansion in small g. After all, the basis vectors are eigenstates for $g = 0$ and when g is gradually turned on, these new eigenstates originate as a continuous deformation of the initial basis vector. In Appendix D, a small g treatment is discussed for the exact solutions and the eigenstate energies can be calculated, starting from an initial distribution (or UPF basis vector). This ultimately boils down to finding the zeroes of the associated Laguerre polynomials. In this way, it can be determined which basis vector has the best chance of having the largest contribution to the ground state. This method is based on a Heine-Stieltjes connection [52, 53].

For the N-particle sector, it is always best to choose an initial guess that *fully connects* with a guess of the $(N-2)$-sector. With this term we mean that the N-sector basis vector can be constructed from the $(N-2)$-sector basis vector by applying an $S^\dagger$-operator. Let's consider g to be very small so that the calculated eigenstates are very close to the UPF basis vectors. Consequently, the overlap of the obtained N-sector ground state with the N-sector initial guess should be very large. Applying the truncated identity operator after the first creation operator of the overlap gives us following expression for the overlap, which has to be close to unity:

$$\frac{1}{\text{Norm}} \langle N_{GS}| S^\dagger_{j_1} |(N-2)_{\tilde{\gamma}}\rangle \langle (N-2)_{\tilde{\gamma}}| S^\dagger_{j_2} ... |\theta\rangle \approx 1. \tag{4.28}$$

[3]Note that this 'one' solution includes information of **all** states $|\alpha\rangle$ with the number of states depending on truncation.

The symbol 'Norm' represents the normalization factor of the UPF basis vector and can be calculated with the help of (2.8). It is now clear that, when no vector connects in the right way, the overlap becomes zero and the approximation becomes meaningless. This bad ground state will then be used as an initial guess for the next g in the recursion scheme. It can be concluded that it is best that the initial guesses are connected through the creation operators so expressions like (4.28) have maximal overlap.

4.4 Equivalence theorem and relation with standard BCS theory

Equivalence of full truncation

Just like for standard BCS theory, the equivalence theorem for the conserved charges can be proven in the fully truncated case, where the dimensions of all particle-number sectors are set to 1 like in the Volya method. However, in order for the theorem to hold, the SEOM must be used so that only S^0-operators with the same particle-number dependence appear in each equation.

Theorem 7. *(SEOM equivalence theorem) The fully truncated symmetrized EOM are equivalent for every conserved charge of an integrable m-level pairing system.*

To fix ideas, the SEOM of 2 conserved charges R_i and R_k of a 3-level system with levels i, k, k' are written down below. The particle-number dependence of the S^0-operators is omitted for ease of notation. The conserved charges share the same number- and Casimir equations.

- R_i :

$$\begin{cases} \Big[E^i_\alpha(N) - E^i_{\tilde\beta}(N-2) - 1\Big]\,(S^\dagger_i)_{\alpha\tilde\beta} = -gX_{ik}(S^\dagger_k)_{\alpha\tilde\gamma}(S^0_i)_{\tilde\gamma\tilde\beta} + gZ_{ik}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_k)_{\tilde\gamma\tilde\beta} \\ \qquad\qquad\qquad\qquad\qquad\qquad - gX_{ik'}(S^\dagger_{k'})_{\alpha\tilde\gamma}(S^0_i)_{\tilde\gamma\tilde\beta} + gZ_{ik'}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_{k'})_{\tilde\gamma\tilde\beta} \\ \Big[E^i_\alpha(N) - E^i_{\tilde\beta}(N-2)\Big]\,(S^\dagger_k)_{\alpha\tilde\beta} = -gX_{ik}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_k)_{\tilde\gamma\tilde\beta} + gZ_{ik}(S^\dagger_k)_{\alpha\tilde\gamma}(S^0_i)_{\tilde\gamma\tilde\beta} \\ \Big[E^i_\alpha(N) - E^i_{\tilde\beta}(N-2)\Big]\,(S^\dagger_{k'})_{\alpha\tilde\beta} = -gX_{ik'}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_{k'})_{\tilde\gamma\tilde\beta} + gZ_{ik'}(S^\dagger_{k'})_{\alpha\tilde\gamma}(S^0_i)_{\tilde\gamma\tilde\beta}. \end{cases} \tag{4.29}$$

- R_k :

$$\begin{cases} \Big[E^k_\alpha(N) - E^k_{\tilde\beta}(N-2) - 1\Big]\,(S^\dagger_k)_{\alpha\tilde\beta} = -gX_{ki}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_k)_{\tilde\gamma\tilde\beta} + gZ_{ki}(S^\dagger_k)_{\alpha\tilde\gamma}(S^0_i)_{\tilde\gamma\tilde\beta} \\ \qquad\qquad\qquad\qquad\qquad\qquad - gX_{kk'}(S^\dagger_{k'})_{\alpha\tilde\gamma}(S^0_k)_{\tilde\gamma\tilde\beta} + gZ_{kk'}(S^\dagger_k)_{\alpha\tilde\gamma}(S^0_{k'})_{\tilde\gamma\tilde\beta} \\ \Big[E^k_\alpha(N) - E^k_{\tilde\beta}(N-2)\Big]\,(S^\dagger_i)_{\alpha\tilde\beta} = -gX_{ki}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_i)_{\tilde\gamma\tilde\beta} + gZ_{ki}(S^\dagger_i)_{\alpha\tilde\gamma}(S^0_k)_{\tilde\gamma\tilde\beta} \\ \Big[E^k_\alpha(N) - E^k_{\tilde\beta}(N-2)\Big]\,(S^\dagger_{k'})_{\alpha\tilde\beta} = -gX_{kk'}(S^\dagger_k)_{\alpha\tilde\gamma}(S^0_{k'})_{\tilde\gamma\tilde\beta} + gZ_{kk'}(S^\dagger_{k'})_{\alpha\tilde\gamma}(S^0_k)_{\tilde\gamma\tilde\beta}. \end{cases} \tag{4.30}$$

- Shared equations:

$$\begin{cases} (S^\dagger_l)_{\alpha\tilde\gamma}(S_l)_{\tilde\gamma\beta} - (S^0_l)_{\alpha\beta} + (S^0_l)^2_{\alpha\beta} = d_l(d_l+1)\delta_{\alpha\beta}, \qquad l = i,k,k'. \\ \sum_l \left(S^0_l\right)_{\alpha\alpha}(N) = \frac{N}{2} - \frac{1}{2}\sum_l \Omega_l, \qquad \forall\alpha. \end{cases} \tag{4.31}$$

Proof. The upper index on the energies refers to the type of conserved charges. The notion of full truncation means that the lower Greek index dependence is omitted and the matrices become numbers,

for example

$$\begin{aligned} E^i_\alpha(N) &\to E^i(N) \\ (S^\dagger_i)_{\alpha\tilde{\beta}} &\to S^\dagger_i. \end{aligned} \tag{4.32}$$

To ease notation, a chemical potential[4] $E^i(N) - E^i(N-2) \equiv \lambda^i$ will be defined. Just as in the equivalence theorem of BCS, the first equation of R_i, for example, will be denoted as $(1)^i$.

Now, all equations $(n)^i$ for R_i, except for the first one, can be written as

$$\frac{\lambda_i}{gS^\dagger_i} = -X_{in}\frac{S^0_n}{S^\dagger_n} + Z_{in}\frac{S^0_i}{S^\dagger_i}, \qquad \forall n \neq i. \tag{4.33}$$

The left-hand sides of these equations are equal, so we can write down the following:

$$-X_{ik}\frac{S^0_k}{S^\dagger_k} + Z_{ik}\frac{S^0_i}{S^\dagger_i} = -X_{ij}\frac{S^0_j}{S^\dagger_j} + Z_{ij}\frac{S^0_i}{S^\dagger_i}, \qquad \forall k, j \neq i. \tag{4.34}$$

From here on, the proof is completely analogous to the BCS case if the following substitution is performed:

$$\begin{cases} S^\dagger \to uv \\ S^0 \to u^2 - v^2 \\ \lambda \to -\dfrac{2\lambda}{\Omega}. \end{cases} \tag{4.35}$$

Consequently, the theorem can be considered proven. □

Just like in the case of the equivalence theorem in chapter 3, the chemical potentials can be seen as fine-tuning parameters. They adjust themselves in such a way that an equivalence of the S^0- and $S^\dagger$-quantities is reached. The substitution (4.35) doesn't appear out of the blue, as will be demonstrated in the next theorem. It turns out that the BCS equations and the EOM are equivalent in a certain simplification limit, analogous to the Volya method:

Theorem 8. *The fully truncated equations of motions reduce to the standard BCS equations in the limit where*

1. *the particle-number dependence of the S^0_j-operators is neglected*
2. *$\Omega_j \to \infty$*

for each energy level with index j.

Proof. A (discrete) chemical potential can be defined as $\lambda = \frac{E(N)-E(N-2)}{2}$. In this simplification limit the (N)- and $(N-2)$-dependence of the S^0 operators is neglected:

$$S^0(N) \approx S^0(N-2) \equiv S^0. \tag{4.36}$$

[4]This can be regarded as the discrete version of the classical definition of a chemical potential: $\lambda = \frac{\partial E}{\partial N}$, hence the name.

The fully truncated EOM reduce to

$$[2\lambda - (1 + \sum_{k\neq i} Z_{ik} S^0_k)] S^\dagger_i = \Delta_i S^0_i \tag{4.37}$$

$$\left[2\lambda - g Z_{ik} S^0_i\right] S^\dagger_k = \Delta_k S^0_k, \qquad \forall k \neq i \tag{4.38}$$

$$\sum_j S^0_j = \frac{N}{2} - \frac{1}{2}\sum_j \Omega_j \tag{4.39}$$

$$(S^\dagger_j)^2 + (S^0_j)^2 = \frac{1}{2}\Omega_j(\frac{1}{2}\Omega_j + 1), \qquad \forall j, \tag{4.40}$$

where we defined the gaps to be

$$\begin{aligned} \Delta_i &= -g \sum_{k\neq i} X_{ik} S^\dagger_k \\ \Delta_k &= -g X_{ik} S^\dagger_i, \end{aligned} \tag{4.41}$$

and we made use of the fact that $(S^\dagger)^T = S^\dagger = S$ in the fully truncated approximation where matrices reduce to numbers. The BCS equations and the EOM share the same particle-number equation (4.39). Now the Casimir identity will be used to show that (4.37) and (4.38) are equivalent to the BCS equations (3.6). Let's start by rewriting the S^0-matrix element in the following way[5] ($\Omega = j+1/2$)

$$\begin{aligned} \left(\frac{S^0}{\Omega}\right) &\overset{(2.1)}{=} \frac{1}{2\Omega}\,(n - \Omega) \\ &= \frac{1}{2}\left(\frac{n}{\Omega} - 1\right) \\ &= \frac{1}{2}\left(2v^2 - 1\right) \\ &= \frac{1}{2}\left(v^2 - u^2\right), \end{aligned} \tag{4.42}$$

where $v^2 (= \frac{n}{2\Omega})$ is the occupation probability of the j'th energy level. The Casimir identity imposes following expression for $S^\dagger$:

$$\left(\frac{S^\dagger}{\Omega}\right)^2 = \frac{n}{2\Omega} - \left(\frac{n}{2\Omega}\right)^2 + \frac{1}{2\Omega}. \tag{4.43}$$

In the BCS equations the term u^2v^2 appears. This can be rewritten as $\frac{n}{2\Omega} - \left(\frac{n}{2\Omega}\right)^2$. From these results we see that, in the proposed limit

$$\frac{S^\dagger}{\Omega} \to uv. \tag{4.44}$$

Collecting all these results and taking into account the multiplication factor $R_i \to 2R_i$, we are left with the modified BCS equations (3.6). □

It is important to note that the omittance of particle-number dependence is a simplification which is not the result of a limit where the system size goes to infinity: Let's consider all degeneracies and the particle number going to infinity. Then of course, it is probable that the number of particles n_j in a certain energy level j also goes to infinity. If both n_j and Ω_j go to infinity, the eigenvalues of the

[5] with the energy index j omitted to ease the notation.

S_j^0 operator take the form of $\infty - \infty$ which of course can be finite. In that case $S^0(N-2)$ does not necessarily converge towards $S^0(N)$:

$$S^0(N-2) \nrightarrow S^0(N). \tag{4.45}$$

Consequently, the simplification of the EOM is not trivial and therefore not the result of a limit where the system size goes to infinity.

Equivalence of partial truncation

Now, the question arises whether the truncated EOM are equivalent even in the partially truncated case. Our conjecture is that the EOM are equivalent if the same amount of truncation is applied for each particle-number sector. This can be checked numerically by switching levels of a pairing system and using the same initial guesses. For example, it was checked and found to be true for example 3 below. The amount of truncation is depicted in an array $[\zeta_1, \zeta_2, ..., \zeta_{\frac{N}{2}-1}]$. The array elements depict the dimension of the truncated Hilbert space for each particle number sector. The first element ζ_1, for example, always denotes the dimension of the vacuum which is of course always 1. The second element ζ_2 denotes the dimension of the $N = 2$-sector, etc...

Example 3

$$\begin{cases} m = 3 \\ \text{COM 1 : } \epsilon_1 = [6, 4, 2] \\ \text{COM 2 : } \epsilon_2 = [4, 6, 2] \\ \Omega = [4, 4, 4] \\ N_{\text{part}} = 4 \\ g = -5 \\ \text{truncation} = [1, 1, 2]. \end{cases}$$

If the right guess is used to obtain the ground state of COM 1, that same initial guess gives rise to the same set of S^0- and $S^\dagger$-matrices as a solution for the equations of COM 2. The equivalence of this system has also been checked for the hyperbolic parametrization of RG integrability, introduced in subsection 2.1.4. The truncation technique involves shrinking the Hilbert space and consequently shrinking the identity operator. However, when deriving the truncated EOM it was assumed that these truncated solutions are also eigenvectors of the conserved charge: the property $H|N_\alpha\rangle = E_\alpha|N_\alpha\rangle$ was used. Basically this comes down to taking a full basis set, constructing the Hamiltonian matrix, then leaving out the rows and columns corresponding to the basis vectors that we want to eliminate and then diagonalizing the smaller matrix. On a general note, 2 matrices can be considered that commute $[A, B] = 0$. We can now eliminate, for example, the last row and column of the matrices. In general, these matrices won't commute any more which in turn means that they don't share a common eigenbasis. An example of this can be found by looking at the matrices (3.62). These matrices commute but omitting their last row and column doesn't preserve this property. This means that applying the truncating technique to commuting operators doesn't necessarily result in equivalent equations of motions. This equivalence thus appears to be typical for the conserved charges of the pairing Hamiltonian. The same conclusion was reached with standard BCS theory in section 3.7. In general, the same variational ansatz of 2 commuting operators doesn't necessarily result in the same parameter equations as a counterexample was found.
As already shown, the equivalence of the fully truncated EOM is proved using the same approach as in the standard BCS case. When not truncating fully, this approach can't be applied any more because

of the fact that all algebraic operations over $\mathbb{R}$ in the proof of theorem 7 need to be replaced with matrix algebra. A proof of the equivalence conjecture of partial truncation hasn't been found yet.

4.5 Examples of many-body systems

In [40] it is commented that an EOM approach can result in a considerable gain in accuracy with respect to standard BCS theory for smaller many-body systems. Also, the large freedom of choice for the initial guess provides good hopes of an accurate treatment for (partially) repulsive constants of motions. In this section, a few examples will be given and it will be shown that this treatment is indeed accurate for repulsive Hamiltonians.

- Let's consider a *fully repulsive* example:

  Example 4

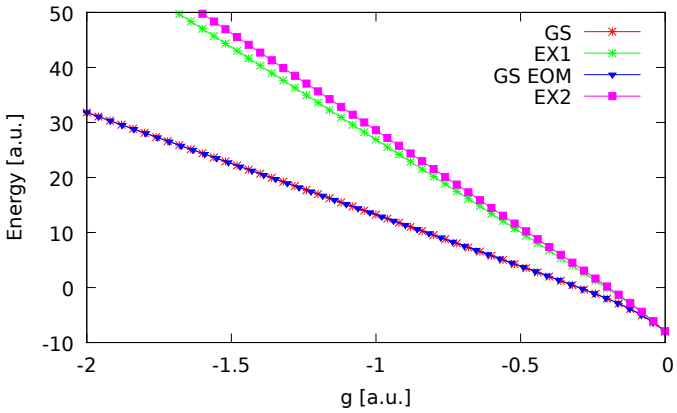
  $$\begin{cases} m = 4 \\ \epsilon = [1, 3, 2, 4] \\ \Omega\,(= j + 1/2) = [8, 8, 8, 8] \\ N_{\text{part}} = 4 \\ g = [-2 : 0] \\ \text{truncation} = [1, 1, 1]. \end{cases}$$

  The fully truncated EOM are solved and compared with the exact results in Figure 4.2. The ground-state energy comparison is shown together with the first exact excited states. It can be seen that the truncated solution is in excellent agreement with the exact case. When utilizing the developed PYTHON routine, it's quickly noticeable that it becomes more challenging to find a solution for conserved charges with repulsive pairing parts. Sometimes convergence is not achieved and more ingenious initial guesses need to be used. Anyhow, it can always be checked if the obtained solution approximates the ground state when g is turned on by looking at the occupation amplitudes for small g. For this particular example, the Heine-Stieltjes method in Appendix D predicts that for small g, the ground state is a perturbation on top of the `[0,0,2,0]` basis vector. Let's explain this basis vector notation first. The value N_{pair} of array element l denotes the number of pairs that occupy energy level l. Since 8 pairs can occupy every level ($\Omega_j = 8$, $\forall j$), the occupation amplitude of the second non-principal level should lie close to and evolve continuously from 0.25 for small g. This can indeed be observed in Figure 4.2.

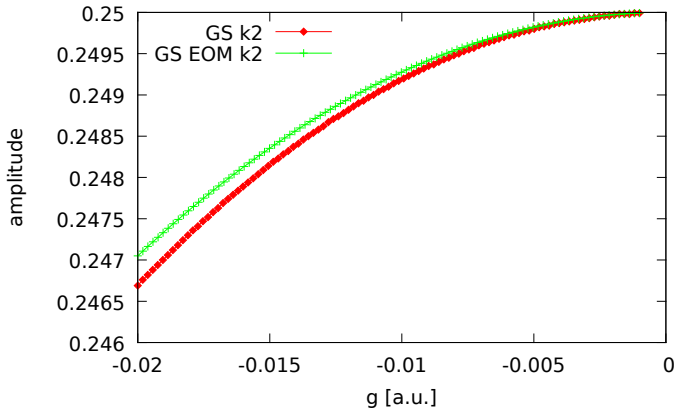
- The following example is one with both *attractive and repulsive parts* and full truncation. The result are shown in Figure 4.3. Again, the EOM results are in good agreement with the exact results.

  Example 5

  $$\begin{cases} m = 4 \\ \epsilon = [3, 4, 2, 1] \\ \Omega = [8, 8, 8, 8] \\ N_{\text{part}} = 6 \\ g = [-2 : 0] \\ \text{truncation} = [1, 1, 1, 1] \end{cases}$$

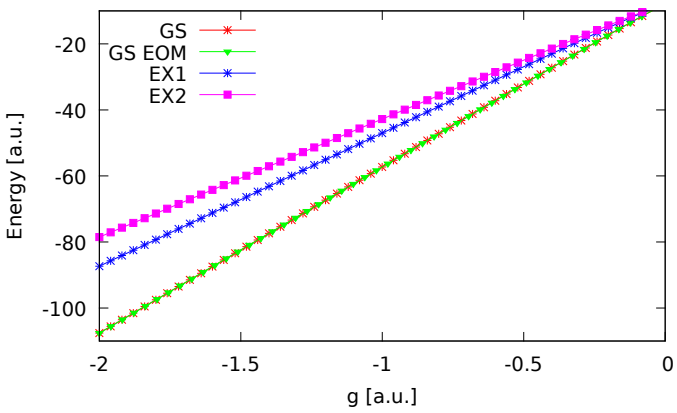


(a) Exact energy spectrum of the low-lying states together with the EOM approximation of the ground state (GS EOM).

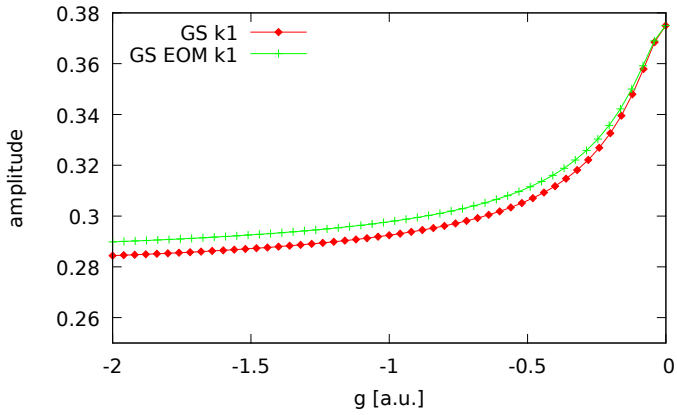


(b) Exact occupation amplitude of the second non-principal level (k2) for small g, together with its EOM approximation

Figure 4.2: Energy spectrum and small g depiction of the occupation amplitude of the second non-principal level (k2) of example 4.



(a) Low-lying energy spectrum.



(b) Occupation amplitude of the second non-principal level (k2).

Figure 4.3: Exact energy spectrum and occupation amplitude of the first non-principal level (k1) of example 5, together with the EOM approximation.

- *Partial truncation:* We can always take into account more than one basis vector in each particle sector. If the last particle-number sector is only partially truncated, excited states can also be approximated. Moreover, one can experiment with different initial guess basis vectors added to the 'ground-state-induced' basis vector predicted by the Heine-Stieltjes small g treatment. In this way, it can be determined if a newly added basis vector has a big contribution on the ground state (or excited state). This is done in the next example.

Example 6

$$\begin{cases} m = 3 \\ \epsilon = [6, 4, 2] \\ \Omega = [4, 4, 4] \\ N_{\text{part}} = 4 \\ \text{trunc } 1 = [1, 1, 1] \\ \text{trunc } 2 = [1, 2, 2] \\ \text{trunc } 3 = [1, 3, 3]. \end{cases}$$

Here, a full truncation is first performed and then 2 partial truncations are performed. For the full truncation, basis vectors were chosen that are not predicted through the Heine-Stieltjes connection to be the onset of the ground state, for instructional purposes. In this way, the full-truncation approximation is not so accurate and a distinctive improvement is noticeable when adding basis vectors. The two partial truncations are constructed by adding basis vectors on top of the vectors that were already used in the previous truncation. The results for the ground-state energy are shown in Figure 4.4. Here it can be seen that the firstly added basis vectors (trunc 2) on top of trunc 1 have little contribution to the ground state but the secondly added basis vectors (trunc 3) result in a distinct improvement of the ground-state approximation.

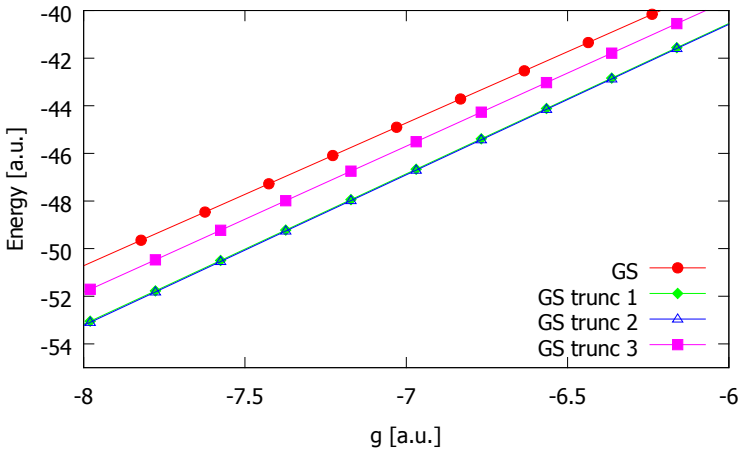


Figure 4.4: Ground-state EOM approximation of example 6 with different types of truncation.

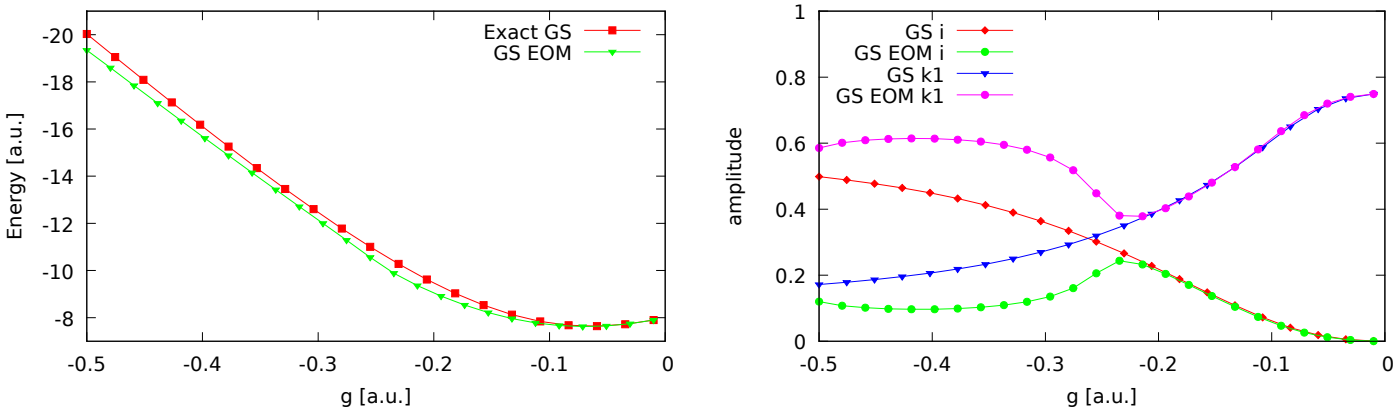
- The examples discussed so far don't contain many particles. In the next example, an attempt is made to treat a more intricate example with 12 particles:

Example 7

$$\begin{cases} m = 4 \\ \epsilon = [1, 2, 3, 4] \\ \Omega = [8, 8, 8, 8] \\ N_{\text{part}} = 12 \\ g = [-2 : 0] \\ \text{full truncation.} \end{cases}$$

It is seen in Figure 4.5 that the result of the ground-state energy is in fairly good agreement with the exact solution but a peculiar thing happens with the occupation amplitudes: At $g \approx -0.2$ the amplitudes begin to severely deviate from the exact solution and even seem to converge towards the other level occupation beyond $g = -0.5$. The reason why no results are shown beyond this value is because the PYTHON solver hasn't reached convergence for these values. Playing around with the initial guess values and partial truncation didn't produce the desired results as no solutions were found. Clearly, the EOM approach can't handle the crossing of the level amplitudes. Also, for more than 12 particles no solutions are found as the Python solver again hasn't reached convergence for both full truncation and partial truncation in the $N_{part} = 14$-sector.

Of course, the EOM approach is an approximation method and one can relax the condition that says that the truncated EOM have to be solved exactly to obtain reasonable approximations. If these truncated EOM are 'approximately' solved, maybe some good energy approximations can come out of it. This can be done with an optimization procedure of a functional, which will be discussed in the next section. The advantage of an optimization procedure with respect to an exact solving method is that a minimum will (almost) always be found. Of course this minimum won't necessarily be the global minimum of the functional, depending on the initial guess that is passed to the minimizer.



(a) Exact ground-state energy together with the fully-truncated EOM approximation for 12 particles.

(b) Exact and approximate occupation amplitudes for the principal level (i) and the first non-principal level (k1).

Figure 4.5: Energy spectrum and occupation amplitudes of example 7.

4.6 Generalization of the EOM approach

4.6.1 General theory

In the last example it became clear that the EOM approach can't seem to handle amplitude level crossings and the difficulty of finding solutions to the truncated equations is an undesirable feature. As already stated above, it is not clear whether solutions to the equations actually exist or if the solution can't be found due to a failure of the NR-method. A more efficient approach would be to convert the problem to an optimization problem instead of solving a set of non-linear equations exactly. This is essentially what is done in [41]. Let's consider the most general form of this method by introducing a time-independent Hamiltonian $\mathcal{H}$ that can be written in terms of a set of operators

$\{X_\nu\}$ belonging to a certain Lie-algebra with commutation relations[6]

$$[X_\mu, X_\nu] = C^\sigma_{\mu\nu} X_\sigma. \tag{4.46}$$

Again, the commutators $[\hat{X}_\nu, \hat{H}]$ can be calculated and a set of equations with matrix elements can be constructed. This is formally done by introducing an irrep $|p\rangle$ and evaluating the equations of motions with respect to this irrep, just like in (4.24). However, instead of solving these equations exactly for the algebra matrix elements, the following functions can be defined:

$$f^{(2)}_{pq}(\nu) =: \langle p| \left[\mathcal{H}, X_\nu\right] |q\rangle - (E_p - E_q) \langle p| X_\nu |q\rangle . \tag{4.47}$$

Additional functions can be defined by taking into account the irrep of the algebra:

$$f^{(1}_{pq}(\mu, \nu) =: \langle p| \left[X_\mu, X_\nu\right] |q\rangle - C^\sigma_{\mu\nu} \langle p| X_\sigma |q\rangle . \tag{4.48}$$

Then the functional $\mathcal{F}$ can be defined as

$$\mathcal{F} =: \sum_{p,q}^{\mathcal{D}} \left\{ \sum_\nu \left| f^{(2)}_{pq}(\nu) \right|^2 + \sum_{\mu\nu} \left| f^{(1)}_{pq}(\mu, \nu) \right|^2 \right\}, \tag{4.49}$$

with $\mathcal{D}$ the dimension of the Hilbert space. At this point the Hilbert space includes all particle-number sectors. The truncation process now simply consists of choosing $\mathcal{D}$ smaller than the actual dimension. This functional now has to be minimized and an approximation of the matrix elements arises. If the Hamiltonian contains particle-number conservation, the desired number of particles can be imposed by constructing an additional expression containing the algebra operator that is connected to the counting operator. The problem can now be seen as a minimization problem with a particle-number constraint. In this way, the same procedure as the EOM approach applies: a recursive procedure, starting from the $N_{\text{part}} = 2$-sector and going up to the desired particle number, can be performed. It has to be noted that (4.49) is only a symbolic/schematic portrayal of the functional if the fixed particle-number approach is used: the dimension symbol $\mathcal{D}$ of course will depend on the N_{part}-sector. One can also choose not to use such recursive approach and construct the functional with all particle sectors simultaneously. The drawback of this method is that S^0-matrices will be obtained that don't conserve particle number exactly, as this is not imposed explicitly. The advantage of a minimization method is that a minimum can always be found even if the functional does not reach zero exactly. Instead of ,or additional to the functions $f^{(1)}$ the Casimir identities of the Lie-algebra can be imposed as an extra function so the total functional becomes

$$\mathcal{F} =: \sum_{p,q}^{\mathcal{D}} \left\{ \sum_\nu \left| f^{(2)}_{pq}(\nu) \right|^2 + \sum_{\mu\nu} \left| f^{(1)}_{pq}(\mu, \nu) \right|^2 + \sum_n \langle p| (\hat{\mathscr{C}}_n - c_n)\delta_{pq} |q\rangle \right\}, \tag{4.50}$$

with $\hat{\mathscr{C}}_n$ and c_n respectively the Casimir operators and their eigenvalues of the Lie-algebra. It is up to the user to decide how many functions are used in the functional. Computational minimization routines are widespread: Maple and Matlab offer excellent minimization procedures and in this thesis the function `minimize` of the Scipy-package [54] was used.

A consequence of truncating the Hilbert space to smaller dimensions is that the most significant errors are made in the outer corners of the truncation matrices[7], as explained in [41]. The elements

[6] Einstein summation implied.

[7] By truncation matrices, we mean the matrix form of the EOM (4.24) and all the quasispin operators.

closest to the outer row and column of the truncation matrix are most severely affected by truncation and therefore least reliable. The contribution of the largest errors can be reduced by introducing an appropriate weighting scheme: The functional can be provided with a weight factor w_{pq}:

$$\mathcal{F} =: \sum_{p,q}^{\mathcal{D}} w_{pq}^2 \left\{ \sum_{\mu} \left| f_{pq}^{(2)}(\nu) \right|^2 + \sum_{\mu\nu} \left| f_{pq}^{(1)}(\mu,\nu) \right|^2 \right\}, \tag{4.51}$$

with $w_{pq} = \frac{1}{(p+1)(q+1)}$. Basically this means that the there is less contribution of the outer rows and columns in the functional, where the interaction with the discarded states is most important.

4.6.2 Application of the functional approach

For the conserved charges, the previously used equations were constructed as a functional and equations (4.21) and (4.22) were also added to the functional. First of all, we shall illustrate that this optimization approach can be prone to multiple local minima. As an example, the solutions of the fully truncated EOM approach of example 7 for $g = 0.01$ were given as an initial guess for the fully truncated optimization function without the usage of (4.21) and (4.22 . Because the EOM were solved exactly, the functional obviously reaches its lowest value at exactly zero for this solution. Inserting the solution in the functional indeed resulted in a value of order 10^{-20}. Then the optimization procedure was performed with this initial guess and another local minimum was found, with function value of order 0.001, and mismatching occupation amplitudes: the first non-principal level has an amplitude of $v_{k1}^2 \approx 0.538$, while the exact solution of the truncated EOM resulted in $v_{k1}^2 \approx 0.749$. It is clear that non-trivial local minima exist that don't necessarily resemble the real physical situation.

A first attempt to an improvement is made by truncating all sectors fully, except for the last one. In the $N_{\text{part}} = 12$-sector the Hilbert space dimension is set to 2. This can be summarized in the following truncation array: `[1,1,1,1,1,1,2]`. The results are depicted in Figure 4.6. It can be seen that the energy approximation of the ground state (GS EOM) is worse than in the exact solving approach in the fully truncated case (Figure 4.5). Also, the second energy state denoted by (EX1 EOM) doesn't seem to make a lot of sense as an approximation of an excited state or the ground state. The solution seems to be stuck in some local minimum that doesn't resemble a physical situation. Several attempts were made to obtain a different local minimum by playing around with the initial guess values but no valid approximation values were found.

Another approach is to take more basis vectors into account in the lower particle sectors. As an example, the following truncation array was used: `[1,2,2,2,2,2,2]`. The results of this approach are given in Figure 4.7. It can be seen that the results in the $N_{\text{part}} = 10$-sector are still reasonable and the EOM-minimizing approach seems to handle the level crossing rather well. However, it is also seen that the results are less accurate than the previously discussed examples in this section with less number of particles. In the $N_{\text{part}} = 12$-sector the results are not so promising. The ground-state energy is pretty far off and the occupation amplitude of the principal level doesn't resemble the exact solution in any way. It seems that a local minimum was reached that doesn't resemble the real physical situation.

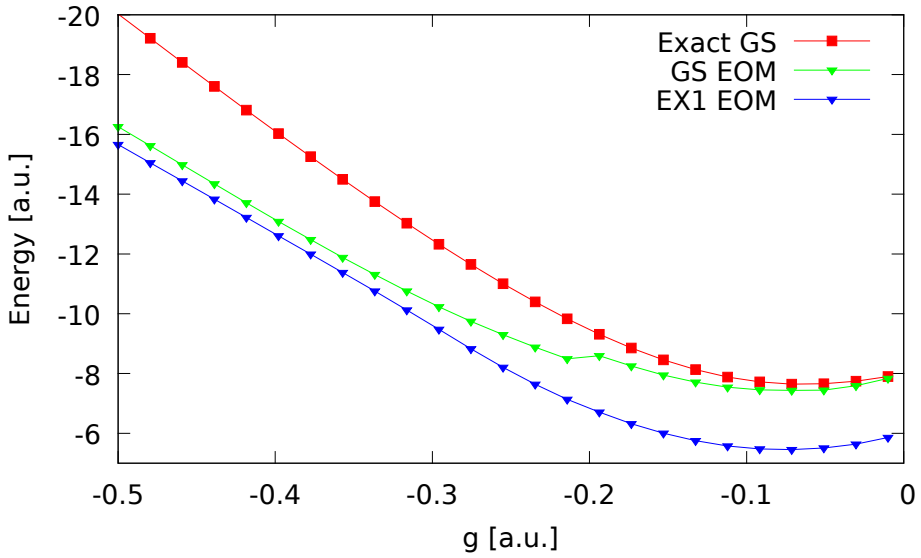
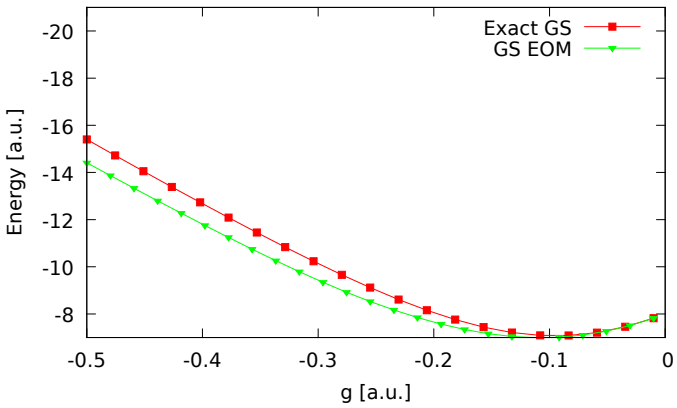


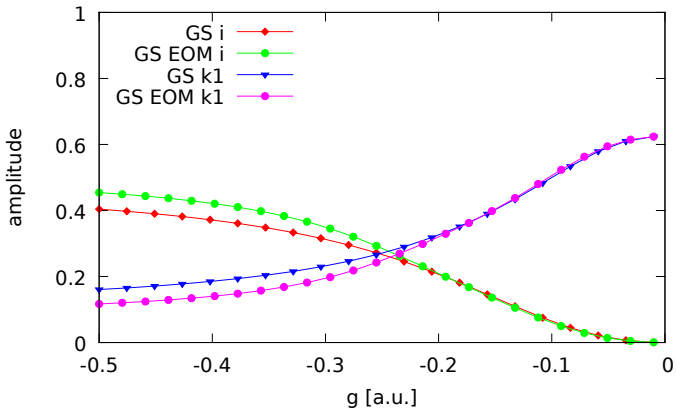
Figure 4.6: Energy values of the optimization procedure with truncation array `[1,1,1,1,1,2]`. The results are worse than the original exact-solving method with full truncation, depicted in Figure 4.5

4.7 Symmetrization of the EOM (SEOM) revisited

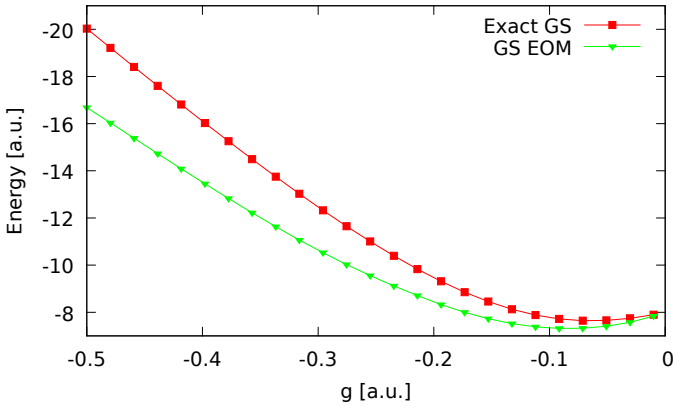
In section 4.2 it was discussed how the EOM on operator level can be made more symmetrical by swapping factors. In this way, we can write the EOM in such a way that only $S^0(N)$-terms or $S^0(N-2)$-terms enter the equations and there is no mixing between them. So far, the EOM (4.24) were used to perform the calculations in this chapter, except for illustrating the equivalence theorem. It turns out that using the SEOM provides a considerable gain in accuracy. Let's take a look back at example 7, recalculated with the SEOM with only $S^0(N-2)$-dependence in the first two equation sets of (4.24). The calculations were done by solving the SEOM exactly and using full truncation. The results are given in Figure 4.8. It can be concluded that the symmetrized approach provides very good results in areas where EOM fails. The reason why a more symmetrized version of the equations offers a considerable gain in accuracy is not known to this day.



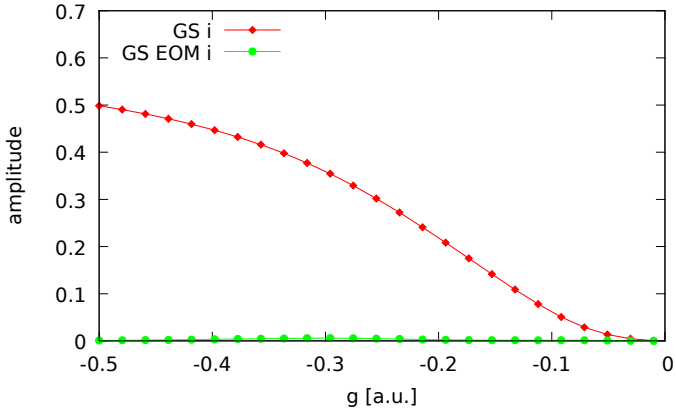
(a) Ground-state energy in the $N_{\text{part}} = 10$-sector.



(b) Occupation amplitudes in the $N_{\text{part}} = 10$-sector.

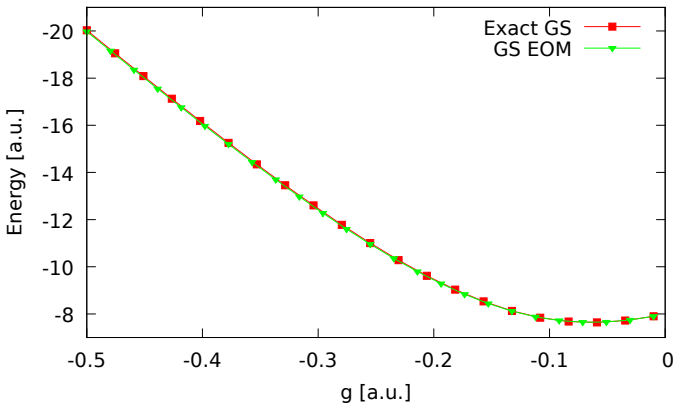


(c) Ground-state energy in the $N_{\text{part}} = 12$-sector.

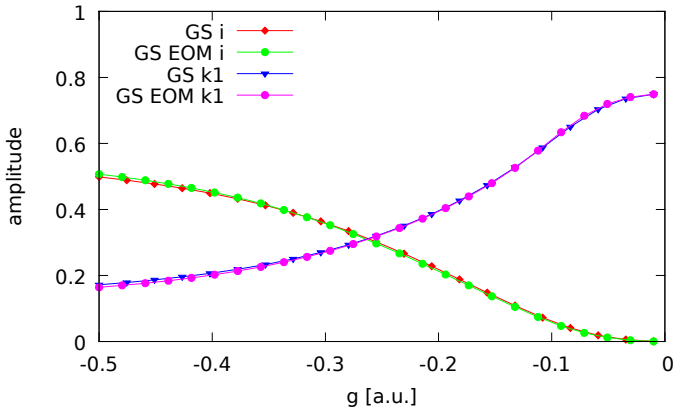


(d) Occupation amplitudes in the $N_{\text{part}} = 12$-sector.

Figure 4.7: Exact ground-state energy in the $N_{\text{part}} = 10$-sector and $N_{\text{part}} = 12$-sector together with the EOM-minimizing approach using a partial truncation array `[1,2,2,2,2,2]`. The occupation amplitude comparisons of the principal (i) and first non-principal level (k1) are also given.



(a) Exact ground-state energy together with the SEOM approximation.



(b) Exact and approximate occupation amplitudes for the principal level (i) and the first non-principal level (k1).

Figure 4.8: Energy spectrum and occupation amplitudes of example 7, recalculated with the fully truncated SEOM.

Chapter 5

Application to the Heisenberg model

After applying the (S)EOM truncation method on the conserved charges, one can move on to different Hamiltonians and see if the approximation still gives reasonable results. One can start, for example with the 1-dimensional Heisenberg spin-1/2 chain with only nearest neighbour interaction and periodic boundary conditions

$$\begin{aligned}\mathcal{H} &= J\sum_{i=1}^{m}\vec{S}_i.\vec{S}_{i+1} \\ &= J\sum_{i=1}^{m}\left[\frac{1}{2}(S_i^\dagger S_{i+1}+S_iS_{i+1}^\dagger)+S_i^0S_{i+1}^0\right],\end{aligned} \tag{5.1}$$

with $S_{m+1}=S_1$. The vacuum state will be chosen as the state where all spins are down: $|\theta\rangle = |\downarrow\downarrow ... \downarrow\rangle$. The fermion spin operators obey the same algebra as the quasispin operators so the analogy can be made that a spin up, i.e. $|\uparrow\rangle = S^\dagger|\theta\rangle$, equals the creation of two fermion particles. Solutions of this model already exist in the form of a Bethe Ansatz and this will be briefly discussed in the section below. If the EOM truncation method turns out to be successful for the Heisenberg model, one could in principle move on to the more complex J_1-J_2 model with J_1 and J_2 interaction strengths for respectively nearest- and next-to-nearest interaction. This could be done by first solving the Heisenberg model and then gradually turn on the next-to-nearest interaction J_2. If J_1 and J_2 have the same sign, this model resembles a frustrated system in the classical point of view [55]. Indeed, let's consider $J_1, J_2 > 0$ and a chain with 3 spins (1), (2) and (3). The nearest (2)- and next-to-nearest (3) neighbour of a certain spin position (1) want to arrange themselves in the opposite direction with respect to (1), resulting in a parallel direction of (2) and (3) that counteracts with the nearest neighbour interaction between the 2 spin positions. A graphical representation of this is given in Figure 5.1. In general, the J_1-J_2-model has no analytic solution, except for certain specific values for the interaction strength like $J_2 = J_1/2$. This model is called the *Majumdar-Ghosh model* (MG) and it was shown that this model has a degenerate ground state of linearly independent dimer states [55].

5.1 Bethe ansatz of the Heisenberg model

Just like in the case of the conserved charges, the operator $S^0 =: \sum_j S_j^0$ commutes with the Heisenberg Hamiltonian so the solutions can be subdivided in sectors with definite spin projection number[1]. The Heisenberg chain can be solved by means of a Bethe Ansatz and this was in fact the first application

[1] or equivalently, particle pair number.

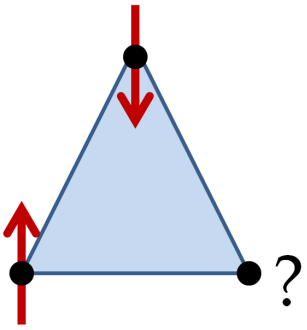


Figure 5.1: Graphical depiction of a frustrated system with 3 spins and an antiferromagnetic neighbouring force between them.

of this method for quantum many-body systems. Without going into detail, the results of the Bethe Ansatz [26, 56] will now be given. For a number of r flipped spins on top of the vacuum, the eigenstates take the form of

$$|\psi\rangle = \sum_{1\leq n_1<\ldots<n_r\leq N} a(n_1,...,n_r)\,|n_1,...,n_r\rangle\,. \tag{5.2}$$

The symbol n_i denotes the position of a spin up in the chain. For example $|n_1,n_2\rangle = S^\dagger_{n_1}S^\dagger_{n_2}\,|\theta\rangle$. The sum goes over all possible configurations of r spins up on top of the vacuum. The coefficient a can always be written as

$$a(n_1,...,n_r) = \sum_{\mathcal{P}} \exp\left[i\sum_{j=1}^{r} k_{\mathcal{P}j}n_j + \frac{i}{2}\sum_{i<j}\theta_{\mathcal{P}i\mathcal{P}j}\right]. \tag{5.3}$$

The operator $\mathcal{P}$ maps the set $\{1,2,...,r\}$ onto a permutation of this set and the sum $\sum_{\mathcal{P}}$ goes over all possible permutation sets. The wave numbers k and phase angles θ are governed by the following set of equations:

$$\begin{aligned} 2\cot\frac{\theta_{ij}}{2} &= \cot\frac{k_i}{2} - \cot\frac{k_j}{2}, \qquad i,j = 1,...,r \\ Nk_i &= 2\pi\lambda_i + \sum_{j\neq i}\theta_{ij}, \qquad i = 1,...,r, \end{aligned} \tag{5.4}$$

with integers $\lambda_i \in \{0,1,...,N-1\}$, called *Bethe quantum numbers*. The Heisenberg problem then reduces to finding those sets of Bethe numbers which yield solutions of the equations mentioned above. The energy eigenvalue is then given by

$$E = J\sum_{j=1}^{r}(\cos k_j - 1) + \frac{JN}{4}. \tag{5.5}$$

It can be shown that the absolute ground state will be found in the subspace $\sum_j S^0_j = 0$ [26]. In the particle language, this corresponds to the $N = m$-particle sector, or half filling of the system.

Special case: $r = 1$

A single spin excitation can be easily solved analytically. It can be checked that following wave function

$$|\psi\rangle = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{ikn}\,|n\rangle\,, \tag{5.6}$$

is an eigenvector for wave numbers $k = 2\pi m/N, m = 0, ..., N-1$. The eigenvalues are given by

$$E_k = J(\cos k - 1) + \frac{JN}{4}. \tag{5.7}$$

Because of translational invariance, the occurrence of e^{ik}-factors could be expected. However, since the Heisenberg Hamiltonian is Hermitian, it's eigenvalues are real. This means that the occurrence of complex numbers has to be the result of complex linear combinations in the eigenspaces of the total vector space, which signals degenerate eigenvalues. Even though the Bethe Ansatz incorporates complex combinations, one could always assume the S^0- and $S^\dagger$ matrices to be real.

5.2 Equations of motion approach

The commutator $[\mathcal{H}, S_j^\dagger]$ can be calculated to be

$$[\mathcal{H}, S_j^\dagger] = J\left[-S_j^0\left(S_{j-1}^\dagger + S_{j+1}^\dagger\right) + S_j^\dagger\left(S_{j-1}^0 + S_{j+1}^0\right)\right], \qquad \forall j. \tag{5.8}$$

This can be evaluated between the appropriate eigenstates $\langle N_\alpha| \, ... \, |(N-2)_{\tilde{\beta}}\rangle$ and together with the particle-number condition (4.26) and the Casimir identity (4.23), this leads to a closed set of equations that have to be solved in a recursive manner. Like in chapter 4, the excitation index of the $(N-2)$-particle sector will be denoted with a tilde. The particle number condition takes the following form:

$$\sum_j \left(S_j^0\right)_{\alpha\alpha}(N) = \frac{N-m}{2}, \qquad \forall \alpha. \tag{5.9}$$

with $N/2$ the total number of spins up and m the number of spin positions. Just like in the case of the conserved charges, the order of the S^0- and $S^\dagger$-operators can be freely chosen, leading to regular or the symmetrized version of the EOM. In theory, it suffices to start the recursive algorithm at $N = 4$ because the information on $N = 2$, or a single spin-up excitation is already known analytically. However, it can be instructive to start at the vacuum sector as the Hilbert space of $N = 2$ is very small and the equations can be solved relatively fast. Moreover, if there are issues with this technique it should already be visible in the $N = 2$ sector. The EOM PYTHON routine was extended to the Heisenberg chain and an exact diagonalization routine was also written in PYTHON. In order to be able to calculate larger spin chains in a fast manner, a C++ routine was put at disposal which can calculate the ground state energy by means of a *density-matrix renormalization group method* (DMRG)[2] [57].

5.3 Problems with the EOM approach

It quickly became clear that the EOM solver had much difficulty solving the equations, in the truncated case as well as the exact case. This is as expected since the initial guess values were almost chosen randomly. The only prior knowledge available is that, because of translational invariance, the S_j^0-elements of the ground state should be equal for all j. To this day, no satisfactory results could be obtained with random initial guess values. In that case, it is best to start from a simple model which is analytically solvable and turn on an interaction parameter gradually, just like in the case of the

[2]Many thanks to dr. Brecht Verstichel, who prepared this code.

conserved charges. For example, two anisotropy parameters Δ_1 and Δ_2 can be introduced in the Hamiltonian:

$$\mathcal{H} = J\sum_{i=1}^{m}\left[\frac{1}{2}\Delta_2(S_i^\dagger S_{i+1} + S_i S_{i+1}^\dagger) + \Delta_1 S_i^0 S_{i+1}^0\right]. \tag{5.10}$$

Now 2 limit cases can be considered

$\Delta_2 = 0$, the Ising model

Setting $\Delta_2 = 0$ results in the famous Ising chain where the Hamiltonian is diagonal in the UPF basis and the absolute ground state is a degenerate Néel state $|\uparrow\downarrow\uparrow\downarrow\uparrow ...\rangle$ for $J\Delta_1 > 0$. The UPF basis set could provide a good starting point for solving the equations. Let's consider an example of a chain with 4 positions and two spin-up excitations (or equivalently 4 fermion particles):

Example 8

$$\begin{cases} m = 4 \\ N_{part} = 4 \\ \Delta_2 = 0 \\ \Delta_1 = 1 \\ J = 1 \end{cases} \tag{5.11}$$

The 2 Néel states of the form $|\uparrow\downarrow\uparrow\downarrow\rangle$ make up the ground state space with degenerate eigenvalue equal to -1. It is expected that, when turning on the Δ_2 parameter, the ground state will be a small deformation on a linear combination of these Néel states. Indeed, setting $\Delta_2 = 0.01$ results in the following ground state:

$$\begin{aligned} |\psi_0\rangle =& 0.0071(|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle) \\ & -0.7070(|\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle), \end{aligned} \tag{5.12}$$

and setting $\Delta_2 = 0.1$ gives

$$\begin{aligned} |\psi_0\rangle =& 0.0687(|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle) \\ & -0.7004(|\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle). \end{aligned} \tag{5.13}$$

It is evident that in the $r = m/2$-sector a truncation can be performed where only the Néel states are used as initial guesses and the Δ_2-parameter can be gradually turned on. However, in order to reach this sector, all the other sectors with $\{1, 2, ...m/2 - 1\}$ spins up have to be successfully calculated. This turns out to be a very cumbersome task as the NR solver almost never seems to reach convergence and when it does, the energy results of every particle sector are in very bad agreement with the exact results. Our conjecture for the failing of this approach is that the translational invariance of this system is broken when truncating the Hilbert spaces and omitting UPF basis vectors. Indeed, a look can be taken at the $r = 1$-sector to clarify this statement. Truncating this sector and omitting basis vectors inevitably results in the breaking of translational invariance as certain spin positions are 'favoured' with a spin up and others are not. This causes the NR solver to not reach convergence or produce mismatching results. The $r = m/2$-sector is an exception of this 'favouring' situation with its 2 Néel states, but to reach this sector all other sectors have to be calculated successfully.

Therefore, it can be concluded that the UPF basis is a poor starting point for a truncated EOM approach. These problems didn't occur for the conserved charges: the degeneracy for $g = 0$ is immediately lifted when turning on the interaction and because of the absence of translational invariance,

it was clear which basis vector continuously deformed into the ground state by performing a small g treatment. The absence of translational invariance also made it possible to omit certain basis vectors without breaking a fundamental ground state symmetry.

$\Delta_1 = 0$, the XX model

A different approach can be taken by setting Δ_1 equal to zero. In this case, the Hamiltonian becomes the *Heisenberg XX chain* and this model can be solved analytically by means of a *Jordan-Wigner fermionization transformation* [58]: a unitary transformation on the operators can be performed to convert the Hamiltonian in a free Fermi gas model which can be easily diagonalized[3]. As a test, this model was solved with the exact diagonalization scheme for various chain lengths and spin excitations and the solutions were used as input for the truncated EOM approach: the input matrices were truncated simply by reducing its dimensions and the equations were solved with this initial guess. However, no reliable results were obtained. In most cases, the solver couldn't reach convergence and if convergence was reached, the energy approximation was way off or the translational invariance of the ground state in the S^0-matrices was broken[4].

5.3.1 EOM Generalization

The difficulty of obtaining solutions can be neatly avoided by using the minimization approach discussed in section 4.6. The functional was constructed with the equations of the EOM approach in section 5.2 and the matrix form of the following expressions were added:

- The commutation of the Hamiltonian with the S^0-operators:

$$[\mathcal{H}, S_j^0] = J\left[S_{j-1}^\dagger S_j - S_j^\dagger S_{j+1} + S_{j+1}^\dagger S_j - S_j^\dagger S_{j-1}\right]. \tag{5.14}$$

- The quasispin algebra commutation relations:

$$\begin{aligned}[S_j^\dagger, S_{j'}] &= 2S_j^0\delta_{jj'} \\ [S_j^0, S_{j'}^\dagger] &= S_j^\dagger\delta_{jj'}.\end{aligned} \tag{5.15}$$

Example 9 As an example, the ground state of the Heisenberg spin chain with 20 positions is calculated with this technique with full truncation. The results can be found in Table 5.1. It can be seen that in the lower particle sectors, big errors are already made because of the relatively large value of the minimized functional. This error is carried along the higher particle sectors because of the E_{N-2}-dependence in the functional of the N-particle sector. In the particle sector of the absolute ground state ($N = 20$ or $r = 10$), the functional seems to have a small value, thus signalling a valid attempt to approximate the relative energy $E_N - E_{N-2}$. However it is seen that the exact value is still twice the approximated value. It can be concluded that no reliable results are realised with this full truncation method. An attempt was also made to perform a truncation array of `[1,2,2,...,2]` but it was quickly clear that very little improvement was made for the energy corrections and the computation time was already very high (more than 2 hours for the PYTHON routine). Also, the translational invariance appeared to be broken as this

[3] Discussing the Jordan-Wigner fermionization transformation in detail lies beyond the scope of this thesis.

[4] The translational invariance of the ground state (S_j^0 is equal $\forall j$) can be easily programmed into the EOM equations but this wasn't done as it provides a good check for the the EOM approach.

was visible in the S^0-matrix elements: the occupation amplitudes in the calculated states were position-dependent and not identical.

It can be concluded that a truncated EOM approach doesn't seem to be an efficient method for the Heisenberg spin chain, as energy estimates are always way off for every attempt made so far. The reason for the failure of this method is not really clear, but the conjecture is that truncating the Hilbert space results in the breaking of translational invariance as explained with the UPF basis vectors. Even if this method would work, it isn't a very efficient way of treating spin chain problems with multiple interaction strength parameters like the J1-J2 model: an EOM or optimizing approach always requires an initial guess that is fairly close to the solution (or global minimum). With no prior knowledge of the solutions, the only way to solve this problem is starting from a situation where the exact solutions are known. If the XX-model or the Ising model is taken as a starting point, 2 interaction parameters have to be switched on and this contributes greatly to the computer time. Of course, one can start from the MG model and turn on the J_2-parameter. This was also done but again, no reliable results were found. Also, when interaction parameters are turned on in frustrated spin systems, the character of the ground state can sometimes change abruptly due to the occurrence of a phase transition [59]. This of course complicates the approach of turning on interaction parameters when solving equations, because the ground-state solution will not deform continuously during this phase transition. It can be concluded that methods like DMRG are way more efficient and reliable for (1-dimensional) spin chains.

Particle-number sector	Exact GS energy	EOM optimized energy	minimized function value
2	3.0	4.71242	16.23647
4	1.02728	4.53843	12.87852
6	-0.88571	4.09742	10.02997
8	-2.70127	3.91251	7.38489
10	-4.37664	3.62985	5.31204
12	-5.86456	3.20397	3.39609
14	-7.11417	2.69019	2.10257
16	-8.07251	2.43612	1.13406
18	-8.686441	2.21223	0.29913
20	-8.90438	2.10992	0.00426

Table 5.1: Comparison of the ground state energy obtained with a DMRG method and the full truncation optimization routine for each sector. The obtained minimal value of the functional is also given.

Chapter 6

Conclusion and future prospects

In the first part of this thesis, the conserved charges of the BCS pairing Hamiltonian were treated with standard BCS theory. It was shown that this approximation scheme is very accurate for fully attractive conserved charges but lacks accuracy for mixed and fully repulsive ones: their ground-state energy and occupation amplitudes could not be predicted in an accurate manner with standard BCS theory. A theorem was also proved which states that the BCS equations are equivalent for all conserved charges in a BCS pairing system. In this way it became clear why BCS theory fails for certain conserved charges: all the conserved charges of a pairing system share the same set of BCS occupation amplitudes. However, the non-trivial BCS solution that accurately describes the ground state of an attractive conserved charge will rather describe excited states for the other conserved charges. Of course, knowledge of a certain excited state instead of the ground state is not very desirable. An attempt was made to search for other non-trivial BCS solutions by means of a generalized Bogoliubov transformation which allows for negative occupation amplitudes. However, this resulted in approximations that were far less accurate than standard BCS theory for attractive constants of motion. The EOM method as an extension of the Volya method was proven to be adequate to describe these repulsive interactions. It was also shown that in a certain simplification limit, the fully truncated EOM reduce to the standard BCS equations. However, the application of this method on the Heisenberg spin chain proved to be unsuccessful. Our assumption is that this failure is attributed to the translational invariance of the model, which the EOM method ultimately breaks. The conserved charges of the BCS pairing Hamiltonian do not possess such translational invariance so this didn't cause any problems.

During the making of this master thesis, a few problems and conjectures were encountered that could not be solved or proven.

- The equivalence of the BCS equations for the conserved charges is proven, but it is not entirely clear why such theorem exists. In general, the equations arising from a variational ansatz wave function for 2 arbitrary commuting operators are not necessarily equivalent as a counterexample was easily found.
- The same questions arise with the EOM method. For the full truncation procedure, the proof of equivalence is identical to the normal BCS case. It is computationally illustrated that such equivalence also seems to apply for partial truncation, but a proof is not found yet. The equivalence proof in the fully truncated case couldn't be generalized because of the occurrence of matrix algebra.
- Conserved charges with repulsive interaction parts can be accurately described with the EOM

approach, but convergence of the NR solver seems to be difficult in some cases. A way out is to use an optimization method by constructing a functional, as discussed in section 4.6. However, this method also has limitations and a local minimum can be easily mistaken for the global minimum, which was illustrated in subsection 4.6.2. A possible continuation could be to investigate more intricate root algorithms to ensure oneself that the obtained minimum really is the global minimum.

- In section 4.7 it was illustrated that the SEOM approach seems to work better in some cases than the EOM approach. The reason of this is still not clear to this day.
- The EOM approach failed to describe the Heisenberg model, but there are of course many different approximation schemes in many-body physics. In the future, a look could also be taken at schemes like the *Random phase approximation* (RPA) or the *Shifted Harmonic Approximation* (SHA).

Appendix A

Newton-Raphson method for solving systems of non-linear equations

Consider a system of n non-linear equations with an equal amount of unknowns described as

$$\begin{aligned} &f_1(x_1, x_2, ..., x_n) = 0 \\ &f_2(x_1, x_2, ..., x_n) = 0 \\ &... \\ &f_n(x_1, x_2, ..., x_n) = 0, \end{aligned} \tag{A.1}$$

or in vector notation as $\mathbf{f}(\mathbf{x}) = \mathbf{0}$. A differential vector $\delta\mathbf{x}$ can be defined and the functions $f_i(\mathbf{x} + \delta\mathbf{x})$ can be Taylor-expanded around $\mathbf{x}$ to linear order. The vector expression of this expansion becomes

$$\mathbf{f}(\mathbf{x} + \delta\mathbf{x}) = \mathbf{f}(\mathbf{x}) + \mathbf{J} \cdot \delta\mathbf{x} + O(\delta\mathbf{x}^2), \tag{A.2}$$

with the Jacobian matrix $\mathbf{J}$ defined as

$$J_{ij} =: \frac{\partial f_i}{\partial x_j}. \tag{A.3}$$

It is now assumed that $\mathbf{x} + \delta\mathbf{x}$ is the solution vector of the equations such that (A.2) can be set equal to $\mathbf{0}$ and in first order we are left with

$$\delta\mathbf{x} = -\mathbf{J}^{-1}(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}). \tag{A.4}$$

This means that if an initial guess $\mathbf{x}$ is given to approximate the solution of the set of equations, this guess can be updated as follows:

$$\mathbf{x}_{new} = \mathbf{x}_{old} + \delta\mathbf{x} = \mathbf{x}_{old} - \mathbf{J}^{-1}(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}). \tag{A.5}$$

Starting from an initial guess, the updating of the guess has to be repeated until the desired convergence is achieved [60]. In Figure A.1, a graphical representation of this method is given for a 1-dimensional function. Sometimes the method can fail as no convergence is reached. The cause of this can be a poor initial estimate or a very small derivative at a certain point resulting in divergence of the updated values. An example of this is also given in Figure A.1.

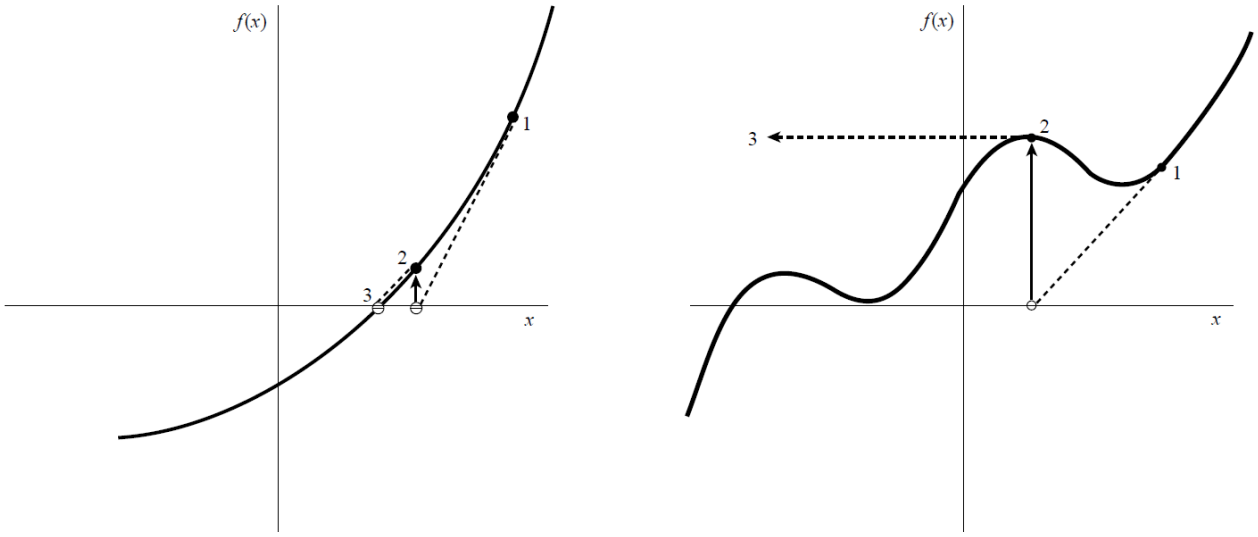


Figure A.1: Graphical representation of the Newton-Raphson algorithm for finding the roots of a 1-dimensional function. *Left figure:* The Taylor approximation to linear order results in an extrapolation of the initial guess along the tangent line at that point. The abscis value of the intersection of this extrapolation with the X-axis is the updated guess. *Right figure:* Illustration of a possible failure of the method. The tangent line in point 2 is horizontal so the 'updated value' becomes ∞. The figure is taken from [60].

Appendix B

Treatment of temperature dependence in BCS theory

When the temperature in a metal is non-zero, thermal vibrations can scatter pairs into higher energy levels and partially break the boson condensate. This can be modelled with a temperature- and level-dependent factor $f_\mu \equiv f_\mu(T)$ alongside the occupation probabilities. In this way, the gap parameter is modified:

$$\Delta = G \sum_{\mu>0} u_\mu v_\mu f_\mu(T). \tag{B.1}$$

This factor should obey the following limiting conditions:

$$\begin{aligned} \lim_{T\to+0} f_\mu(T) &= 1 \\ \lim_{T\to+\infty} f_\mu(T) &= 0. \end{aligned} \tag{B.2}$$

This means that the gap disappears completely as the temperature goes to infinity. In practice, the gap will disappear at the critical temperature T_c. In [3] it is proven that this function takes the following form:

$$f_\mu(T) \equiv f_\mu(T, E_\mu) = 1 - \frac{2}{e^{\frac{E_\mu}{kT}} + 1}, \tag{B.3}$$

with k the Boltzmann constant and E_μ the quasiparticle energy (1.33) of orbital μ. The derivation of this function (B.3) relies on constructing and minimizing the Helmholtz Free energy, as done in [3], but this lies outside the scope of this thesis. The second term can be identified as the famous Fermi-Dirac distribution containing the Boltzmann-factor. With the help of (1.25), (B.1) can be rewritten as

$$\frac{1}{G} = \sum_{\mu>0} \frac{1}{2E_\mu} \left[1 - \frac{2}{e^{\frac{E_\mu}{kT}} + 1} \right]. \tag{B.4}$$

The critical temperature is now defined as the temperature where the Fermi gas stops to be superconductive and $\Delta \to 0$. In this limit, the quasiparticle energies reduce to

$$E_\nu \to |\xi_\nu| =: |\epsilon_\nu - G v_\nu^2 - \lambda|. \tag{B.5}$$

The quantity ξ_ν can be interpreted as the new single-particle energy obtained after a renormalization correction of the original single-particle energies due to the interaction with the other particles [9, 15]. In this way, the sum over all orbitals $\sum_\nu$ can be interpreted as the sum over all single-particle energies.

In a macroscopic piece of metal, the assumption can be made that the single-particle energy spectrum is a quasi-continuum. In this continuum limit, the gap equation at the critical temperature becomes:

$$\frac{1}{G} = \int d\xi \frac{N(\xi)}{2|\xi|} \left[1 - \frac{2}{e^{\frac{\xi}{kT_c}} + 1} \right], \tag{B.6}$$

with $N(\xi)$ the density of states of the electrons. This integral has a logarithmic divergence for $\xi \to \pm\infty$ and the introduction of a cut-off ϵ_c is needed to obtain physical results. Assuming that $N(\xi)$ is a rather constant quality, we obtain the following integral:

$$\frac{1}{GN(0)} = \int_0^{\epsilon_c} \frac{d\xi}{|\xi|} \left[1 - \frac{2}{e^{\frac{\xi_\mu}{kT_c}} + 1} \right], \tag{B.7}$$

with $N(0)$ the electron density at the Fermi surface. Here we have made use of the symmetry of the integrandum to integrate from 0 instead of $-\infty$. After some calculus we obtain

$$kT_c \approx 1.14\epsilon_c e^{-\frac{1}{N(0)G}}. \tag{B.8}$$

The quantity ϵ_c, which is the upper limit of the renormalized single-particle energies can be interpreted as the energy cutoff of the attractive interaction mechanism in a metal: the Debeye frequency $\hbar\omega_D$. This derivation was based on [61].

Appendix C

General info on Casimir operators

In general, a Casimir operator of a Lie group can be constructed in the following way [62, 63]: Suppose $\mathcal{T}_a$ are the generators of a Lie group satisfying the following commutation relations[1]

$$[\mathcal{T}_a, \mathcal{T}_b] = f_{ab}^c \mathcal{T}_c \qquad \forall a, b, c = 1, ...d_G. \tag{C.1}$$

with d_G the dimension of the group and f_{ab}^c the tensor or *structure constants* defining the algebra. The Killing form can now be defined as

$$g_{ab} =: f_{ac}^d f_{bd}^c. \tag{C.2}$$

and its inverse is defined as $g_{ab}g^{bc} = \delta_a^c$. Now the quadratic Casimir operator can be defined as

$$\mathscr{C}_2 =: g^{ab}\mathcal{T}_a\mathcal{T}_b. \tag{C.3}$$

It can easily be proved that

$$[\mathscr{C}_2, T_a] = 0, \qquad \forall a. \tag{C.4}$$

Now, Schur's lemma states that an operator that commutes with all the generators $\mathcal{T}$ in an irrep must be a multiple of the identity operator. We can thus write the Casimir operator as

$$\mathscr{C}_2(R) = c_R \mathbf{1}, \tag{C.5}$$

with R an irrep of the Lie group and c_R the constant value belonging to this irrep.

[1] Einstein summation is implied

Appendix D

Weak coupling limit of the conserved charges

For small g, one can assume the pairs to be almost condensed in the Fermi sea, as the exact eigenstate is a small perturbation on top of an uncorrelated pair filling of the vacuum. If a pair is condensed into a single-particle level, the rapidity belonging to that pair will approach the single-particle energy, i.e. $x_\alpha \to \epsilon_j$. Indeed, a Cooper pair in a pairing system is denoted as the Gaudin pair creation operator acting on the vacuum:

$$S_\alpha^\dagger |\theta\rangle = \sum_{j=1}^{m} \frac{1}{\epsilon_j - x_\alpha} S_i^\dagger |\theta\rangle \,, \tag{D.1}$$

and as $x_\alpha \to \epsilon_i$, the $S_i^\dagger$-term dominates and the pair is fully condensed in the i-level. An example of this was discussed in subsection 2.1.5 and Figure 2.3. With this in mind, the RG equations (2.27) for N pairs with rapidities x_α condensing in the j'th level can approximately be written as

$$1 + 2g\frac{d_j}{2\epsilon_j - E_\alpha} + 2g\sum_{\beta\neq\alpha}^{N} \frac{1}{E_\alpha - E_\beta} = 0, \qquad \alpha = 1, ..., N, \tag{D.2}$$

because these terms predominate. Again, a rescaling of the rapidities was performed $x_\alpha \to E_\alpha/2$. One can now define the following polynomials

$$\begin{aligned} P(x) &= \prod_{\alpha=1}^{N} (x - E_\alpha) \\ P'(x) &= \sum_{\alpha=1}^{N} \prod_{\beta\neq\alpha}^{N} (x - E_\beta) \\ P''(x) &= \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \prod_{\gamma\neq\alpha,\beta}^{N} (x - E_\gamma), \end{aligned} \tag{D.3}$$

where the rapidities E_α are the zeros of $P(x)$. (D.2) can now be multiplied with $(2\epsilon_j - E_\alpha)P'(E_\alpha)$ and this leads to the following equation

$$(2\epsilon_j - E_\alpha + 2gd_j)P'(E_\alpha) + g(2\epsilon_j - E_\alpha)P''(E_\alpha) = 0, \qquad \alpha = 1, ...N. \tag{D.4}$$

This means that E_α is the root of the following polynomial which has the same degree as $P(x)$.

$$(2\epsilon_j - x + 2gd_j)P'(x) + g(2\epsilon_j - x)P''(x). \tag{D.5}$$

Because of the fact that this function and P share the same root E_α they have to be equal up to a scaling factor λ. Comparing the highest degree of (D.5) and P one can identify $\lambda = -N$ and therefore write

$$g(2\epsilon_j - x)P''(x) + (2\epsilon_j - x + 2gd_j)P'(x) + NP(x) = 0. \tag{D.6}$$

With the substitution $z = (2\epsilon_j - x)/g$ this leads to

$$zP''(z) + (-2d_j - z)P'(z) + NP(z) = 0. \tag{D.7}$$

This equation can be recognized as associated Laguerre differential equations so the unknown rapidities are the zeros of the associated Laguerre polynomials L_N^α with $\alpha + 1 = -2d_j$ (taking into account the substitution $x \to z$). With the help of the well-known Laguerre recursive relation [64]

$$nL_n^\alpha(x) = (2n - 1 + \alpha - x)L_{n-1}^\alpha(x) - (n - 1 + \alpha)L_{n-2}^\alpha(x), \tag{D.8}$$

and the first two polynomials

$$\begin{aligned} L_0^\alpha(x) &= 1 \\ L_1^\alpha(x) &= 1 + \alpha - x, \end{aligned} \tag{D.9}$$

the Laguerre polynomial $L_n^\alpha(x)$ can be written in a determinant form

$$L_n^\alpha(x) = \frac{1}{n!}\begin{vmatrix} 1+\alpha-x & \sqrt{1+\alpha} & \dots & 0 \\ \sqrt{1+\alpha} & 3+\alpha-x & \dots & 0 \\ 0 & \dots & \dots & 0 \\ \vdots & & & \vdots \\ 0 & \dots & \dots & \sqrt{(n-1+\alpha)(n-1)} \\ 0 & \dots & \sqrt{(n-1+\alpha)(n-1)} & 2n-1+\alpha-x \end{vmatrix}, \tag{D.10}$$

which resembles an eigenvalue equation in x of the corresponding matrix when set to zero. This can be seen if one develops the determinant to the outer row or column. As a result, finding the rapidities of N pairs condensing in the j'th energy level boils down to searching the eigenvalues of this matrix. In this way, the energy of an UPF basis vector can be calculated by solving (D.10) for every energy level and once all the rapidities are known, the eigenvalue energy can be calculated with (2.19). Therefore, one can determine which uncorrelated pair filling vector will give rise to the ground state energy for small g. The determinant and the eigenvalue equation was programmed in a PYTHON routine. One can notice that the above matrix contains complex values, but python handles complex matrices well. This approach of transforming a problem of non-linear equations into finding the zeros of a polynomial is called a *Heine-Stieltjes connection* [52, 53].

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