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# The Many-Electron Problem in Novel Low-Dimensional Materials

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# Contents

# Preface

The work contained in this Thesis has mostly been done at the University of Évora, Portugal. Some developments took place at the University of Urbana-Champaign, U. S. A.. I had Prof. José Manuel Pereira Carmelo as supervisor, and with him I did most of my research work. To him I want to express my gratitude for suggesting me the topic of research developed in this Thesis. With Prof. José Carmelo I have learned valuable tools in theoretical physics.

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J. M. P. Carmelo and N. M. R. Peres, *Topological Ground-State Excitations and Symmetry in the Many-Electron One-Dimensional Problem*, Nucl. Phys. B **458**, 579 (1996).

N. M. R. Peres, J. M. P. Carmelo, D. K. Campbell, and A. W. Sandvik, *Pseudoparticle Description of the 1D Hubbard Model Electronic Transport Properties*, Z. Phys. B **103**, 217 (1997).

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**To Augusta,**
**Filipa**
**and**
**Augusto Luis.**

Uno puede escribir un artículo o
un cuento porque se lo encomiendan (...);
a veces se le propone haste el tema,
y nada de ello me parece grave si uno
logra hacer suyo el proyeto y se
divierte escribiéndolo.
Es más, sólo concibo escribir
algo si me diverto, y sólo puedo
divertirme si me intereso.

Javier Marías,
in *Cuando fui mortal*,
Alfaguara, Madrid, 1996.

# Chapter 1

# Introduction

This Thesis deals with the one-dimensional (1D) Hubbard model [1, 2, 3], which describes single-band interacting (correlated) electrons in a (1D) lattice. According to Lieb [4]:

" The Hubbard model is to the problem of electron correlations as the Ising model is to the problem of spin-spin interactions; it is the simplest possible model displaying many "real world" features."

The model depends on the parameter $t$, the hopping integral, characterizing the kinetic energy of the electrons when they hop between two adjacent lattice sites, and on the parameter $U$, the on-site Coulomb integral, characterizing the Coulomb interaction energy when two electrons occupy the same lattice site (Chapter 2).

Strictly one-dimensional systems are not found in real solid-state materials, however there are quasi-one-dimensional materials in nature. Theoretically, a quasi-one-dimensional solid – the definition of which is quite broad [5]– may be represented by a three-dimensional array of one-dimensional chains, such that the hopping integrals between the chains are much smaller than the hopping integral along them [6]. The correspondence with real materials – for which $t$ and $U$ can be estimated from infrared spectroscopy data [7, 8, 9]– is then made by means of quantum chemistry calculations [10], where the hopping integrals and the Coulomb on-site energy are computed by means of the atomic (molecular) wave functions of the atoms (molecules) of the solid under consideration.

Obviously, approximating real materials by a simple one-dimensional model is not enough in general to make a quantitative description of the solid properties. In spite of this, a description based on the parameters $t$ and $U$ contains many "real

world" features [7, 8]. On the other hand, effects like electron-phonon coupling and more general Coulomb interactions, for example, are needed to account for a more quantitative description of the physical properties of real quasi-one-dimensional materials [11, 12, 13, 14, 15, 16, 17].

The systems described by the 1D Hubbard model (and its generalizations) have narrow energy bands, and, therefore, the tight-binding approximation for independent electrons can be applied [18].

## 1.1 Materials

There are several classes of quasi-one-dimensional materials in nature which can can be described by 1D electron models, the benzene molecule ($C_6H_6$) being one of the simplest systems to which the Hubbard model can be applied. [The molecular $\pi$ orbitals of the six carbon atoms can be thought of as a lattice with six sites populated by six electrons. The Coulomb interaction have been computed by Parr *et al.* [10] and are $U = 16.93$ eV, for the on-site Coulomb integral, and $V = 9.027$ eV, for the next-nearest-neighbour Coulomb integral (Chapter 2).]

In what follows we describe very briefly some of the most typical quasi-one-dimensional materials.

**1.)Inorganic Materials**

**1.a) Potassium cyanoplatinates**: a typical example is $K_2Pt(CN)_4Br_{0.3}.3H_2O$ which was synthesized during the 19th century. The chains are built by the superposition of the $d$ orbitals of the Pt atoms. The ratio of the conductivity along the chains ($\sigma_\parallel$) over the conductivity perpendicular to the chains ($\sigma_\perp$) is $\sigma_\parallel/\sigma_\perp \sim 10^5$, and the electronic density $n$ – the ratio of the number of electrons $N$ over the number of lattice sites $N_a$ – is 0.85 [19]. The values of $\sigma_\parallel$ and $\sigma_\perp$ are a measure for the atomic (or molecular) orbitals overlap along and perpendicular to the chain direction, respectively [20]. Therefore, $\sigma_\parallel/\sigma_\perp$ provides a measure of the relative values of the hopping integrals.

**1.b) Transition metalchalcogenides**: $MX_3$ and $(MX_4)_nY$, with the metals M=Nb,Ta, the chalcogenides X=S,Se, and the halides Y=I,Br,Cl. The basic units of the chains in $MX_3$ are $MX_6$ triangular prisms stacked on top of each other, and in $(MX_4)_2Y$ are $M_2X_4$ octaedra. Typical examples are $NbSe_3$, $TaS_3$, $(TaSe_4)_2I$, and

$(NbSe_4)_2I$, with $\sigma_\parallel/\sigma_\perp \sim (10 - 10^3)$ and $n \sim 1/4$ [19].

**1.c) Transition metal bronzes**: $A_{0,3}MoO_3$, with A=K,Rb,Tl. These materials are called blue bronzes due to their metallic blue brightness. The chains are formed by the $MoO_6$ octaedra, and, in these materials, $\sigma_\parallel/\sigma_\perp \sim$ (10-$10^3$) and $n \sim 3/4$ [19].

**1.d) Copper oxide compounds**: typical examples are the 1D antiferromagnetic $Sr_2CuO_3$ and $SrCuO_2$ materials [21]. These systems can be modeled by the 1D Hubbard Model with $U >> t$ and $n = 1$ (Chapter 2). The Heisenberg exchange interaction $J = 4t^2/U$ for these two compounds is $J = (2200 \pm 200)$ K and $J = (2100 \pm 200)$ K, respectively. The interaction between chains, $J'$, obeys the ratio $J/J' \sim 10^5$ for $Sr_2CuO_3$ and $J/|J'| \sim$ (5 to 10) for $SrCuO_2$. Intimately related to the spin-chain compounds are the spin-ladder compounds. These latter systems can form two, three, or more leg ladders. Typical examples are $SrCu_2O_3$ (a two-leg spin 1/2 systems) and $Sr_2Cu_2O_5$ (a three-leg spin 1/2 ladder) [22]. An interesting result is that the even-leg spin 1/2 ladders present a gap in their excitation spectra, while the odd-leg spin 1/2 ladders do not. Upon doping (this means $n = 1/2 - \delta$, where $\delta$ is usually small when compared to 1/2) these ladder materials present both metallic and superconducting phases [22, 23].

**2.) Organic Linear Chain Compounds**

**2.a) Polymers**: the typical example is polyacetylene. It consists of a long chain of $(CH)_x$ units with alternating single and double bonds between the carbon atoms [11, 13, 24]. The values of the transfer and Coulomb integrals are taken to be $4t \sim 10$ eV and $U \sim 6.5$ eV, respectively, and $n = 1$ [11, 13, 24].

**2.b) Stacks of organic molecules**: these materials are made of planar organic molecules stacked together. The organic molecules have $\pi$ molecular orbitals perpendicular to the plane of the molecule. These orbitals overlap forming a 1D chain. A typical example is the incommensurate (the average number of carriers per molecule can not be expressed by a simple rational number) tetrathiafulvalena- tetracyanoquinodimethane – TTF-TCNQ – with $4t \sim 0.61$ eV, $U \sim 1.1$ eV, and $n \sim 0.55$ [7, 8]. Other examples are the salts $M_2X$, with M=TMTSF,TMTTF (where TMTSF denotes tetramethyltetraselenafulvaleno and TMTTF denotes tetramethyltetrathiafulvaleno) and X=Br,$PF_6$,$ClO_4$. These salts are quarter filling systems (quarter-filled hole band: $n = 1/4$), with the $t$ and $U$ parameters being of the order $t \sim 0.25$

eV and $U \sim 1$ eV ($t_b$ and $t_c$, the interchain couplings, are of the order of 25 meV and 1 meV, respectively) [25]. These materials can also present a superconducting phase [26].

There are still other realizations of quasi-one-dimensional systems like in heterostructures (an example is the AlGaAl-GaAs-AlGaAl material) and in nanotubes (an example is the $B_{1-\delta}C_{2+\delta}N$ material) [27, 28, 29].

Many of the materials we have briefly described are not metals at zero temperature. Usually they are metals at room temperature and undergo some type of phase transition when the temperature is lowered. Depending on the material and on the physical values of certain external parameters (like doping, external fields, pressure and cooling rate) they may, for example, undergo structural, metal-insulator, spin density wave, or superconducting phase transitions [26, 19, 30, 31, 32, 33].

When one performs zero-temperature calculations and applies the results to finite-temperature data, no more than a qualitative agreement is to be expected. Nevertheless, the calculation of, for example, the zero-temperature optical conductivity has for some quasi-one-dimensional materials been used with some success in describing the optical conductivity of these materials in the (finite temperature) metallic phase [7, 8, 17]. However, due to its quasi-one-dimensional character, these materials can only be approximate by an one-dimensional model at moderate temperatures. At low temperatures 3D effects start to play a role. These effects may drive phase transitions in these materials, as those indicated above.

## 1.2 Theoretical results

As the Hubbard chain is the simplest possible model for the study of interacting electrons in a lattice, the theoretical study of the model is by it self of interest [4]. In this section we summarize very briefly some of the previous work on the 1D Hubbard model. This includes its exact solution, as well as recent new results, some of which are presented in this Thesis. The 1D Hubbard model is exactly solvable by the Bethe-ansatz technique, first introduced by Bethe [34] in his solution of the 1D spin 1/2 Heisenberg chain. Roughly speaking, the model has charge and spin excitations – usually called holon and spinon excitations – which are decoupled from each other. This feature is usualy taken as a signature of 1D electronic correlated systems. The experimental observation of the holon and spinon spectra has recently been achieved by photoemission spectroscopy by Kim *et al.* [35] in the 1D $SrCuO_2$

material (but not in the 2D related $Sr_2CuO_2Cl_2$ cuprate). Moreover, these authors find that the Hubbard model in the limit $U \gg 4t$ (the parameters used are $t = 0.60$ eV and $U = 7.2$ eV) "agrees strikingly" with the data.

Using the same method as Yang for a continuum multicomponent model [36], Lieb and Wu [37] computed the ground-state energy at half filling ($n = 1$) and zero magnetization ($m = 0$). They also found that for $n = 1$ the charge excitations have a gap – the Mott-Hubbard gap $\Delta_{MH^-}$, for any value of the on-site Coulomb integral $U$. Thus the model is an insulator at half filling and zero temperature. Experimental evidence of 1D Mott-Hubbard insulating behavior has been found in the quasi-one-dimensional HMTSF-TCNQF$_4$, HMTTF-TCNQF$_4$, and DBTSF-TCNQF$_4$ organic compounds [8, 38] (all these three compounds have $n = 1$, and HMTSF, HMTTF, and TCNQF$_4$ denote hexamethylenetetraselenafulfalene, hexamethylenetetrathifulfalene, tetrafluoro-tetracyano-*p*- quinodimethane, respectively).

Shiba [39] performed some numerical work for densities lower than half filling and computed the ground state energy and the magnetic susceptibility. In the limit $U \gg 4t$, it has been possible to compute analytically the ground-state energy for $n \leq 1$ [40]. The thermodynamics of the Hubbard chain has been described by Takahashi [41], who obtained the full solution of the Lieb and Wu equations [37].

The spectra and the momenta of the low-lying excitations were determined by Ovchinnikov [42] for the half-filled band case and by Coll for any filling [43]. Ovchinnikov [42] also remarked that for $U \gg 4t$ the spin spectrum is the same as for the anti-ferromagnetic Heisenberg chain [44]. This fact is an indication of the factorization of the Bethe-ansatz wave function into a free-spinless fermion Slater-determinant and into the anti-ferromagnetic Heisenberg wave function [34], as discussed later by Ogata and Shiba [45].

In the presence of a magnetic field, the charge and spin low-lying excitations transform into more exotic $c$ and $s$ excitations, and their energy spectra and momenta, as well as the low-energy thermodynamics and static properties have been analytically computed [46, 47, 48] for electronic and magnetization densities such that $n \leq 1$ and $m \leq n$, respectively. The study of excitations of topological character in a finite-size chain has been made by Carmelo and Peres [49, 50]. In addition to the $c$ and $s$ modes, the 1D Hubbard model has finite-energy charge $(c, \gamma)$ and spin $(s, \gamma)$ excitations, which have been considered by Woynarovich [51, 52]. These charge and spin excitations can be seen as bound states of $c$ and $s$ pseudoparticles. Their operator generators, excitation spectra, and momenta have been computed by Carmelo and Peres [53].

Due to its involved form, the Bethe-ansatz wave function is not ideally suitable for the computation of operator mean values and correlation functions. These latter quantities can be obtained in some limits by combining the Bethe-ansatz solution with conformal-field theory [54, 55]. These calculations require a simple representation for the eigenstates of the model. In particular, the possibility of finding a set of operators (in second quantization) which diagonalize the Hamiltonian is a major step in that direction. An example of this general idea is the bosonization technique [56, 57], where the g-ology Hamiltonians [58] can be diagonalized by boson operators. The low-energy correlation functions can then be computed by expressing both the fermionic fields and the eigenstates of these models in terms of the boson operators.

A central problem in this model is the study of the transport properties: quantities like the charge and spin currents and the corresponding conductivity spectra are of importance [59, 60, 61, 62]. The low-frequency properties of the 1D Hubbard model have been studied both by means of bosonization techniques [57] and by means of the pseudoparticle representation [63, 64]. However, the study of the finite-energy transport and spectral properties requires an operator representation for the Bethe-ansatz solution at all energy scales.

Following previous results for the low-energy Hilbert sub-space [65, 66], Carmelo and Peres [53] suceeded in writing the Hamiltonian, the momentum operator, and the generators for all $4^{N_a}$ eigenstates of the Hubbard model in a suitable second quantized operational basis. This basis is defined by the set of operators $a^{\dagger}_{q,\alpha,\beta}$ and $b^{\dagger}_{q,\alpha,\gamma}$, which we call pseudohole and heavy-pseudoparticle operators, respectively (Chapter 3). In this basis the eigenstates of the 1D Hubbard model have a simple Slater-determinant form. In its diagonalized form the model is written as an infinite sum of terms involving only forward scattering interactions among the pseudoparticles at all energy scales.

The use of the pseudohole and heavy-pseudoparticle operational representation allows the evaluation of the charge and spin current mean values, as well as of the charge and spin transport masses of the pseudoparticle carriers [67, 68]. Moreover, combining this operational representation with a new generalized conformal-field theory [69], the optical conductivity of the 1D Hubbard model around some finite energy values can be computed [70]. The set of these energy values, $\omega = \omega_0$, correspond to the new conformal critical theories of $(\omega - \omega_0)$ low energy.

The present Thesis is organized as follows. In Chapter 2, a derivation of the Hubbard model is given and some of its well known properties are discussed. In

Chapter 3, a detailed presentation of the operational representation of the model in terms of pseudoholes and heavy-pseudoparticles is given. The general expressions for the low-lying and finite-energy excitation spectra are provided in Chapter 4. In Chapter 5, the topological excitations in a finite size system are discussed. In Chapter 6, the charge and spin transport currents and the charge and spin transport masses are evaluated. Qualitative results on the optical conductivity of the Hubbard model are discussed and some Monte Carlo calculations are presented. Finally, in Chapter 7, we summarize and discuss future research directions.

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# Chapter 2

# The Hubbard Model

## 2.1 The Hubbard model

The theoretical study of electron correlations in solids requires the use of a suitable Hamiltonian such that it includes, in some way, the Coulomb interaction among the relevant electrons of the solid (those of the outer shells). If one is interested in both the thermodynamics and the transport properties, one must include the necessary external fields to the Hamiltonian. Response to an electric field requires the introduction of a vector potential $\vec{A}$ (taken to be small). In first quantization, the general Hamiltonian including Coulomb interactions reads

$$\hat{H} = \sum_i \left[ \frac{\hbar^2}{2m}(-i\vec{\nabla}_i - \frac{e\vec{A}_i}{c\hbar})^2 + V(\vec{r}_i) \right] + \frac{1}{2}\sum_{i,j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}, \tag{2.1}$$

where $m$ is the electron mass, $e$ is the electron charge ($e < 0$), and $V(\vec{r})$ is the lattice potential, which will have the suitable symmetry (the effects of disorder will not be considered). The treatment of this Hamiltoninan is best accomplished in second quantization. We write the electron fields $\Psi^\dagger_{\sigma,l}(\vec{r})$ ($\sigma$ and $l$ are the spin and band labels, respectively) in terms of Wannier functions which perserve the lattice symmetry (for practical calculations, one uses atomic wave functions). These fields are localized at the lattice sites $\vec{R}_i$ and are of the form $\Psi^\dagger_{\sigma,l}(\vec{r}) = \sum_i \phi(\vec{r} - \vec{R}_i) e^{-i\frac{e}{c\hbar}\int_{\vec{R}_i}^{\vec{r}} \vec{A}(\vec{x})\cdot d\vec{x}} c^\dagger_{i,\sigma,l}$, where $c^\dagger_{i,\sigma,l}$ creates one electron of spin $\sigma$ at the band $l$ and lattice site $\vec{R}_i$. The operators $c^\dagger_{i,\sigma,l}$ and $c_{j,\sigma',l'}$ obey the usual anticommuting fermionic relations and the exponential term in the field definition is required to mantain gauge invariance. As a first approximation we consider only one band and neglect all the band structure of the solid. We then omit the band index in what follows. In the

Wannier representation, the Hamiltonian (2.1) reads

$$\hat{H} = -\sum_{i,j,\sigma} t_{i,j} e^{-i\frac{e}{c\hbar}\vec{A}\cdot(\vec{R}_i-\vec{R}_j)} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \sum_{i,j,l,m}\sum_{\sigma,\sigma'} U_{i,j,l,m} c^{\dagger}_{i,\sigma} c^{\dagger}_{j,\sigma'} c_{l,\sigma'} c_{m,\sigma}\,, \tag{2.2}$$

where the hopping integral $t_{i,j}$ and the Coulomb integral $U_{i,j,l,m}$ are given, respectively, by

$$t_{i,j} = -\int d\vec{r}\phi^*(\vec{r}-\vec{R}_i)\left[\frac{-\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\phi(\vec{r}-\vec{R}_j)\,, \tag{2.3}$$

and

$$U_{i,j,l,m} = \int\int d\vec{r}d\vec{r}'\phi^*(\vec{r}-\vec{R}_i)\phi^*(\vec{r'}-\vec{R}_j)\frac{e^2}{|\vec{r}-\vec{r}'|}\phi(\vec{r'}-\vec{R}_l)\phi(\vec{r}-\vec{R}_m)\,. \tag{2.4}$$

The hopping integral (2.3) gives the amplitude for an electron to jump from the atomic orbital centered at the lattice site $\vec{R}_i$ to the atomic orbital centered at the lattice site $\vec{R}_j$. The Coulomb integral accounts for the electronic correlations among the electrons at the different atomic orbitals. Hubbard estimated [1] that the most important contribution to the Coulomb integral comes from the term where two electrons are at the same atomic orbital, that is $U_{i,i,i,i} \equiv U$ (the order of magnitude of the bare $U$ is roughly of 10-20 eV). The second most important contribuition to the interaction energy, $U_{i,j,i,j}$, comes from the interaction of two electrons at nearest neighbor sites (the order of magnitude is roughly 2 to 3 eV). If the electrons belong to narrow free-electron bands, the most important contribution to the kinetic energy comes from hopping between nearest neighbour sites; this is the usual tight-binding approach. In view of this, the simplest Hamiltonian we can think of for describing correlated electrons in a regular solid is the Hubbard model. It consists in considering, out of all the hopping and Coulomb integrals, only the nearest neighbour hopping $t$ and the on-site Coulomb repulsion $U$. The Hubbard Hamiltonian then reads [1, 2, 3]

$$\hat{H} = -t\sum_{<i,j>,\sigma}^{N_a} e^{-i\frac{e}{c\hbar}\vec{A}\cdot(\vec{R}_i-\vec{R}_j)} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U\sum_{i}^{N_a}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\,, \tag{2.5}$$

where $< i,j >$ means summing over nearest neighbor sites $i$ and $j$ only, $N_a$ is the number of lattice sites, and $\hat{n}_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ is the number operator at site $i$ for $\sigma$ electrons. For the spin label, $\sigma$, we have $\sigma = \uparrow, \downarrow$ when used has an index and

$\sigma = \pm 1$ otherwise. This Hamiltonian has only two parameters, $t$ and $U$, and thus the only energy scale is $U/t$. This ratio is present in all physical quantities. In what follows we consider $c_{N_a+1\sigma} = c_{1\sigma}$, units such that $\hbar = 1$, the lattice spacing $a = 1$, and the electron charge $e = -1$.

## 2.2 The SO(4) symmetry of the Hubbard model

The SO(4) symmetry of the Hubbard model can be traced back to its spin-up/spin-down and particle-hole symmetries [4, 5, 6, 7]. Let us define the number and magnetization operators as $\hat{N} = \sum_{i,\sigma} \hat{n}_{i,\sigma}$ and $\hat{S}^s_z = -\frac{1}{2}\sum_{i,\sigma} \sigma \hat{n}_{i,\sigma}$, respectively. ($N_\sigma$ is the number of $\sigma$ electrons and $N = N_\sigma + N_{-\sigma}$.) If we perform the spin-up/spin-down transformation, $c^\dagger_{i,\sigma} \to c^\dagger_{i,-\sigma}$, the local number operator for $\sigma$ electrons transforms as $\hat{n}_{i,\sigma} \to \hat{n}_{i,-\sigma}$. This implies that the number operator, $\hat{N}$, and the Hamiltonian (2.5) remain unchanged, but that the magnetization operator transforms as $\hat{S}^s_z \to -\hat{S}^s_z$. That is, under this transformation we go from the sector where $N_\sigma > N_{-\sigma}$ to the sector where $N_\sigma < N_{-\sigma}$. This can be accomplished by the ladder operators

$$\hat{S}^s_- = \sum_j c^\dagger_{j\uparrow} c_{j\downarrow}\,, \qquad \hat{S}^s_+ = \sum_j c^\dagger_{j\downarrow} c_{j\uparrow}\,. \tag{2.6}$$

On the other hand, if we perform the particle-hole transformation $c_{i,\sigma} \to (-1)^i c^\dagger_{i,-\sigma}$, the local number $\sigma$ operator transforms as $\hat{n}_{i,\sigma} \to (1 - \hat{n}_{i,-\sigma})$. This transformation implies that the magnetization operator and the kinetic energy ($\vec{A} = 0$) of the Hamiltonian (2.5) remain unchanged, whereas the number operator and the interaction term of the Hamiltonian (2.5) transform as

$$\hat{N} \to 2N_a - \hat{N}\,, \tag{2.7}$$

and

$$U\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} \to U\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + UN_a - UN\,, \tag{2.8}$$

respectively. Therefore, the interaction term can be cast in an invariant form if we write it as $U\sum_i(\hat{n}_{i,\uparrow} - 1/2)(\hat{n}_{i,\downarrow} - 1/2)$. This transformation then takes us from the sector where $N < N_a$ to the sector where $N > N_a$. At half-filling the number operator remains invariant. This change in the electronic density sector without changing the magnetization density can be accomplished by means of suitable operators. The simplest way for generating these operators is to perform the transformation

$c_{i,\uparrow} \to (-1)^i c^\dagger_{i,\uparrow}$ in the $\hat{S}^s_-, \hat{S}^s_+$, and $\hat{S}^s_z$ operators. This leads to the following set of operators

$$\hat{S}^c_z = -\frac{1}{2}[N_a - \sum_\sigma \hat{N}_\sigma]\,, \qquad \hat{S}^c_- = \sum_j (-1)^j c_{j\uparrow} c_{j\downarrow}\,, \qquad \hat{S}^c_+ = \sum_j (-1)^j c^\dagger_{j\downarrow} c^\dagger_{j\uparrow}\,. \quad (2.9)$$

Both the set of generators $\{\hat{S}^s_-, \hat{S}^s_+, \hat{S}^s_z\}$ and $\{\hat{S}^c_-, \hat{S}^c_+, \hat{S}^c_z\}$ form two independent SU(2) algebras. The first set takes into account the spin part and the second set the charge part. If we write the Hamiltonian (2.5) as

$$\hat{H}_{SO(4)} = -t \sum_{\langle j,i\rangle,\sigma} c^\dagger_{j\sigma} c_{i,\sigma} + U \sum_i (\hat{n}_{i,\uparrow} - 1/2)(\hat{n}_{i,\downarrow} - 1/2)\,, \quad (2.10)$$

the Hubbard model becomes SO(4) invariant [4, 6, 7]. Note that the $SO(4)$ symmetry is not fully equivalent to the $SU(2) \otimes SU(2)$ symmetry [4, 6, 7]. All the eigenstates $|\phi\rangle$ of the Hubbard model can be choosen as simultaneous eigenstates of $\hat{H}, \hat{S}^c_z, \hat{S}^s_z, (\hat{S}^s)^2, (\hat{S}^c)^2$, and the lattice translation operator. The commutators

$$[\hat{S}^c_+, \hat{N}] = -2\hat{S}^c_+\,, \qquad [\hat{S}^\alpha_+, \hat{S}^\alpha_z] = -\hat{S}^\alpha_+\,, \qquad \alpha = c, s\,, \quad (2.11)$$

and

$$[\hat{S}^c_+, \hat{P}] = -\pi \hat{S}^c_+\,, \qquad (\hat{P} = \sum_{k,\sigma} k c^\dagger_{k,\sigma} c_{k,\sigma}) \quad (2.12)$$

where $\hat{P}$ is the momentum operator, imply that if a state $|\phi\rangle$ has $N$ electrons, magnetization $(N_\downarrow - N_\uparrow)/2$, and momentum $P$, then the state $\hat{S}^c_+|\phi\rangle$ has $N+2$ electrons and momentum $P+\pi$, and the state $\hat{S}^s_+|\phi\rangle$ has magnetization $(N_\downarrow - N_\uparrow)/2 + 1$ and momentum $P$. These results introduce a enormous simplification in the description of the Hilbert space in any dimension.

The inclusion of terms that break the SO(4) symmetry in a trivial way, like the chemical-potential term and the Zeeman-coupling term, do not change the simplicity of the SO(4) description. The inclusion in the Hamiltonian (2.10) of such terms reduces, in general, the symmetry of the model. The resulting Hamiltonian reads

$$\hat{H} = \hat{H}_{SO(4)} + 2\mu\hat{\eta}_z + 2\mu_0 H \hat{S}_z\,. \quad (2.13)$$

For finite values of both the magnetic field and the chemical potential the symmetry of the quantum problem is reduced to $U(1) \otimes U(1)$, with $\hat{S^c}_z$ and $\hat{S^s}_z$ commuting with $\hat{H}$. The values of $\mu$ and $H$ determine the different symmetries of the Hamiltonian (2.13). When $\mu \neq 0$ and $H \neq 0$ the symmetry is $U(1) \otimes U(1)$, for $\mu = 0$ and

$H \neq 0$ it is $SU(2) \otimes U(1)$, when $\mu \neq 0$ and $H = 0$ it is $U(1) \otimes SU(2)$, and at $\mu = 0$ and $H = 0$ the Hamiltonian symmetry is SO(4).

There are four $U(1) \otimes U(1)$ sectors of parameter space corresponding to $S_z^c < 0$ and $S_z^s < 0$, $S_z^c < 0$ and $S_z^s > 0$, $S_z^c > 0$ and $S_z^s < 0$, and $S_z^c > 0$ and $S_z^s > 0$. We follow the works [8, 9] and call these sectors $(l_c, l_s)$, where

$$l_\alpha = \frac{S_z^\alpha}{|S_z^\alpha|} \, . \tag{2.14}$$

The sectors $(-1,-1)$, $(-1,+1)$, $(+1,-1)$, and $(+1,+1)$ refer to electronic densities and spin densities $0 < n < 1$ and $0 < m < n$, $0 < n < 1$ and $-n < m < 0$, $1 < n < 2$ and $0 < m < (2-n)$, and $1 < n < 2$ and $-(2-n) < m < 0$, respectively.

There are two $(l_s)$ sectors of $SU(2) \otimes U(1)$ Hamiltonian symmetry [and two $(l_c)$ sectors of $U(1) \otimes SU(2)$ Hamiltonian symmetry] which correspond to $S_z^s < 0$ and $S_z^s > 0$ for $l_s = -1$ and $l_s = +1$, respectively, (and to $S_z^c < 0$ and $S_z^c > 0$ for $l_c = -1$ and $l_c = +1$, respectively). There is one SO(4) sector of parameter space [which is constituted only by the $S_z^c = 0$ (and $\mu = 0$) and $S_z^s = 0$ canonical ensemble].

## 2.3 Basic features of the Hubbard model

The Hubbard model (2.5) [or its SO(4) invariant version (2.10)] depends on two parameters, namely the hopping integral $t$ and the Coulomb integral $U$. The model shows very different physical behavior depending on the relative strength of these two parameters and on the band filling $n$. In the case of $U = 0$, the Hubbard model reduces to the simple tight-binding model

$$\hat{H}_0 = -t \sum_{<i,j>,\sigma} e^{-\frac{i}{c}\vec{A}\cdot(\vec{R}_i - \vec{R}_j)} c_{i,\sigma}^\dagger c_{j,\sigma} \, , \tag{2.15}$$

and a simple exact solution follows from [10] the introduction of momentum-space operators $c_{\vec{k},\sigma}^\dagger$ and $c_{\vec{k},\sigma}$. These operators are related to the Wannier representation by $c_{i,\sigma}^\dagger = N_a^{-1/2} \sum_i e^{i\vec{k}\cdot\vec{R}_i} c_{\vec{k},\sigma}^\dagger$. The form of the band then depends on the type of lattice considered. For the one-dimensional case, with one atom per unit cell, the diagonalized Hamiltonian is

$$\hat{H}_0 = -2t \sum_{k,\sigma} \cos\left(k - \frac{A}{c}\right) c_{k,\sigma}^\dagger c_{k,\sigma} \, . \tag{2.16}$$

It is a simple matter to compute both the exact partition function and the conductivity for the Hamiltonian (2.16). This model is a metal for all electronic densities,

exception made to $N/N_a = 2$, where it has two electrons per lattice site, and for $N/N_a = 1$, when the system is fully polarized.

Another limit where the model (2.5) has an exact solution is the atomic limit [1]. In this limit the hopping integral is zero and the electrons are localized at the lattice sites. Since the electrons have zero kinetic energy, the model represents an insulator for all values of $U$, possesing only two (flat) bands, one located at the chemical potencial $\mu$ and another at the energy $\mu + U$. This can be put in a more formal way by means of the Green's function formalism. A very simple calculation of the one-particle Green's function at finite temperature (suitable to deal with the massive degeneracy of the model eigenstates in this limit), leads to

$$\mathcal{G}^{atomic}_{\sigma_i,\sigma_j}(\omega) = \delta_{i,j}\delta_{\sigma_i,\sigma_j}\left[\frac{1-\langle n_\sigma\rangle}{i\omega+\mu} + \frac{\langle n_\sigma\rangle}{i\omega+\mu-U}\right], \tag{2.17}$$

where $i\omega$ is the usual finite-temperature Matsubara frequency and $\langle n_\sigma\rangle$ is the electronic occupation number at finite temperature for the single site Hamiltonian, $\hat{h}_i = \sum_\sigma (U/2\hat{n}_{i,\sigma}\hat{n}_{j,-\sigma} - \mu\hat{n}_{i,\sigma})$.

The question now is whether the system undergoes or not a phase transition when the parameters varie from the tigth-binding $U/t = 0$ limit to the atomic $U/t \to \infty$ limit, for some finite value of $U/t$. In the strong-coupling regime $U \gg t$, the states with two electrons in the same site have a much larger energy – of order $U$ – relatively to those states with single-site occupancy only. Thus, for the half-filled band we expect to have an insulator in the large $U$ limit, and we show below, within perturbation theory, that this is indeed the case.

Let us then divide the Hilbert space of the Hubbard model into three subspaces: the subspace of single-occupied-site states $\{|S\rangle\}$, the subspace of one double-occupied site states $\{|D_1\rangle\}$, and the subspace of more than one double-occupied-site states $\{|D_n\rangle\}$. Since $U \gg t$, the kinetic term of the Hamiltonian (2.5) can be treated as a perturbation. Note that due to the massive degeneracy in each of the three considered subspaces, degenerate perturbation theory must be applied. Moreover, in order to extract information on the nature of the ground state of the model, we compute the average energy relative to the states belonging the subspace $\{|S\rangle\}$.

Let us consider the system away from half filling. All states belonging to the subspace $\{|S\rangle\}$ have zero Coulomb energy. Then, up to second order in perturbation theory, the energy of a given state belonging to the subspace $\{|S\rangle\}$ is given by

$$E_{|S\rangle} = \langle S|\hat{T}|S\rangle - \frac{1}{U}\sum_{|D_1\rangle}\langle S|\hat{T}|D_1\rangle\langle D_1|\hat{T}|S\rangle\,, \tag{2.18}$$

where $\hat{T} = -t \sum_{<i,j>,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma}$. The states belonging to the subspace $\{|D_n\rangle\}$ have not been considered because the operator $\hat{T}$ does not connect that subspace with $\{|S\rangle\}$. The operator $\hat{P}_{D_1} = \sum_{|D_1\rangle} |D_1\rangle\langle D_1|$ can be regarded as the projection operator for the subspace $\{|D_1\rangle\}$. Thus, up to this order in perturbation theory, the operator $\hat{P}_{D_1}$ can be replaced in Eq. (2.18) by $\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}$. It should be emphasized that this substitution is valid only if these calculations are restricted to the subspaces $\{|S\rangle\}$ and $\{|D_1\rangle\}$. From Eq. (2.18), one then arrives to an effective Hamiltonian valid for the subspace $\{|S\rangle\}$ that reads

$$\begin{aligned} \hat{H}^{eff.}_{n<1} &= \hat{P}_s \left[ \hat{T} - \frac{t^2}{U} \sum_{\sigma,\sigma'} \sum_{i,m} c^{\dagger}_{m,\sigma} c_{i,\sigma} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} c^{\dagger}_{i,\sigma'} c_{m,\sigma'} \right. \\ &- \left. \frac{t^2}{U} \sum_{\sigma,\sigma'} \sum_{l \neq i,m} c^{\dagger}_{l,\sigma} c_{i,\sigma} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} c^{\dagger}_{i,\sigma'} c_{m,\sigma'} \right] \hat{P}_s \,, \end{aligned} \tag{2.19}$$

where $\hat{P}_s = \sum_{|S\rangle} |S\rangle\langle S|$ is the projector onto the subspace $\{|S\rangle\}$. The third term in the rhs of Eq. (2.19) is usually neglected and the remaining two terms are called the $t - J$ model [11]. At half filling, the first and the third terms in the rhs of Eq. (2.19) vanish and we are left with another effective Hamiltonian

$$\hat{H}^{eff.}_{n=1} = \frac{J}{2} \sum_{i,j} [\vec{S}_i \cdot \vec{S}_j - \frac{\hat{n}_i \hat{n}_j}{4}] \,, \tag{2.20}$$

with $J = 4t^2/U$. This is the Heisenberg anti-ferromagnetic model. The second term in the rhs of Eq. (2.19) was rewritten by using the electronic representation for the spin operators defined by $\hat{S}^s_z$, $\hat{S}^s_+$, and $\hat{S}^s_-$.

The above results show (assuming that the perturbative treatment holds) that for strong electronic correlations ($U \gg t$) the system is an antiferromagnetic insulator at half filling. Due to the restrictions imposed on electronic movements by the reduced dimensionality, for one-spatial dimension the Hubbard model is an insulator at half-filling for any positive value of $U$ [12]. In one dimension the system is not a simple Fermi liquid. The most difficult problem is the study of the intermediate-$U$ case and of how the model properties change as the ratio $U/t$ goes from small to large values. The study of this regime requires non-perturbative methods. In the following we consider the case of the 1D lattice where the exact Bethe-ansatz solution is available.

## 2.4 Basic ideas on the Bethe ansatz

From here on, we will be dealing with the one-dimensional Hubbard model. Following Yang's solution [13] of the one-dimensional many-body problem with a delta-function interaction, Lieb and Wu [12] computed the ground state of the Hubbard model. Later, Takahashi [14] gave the complete solution of the Lieb and Wu Bethe-ansatz equations. The basic ingredients of the Bethe ansatz are: the simple topology of the 1D space, the continuity condition at the same point of the lattice, the boundary conditions, and Pauli's principle. However, the implementation of these simple concepts in order to achieve the solution of the general eigenvalue problem is a task of considerable complexity [15]. In this section, the Bethe ansatz technique is illustrated by the solution of the two-electron problem in a chain of $N_a$ sites.

The eigenstates $|\Psi\rangle$ of the two-electron problem can be written as a superposition of Wannier states $c^{\dagger}_{x_2,\sigma_2}c^{\dagger}_{x_1,\sigma_1}|0\rangle$

$$|\Psi\rangle = \sum_{x_1,\sigma_1}\sum_{x_2,\sigma_2}\psi(x_1,\sigma_1;x_2,\sigma_2)c^{\dagger}_{x_2,\sigma_2}c^{\dagger}_{x_1,\sigma_1}|0\rangle\,, \tag{2.21}$$

where $|0\rangle$ is the electronic vacuum and $x_i$ stands for the position of the electron $i$. Obviously, the problem consists in determining the coefficients $\psi(x_1,\sigma_1;x_2,\sigma_2)$. The starting point is the eigenvalue equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$ which imposes the following relation among the coefficients $\psi(x_1,\sigma_1;x_2,\sigma_2)$

$$\begin{aligned} - \quad & t[\psi(x_1+1,\sigma_1;x_2,\sigma_2)+\psi(x_1-1,\sigma_1;x_2,\sigma_2)+ \\ + \quad & \psi(x_1,\sigma_1;x_2+1,\sigma_2)+\psi(x_1,\sigma_1;x_2+1,\sigma_2)]+ \\ + \quad & U\delta x_1,x_2\delta\sigma_1,-\sigma_2\psi(x_1,\sigma_1;x_2,\sigma_2) = E\psi(x_1,\sigma_1;x_2,\sigma_2)\,. \end{aligned} \tag{2.22}$$

The spatial dimensionality of the system allows the definition of two regions, I and II, for which $x_1 \leq x_2$ and $x_1 \geq x_2$, repectively. The electronic antisymmetric character under the interchange of positions implies that

$$\psi_I(x_1,\sigma_1;x_2,\sigma_2) = -\psi_{II}(x_2,\sigma_2;x_1,\sigma_1)\,. \tag{2.23}$$

The next step is to choose a simple representation for the anti-symmetric property (2.23). We introduce the Bethe ansatz

$$\psi_I(x_1,\sigma_1;x_2,\sigma_2) = A(p_1,\sigma_1;p_2,\sigma_2)e^{i(p_1x_1+p_2x_2)} - A(p_2,\sigma_1;p_1,\sigma_2)e^{i(p_2x_1+p_1x_2)} \tag{2.24}$$

and

$$\psi_{II}(x_2\sigma_2, x_1, \sigma_1) = A(p_2, \sigma_2; p_1, \sigma_1)e^{i(p_1x_1+p_2x_2)} - A(p_1, \sigma_2; p_2, \sigma_1)e^{i(p_2x_1+p_1x_2)} \,. \quad (2.25)$$

It is clear that the interchange $(x_1, \sigma_1) \leftrightarrow (x_2, \sigma_2)$ in $\psi_I(x_1, \sigma_1; x_2\sigma_2)$ or $\psi_{II}(x_2\sigma_2, x_1, \sigma_1)$ agrees with the antisymmetry condition (2.23). If $x_1 \neq x_2$, introduction of both $\psi_I(x_1, \sigma_1; x_2\sigma_2)$ and $\psi_{II}(x_2\sigma_2, x_1, \sigma_1)$ in Eq. (2.22) leads to $E = -2t\cos(p_1) - 2t\cos(p_2)$ (we are considering the lattice spacing $a$ equal to 1).

At the same lattice point, $x_1 = x_2 = x$, we must have

$$\psi_I(x, \sigma_1; x, \sigma_2) = \psi_{II}(x, \sigma_2; x, \sigma_1) \,, \quad (2.26)$$

which is the continuity equation. Combining Eq. (2.26) with the eigenvalue equation for the two electrons at the same site and imposing the same functional form, $E = -2t\cos(p_1) - 2t\cos(p_2)$, for the energy eigenvalue, after some algebra the following relation among three of the amplitudes $A(p_j, \sigma_i; p_m, \sigma_n)$ (with $j, i, m, n = 1, 2$) is obtained

$$\begin{pmatrix} A(p_2, \sigma_1; p_1, \sigma_2) \\ A(p_2, \sigma_2; p_1, \sigma_1) \end{pmatrix} = \frac{1}{k_{12} + ic} \begin{pmatrix} ic & k_{12} \\ k_{12} & ic \end{pmatrix} \begin{pmatrix} A(p_1, \sigma_1; p_2, \sigma_2) \\ A(p_1, \sigma_2; p_2, \sigma_1) \end{pmatrix} . \quad (2.27)$$

Here $k_{12} \equiv \sin(p_1) - \sin(p_2)$ and $c \equiv U/(2t)$. Solution of the problem in closed form involves the imposition of periodic boundary conditions (other boundary conditions are also possible). Since we have two electrons, we must impose periodic boundary conditions on both $x_1$ and $x_2$ (some care is needed in taking into account the regions I and II). These are

$$\begin{aligned} \text{Region I}: \quad & x_1 < x_2 \rightarrow x_1 + N_a > x_2, \\ & \psi_I(x_1, \sigma_1; x_2\sigma_2) = \psi_{II}(x_1 + N_a, \sigma_1; x_2, \sigma_2) \end{aligned} \quad (2.28)$$

and

$$\begin{aligned} \text{Region II}: \quad & x_1 > x_2 \rightarrow x_2 + N_a > x_1, \\ & \psi_{II}(x_1, \sigma_1; x_2\sigma_2) = \psi_I(x_1, \sigma_1; x_2 + N_a, \sigma_2) \,. \end{aligned} \quad (2.29)$$

Combinig Eqs. (2.24) and (2.25) with Eqs. (2.28) and (2.29), we arrive to the two following relations

$$e^{ip_1 N_a}\begin{pmatrix} A(p_2,\sigma_1;p_1,\sigma_2) \\ A(p_2,\sigma_2;p_1,\sigma_1)\end{pmatrix} = \begin{pmatrix} A(p_1,\sigma_2;p_2,\sigma_1) \\ A(p_1,\sigma_1;p_2,\sigma_2)\end{pmatrix}, \tag{2.30}$$

and

$$e^{ip_2 N_a}\begin{pmatrix} A(p_1,\sigma_1;p_2,\sigma_2) \\ A(p_1,\sigma_2;p_2,\sigma_1)\end{pmatrix} = \begin{pmatrix} A(p_2,\sigma_2;p_1,\sigma_1) \\ A(p_2,\sigma_1;p_1,\sigma_2)\end{pmatrix}. \tag{2.31}$$

By combining Eqs. (2.30) and (2.27), we end up with the simple eigenvalue problem

$$e^{-ip_1 N_a}|A\rangle = \hat{R}|A\rangle\,, \tag{2.32}$$

and equivalently for the eigenvalue $e^{-ip_2 N_a}$. The state $|A\rangle$ and the operator $\hat{R}$ are written as

$$|A\rangle = \begin{pmatrix} A(p_1,\sigma_1;p_2,\sigma_2) \\ A(p_1,\sigma_2;p_2,\sigma_1)\end{pmatrix}, \qquad \hat{R} = \frac{1}{k_{12}+ic}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}\begin{pmatrix} ic & k_{12} \\ k_{12} & ic\end{pmatrix}. \tag{2.33}$$

The solution to this simple problem can be cast in the form

$$e^{ip_j N_a} = \frac{\sin(p_j)-\Lambda+ic/2}{\sin(p_j)-\Lambda-ic/2} \qquad j=1,2\,, \tag{2.34}$$

and

$$\prod_{i=1}^{2}\frac{\sin(p_i)-\Lambda+ic/2}{\sin(p_i)-\Lambda-ic/2} = 1\,, \tag{2.35}$$

where $\Lambda = \sin(p_1)+\sin(p_2)$. These are the Bethe-ansatz equations for one up-spin and one down-spin electron.

Finally, by considering a magnetic flux $\phi$ through the ring, the general Bethe-ansatz equations become [12, 16]

$$e^{ik_j N_a} = e^{i\phi}\prod_{\delta=1}^{N_\downarrow}\frac{\sin(k_j)-\Lambda_\delta+iU/4}{\sin(k_j)-\Lambda_\delta-iU/4}\,, \qquad (j=1,\ldots,N) \tag{2.36}$$

and

$$\prod_{j=1}^{N}\frac{\sin(k_j)-\Lambda_\delta+iU/4}{\sin(k_j)-\Lambda_\delta-iU/4} = -\prod_{\beta=1}^{N_\downarrow}\frac{\Lambda_\beta-\Lambda_\delta+iU/2}{\Lambda_\beta-\Lambda_\delta-iU/2}\,, \qquad (\delta=1,\ldots,N_\downarrow)\,. \tag{2.37}$$

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# Chapter 3

# Algebraic Representation for the Hilbert Space of the 1D Hubbard Model

## 3.1 Introduction

In this chapter we present the algebraic solution for the 1D Hubbard model, which shows some basic similarities with the algebraic solution of the isotropic harmonic oscillator. In order to clarify the basic ideas underlying the problem, we begin by presenting in the following the main results for the algebraic solution of the harmonic oscillator. Afterwards, we discuss the general similarities and differences between the two cases.

The isotropic harmonic oscillator has SO(3) symmetry. The SO(3) group can be defined by the following algebra envolving the angular momentum operators

$$[L_+, L_z] = -L_+ \,, \qquad [L_-, L_z] = L_- \,, \qquad [L_+, L_-] = 2L_z \,, \tag{3.1}$$

where $L = (L_x, L_y, L_z)$ and $L_\pm = L_x \pm iL_y$. Moreover, $[L^2, L] = 0$ and $[H, L] = 0$, where $H$ represents the isotropic harmonic oscillator Hamiltonian. The commutators (3.1) imply that $L^2$, $L_z$, and $H$ can be simultaneously diagonalized. In second quantization, $H$, $L_z$, and $L^2$ can be written as ($\hbar = 1$)

$$H = \frac{\omega}{2}\left(3 + a_0^\dagger a_0 + a_{\frac{1}{2}}^\dagger a_{\frac{1}{2}} + a_{-\frac{1}{2}}^\dagger a_{-\frac{1}{2}}\right) , \tag{3.2}$$

$$L_z = \frac{1}{2}(a^\dagger_{\frac{1}{2}} a_{\frac{1}{2}} - a^\dagger_{-\frac{1}{2}} a_{-\frac{1}{2}})\,, \tag{3.3}$$

$$L^2 = L_- L_+ + L_z^2 + L_z\,, \tag{3.4}$$

with

$$L_- = a^\dagger_{-\frac{1}{2}} a_{\frac{1}{2}}\,, \qquad L_+ = a^\dagger_{\frac{1}{2}} a_{-\frac{1}{2}}\,. \tag{3.5}$$

The operators $a_0^\dagger$, $a_{\frac{1}{2}}^\dagger$, and $a^\dagger_{-\frac{1}{2}}$ are bosonic operators and the angular momentum operators are written in the Schwinger representation [1]. The eigenstates $|n_{\frac{1}{2}}, n_0, n_{-\frac{1}{2}}\rangle$ of $H$, $L_z$, and $L^2$, corresponding to a given $n = n_{\frac{1}{2}} + n_0 + n_{-\frac{1}{2}}$, a given $\ell = n - 2n_0$, and given $m$ (the eigenvalue of $L_z$), read

$$|n_{\frac{1}{2}}, n_0, n_{-\frac{1}{2}}\rangle = \frac{L_+^{(n-2n_0+m)} (a^\dagger_{-\frac{1}{2}})^{2(n-2n_0)} (a_0^\dagger)^{4n_0}}{\sqrt{(4n_0)!}\sqrt{(2n-4n_0)!}\sqrt{(n-2n_0+m)!}}\,|0,0,0\rangle\,. \tag{3.6}$$

For a given value of $n$, the quantum number $n_0$ assumes the values $0, 1, 2, \ldots, n/2$, for $n$ even, and $0, 1, 2, \ldots, (n-1)/2$, for $n$ odd [the number $n_0$ is used to generate, for example, all the LWS ($m = -\ell$, see below) for a given $n$]. The states of the form $|n_{\frac{1}{2}}, n_0, 0\rangle$ are called highest-weight states (HWS's), since $L_+|n_{\frac{1}{2}}, n_0, 0\rangle = 0$, and the states $|0, n_0, n_{-\frac{1}{2}}\rangle$ are called lowest-weight states (LWS's), since $L_-|0, n_0, n_{-\frac{1}{2}}\rangle = 0$. The states such that $L_\pm|n_{\frac{1}{2}}, n_0, n_{-\frac{1}{2}}\rangle \neq 0$ are called non-LWS's or non-HWS's. To go from the LWS of a given tower, characterized by the angular momentum number $\ell = n - 2n_0$, to the respective HWS (or vice-versa), one applies the rising operator $L_+$ (or the lowering operator $L_-$). For a given $\ell$, the number $m$ can have the values $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$. All the states in the $\ell$ tower differ only in the $L_z$ eigenvalue, and all the states with a given $n$ have degeneracy $(n^2+3n+2)/2$.

From the above analysis, we see that the isotropic harmonic oscillator is characterized by three types of particles: the $a_0^\dagger$ bosons, which do not contribute to the angular momentum operators, and the $a_{\frac{1}{2}}^\dagger$ and $a^\dagger_{-\frac{1}{2}}$ bosons. The latter two particles describe the towers of angular momentum. Note that the HWS's (LWS's) have only $a_{\frac{1}{2}}^\dagger$ ($a^\dagger_{-\frac{1}{2}}$) bosons. The non-LWS's or non-HWS's have both types of particles. The ladder operators $L_\pm$ act upon the $\pm\frac{1}{2}$ bosons interchanging the $\pm\frac{1}{2}$ quantum numbers.

A similar algebra occurs in the 1D Hubbard model. Obviously, the algebraic description of this model is much more involved, for we are dealing with a many-body system with discrete translational symmetry. The Bethe-ansatz solution of

the Hubbard model refers usually to the symmetry sector $(-1,-1)$ [2, 3, 4] (Sec. 2.2). In this sector it has been proved by Essler *et al.* [5, 6, 7] that the Bethe-ansatz eigenstates $|\psi\rangle$ are LWS's of the SO(4) algebra, that is $\hat{S}^{\alpha}_{-}|\psi\rangle = 0$. We can then construct the towers of spin and eta-spin by acting onto the states $|\psi\rangle$ with the ladder operators $\hat{S}^{\alpha}_{+}$ and reach the respective HWS's. This procedure generates all the $4^{N_a}$ eigenstates of the Hubbard chain, which span the whole Hilbert space associated with all the nine symmetry sectors of the model.

In the algebraic solution of the Hubbard chain the eigenstates of the model are described by the set of operators $a^{\dagger}_{q,\alpha,\beta}$ and $b^{\dagger}_{q,\alpha,\gamma}$ which refer to the quantum objects that we call pseudoholes and heavy-pseudoparticles, respectively [8, 9, 10]. These operators obey the usual anticommutation relations. The quantum numbers that label the operators $a^{\dagger}_{q,\alpha,\beta}$ and $b^{\dagger}_{q,\alpha,\gamma}$ are the following: a) the $q$ is the pseudomomentum and is to be chosen out of the available pseudo-Brillouin zone values (to be defined later); b) there are two colors of pseudohole and heavy-pseudoparticle, which are called $\alpha = c$ and $\alpha = s$; c) these different types of heavy pseudoparticles can populate different $\gamma$ bands ($\gamma = 1, 2, ..., \infty$). In the case of the $\alpha, \beta$ pseudoholes, the band index number is $\gamma = 0$ (this was omitted for convenience of notation); d) the $\beta = \pm 1/2$ is related to the SO(4) algebra.

In the 1D Hubbard model the Bethe-ansatz eigenstates can be classified as LWS's I and LWS's II [5, 6, 7]. The former have neither heavy-pseudoparticle nor $\alpha, \beta = 1/2$ pseudohole occupancy and all the $\alpha, \beta$ pseudoholes which populate the $\alpha, 0$ band have $\beta = -1/2$. On the other hand, the latter eigenstates have both heavy-pseudoparticles and $\beta = \pm 1/2$ pseudoholes. The SO(4) generators involve only the $a^{\dagger}_{q,\alpha,\beta}$ pseudohole operators, as the SO(3) generators, in the isotropic oscillator, involve only the $a^{\dagger}_{\mp\frac{1}{2}}$ boson operators. The two colors $\alpha = c$ and $\alpha = s$ are directly related to the charge and spin degrees of freedom, respectively. The generators of the SO(4) algebra are given, in the generalized Schwinger representation, by [9, 10]

$$\hat{S}^{\alpha}_{z} = \frac{1}{2}\sum_{q}(a^{\dagger}_{q,\alpha,\frac{1}{2}}a_{q,\alpha,\frac{1}{2}} - a^{\dagger}_{q,\alpha,-\frac{1}{2}}a_{q,\alpha,-\frac{1}{2}})\,, \qquad \hat{S}^{\alpha}_{\pm} = \sum_{q} a^{\dagger}_{q,\alpha,\pm\frac{1}{2}}a_{q,\alpha,\mp\frac{1}{2}}\,. \tag{3.7}$$

The spin and eta-spin "angular" quantum numbers $S^{\alpha}$ are given by

$$S^{\alpha} = \frac{1}{2}(N^{h}_{\alpha} - \sum_{\gamma=1}^{\infty} 2\gamma N_{\alpha,\gamma})\,, \tag{3.8}$$

where $N^{h}_{\alpha} = \sum_{\beta} N^{h}_{\alpha,\beta}$, $N^{h}_{\alpha,\beta}$ is the number of $\alpha, \beta$ pseudoholes, and $N_{\alpha,\gamma}$ is the number of heavy $\alpha, \gamma$ pseudoparticles. As in the SO(3) algebra, the ladder operators

interchange only the $\beta = \pm 1/2$ quantum number. Thus, as in the case of the harmonic oscillator, all the pseudoholes have $\beta = -1/2$ in the LWS's I and $\beta = +1/2$ in the HWS's I. The non-LWS's I (and non-HWS's I) have both $\beta = +1/2$ and $\beta = -1/2$ pseudohole occupancy.

The number of discrete pseudomomentum values in each $\alpha, \gamma$ band ($\alpha, \gamma$-band Fock-space dimension) is given by the Bethe-ansatz solution [4] and reads

$$d_{c,0} = N_a \tag{3.9}$$

$$d_{\alpha,\gamma} = N_\alpha^h + N_{\alpha,\gamma} - \sum_{\gamma'=1}^{\infty} [\gamma + \gamma' - |\gamma - \gamma'|] N_{\alpha,\gamma'} \,, \qquad \alpha, \gamma \neq c, 0 \,. \tag{3.10}$$

In the summations and products over $q$ the pseudomomentum $q$ takes on values

$$q_j = \frac{2\pi}{N_a} I_j^{\alpha,\gamma} \,, \tag{3.11}$$

where in contrast to the usual momentum, $I_j^{\alpha,\gamma}$ are consecutive integers or half-odd integers for $\bar{N}_{\alpha,\gamma}$ odd and even, respectively [3, 4]. Here

$$\bar{N}_{c,0} = \sum_\alpha \frac{N_\alpha^h}{2} - \sum_{\gamma=1}^{\infty} N_{c,\gamma} = \frac{N_a}{2} - N_{s,0} - \sum_{\alpha,\gamma=1}^{\infty} N_{\alpha,\gamma} \,, \tag{3.12}$$

and

$$\bar{N}_{\alpha,\gamma} = d_{\alpha,\gamma} \,, \tag{3.13}$$

for values of $\alpha, \gamma$ other than $c, 0$. It follows that for each $\alpha, \gamma$ band, $q_{\alpha,\gamma}^{(-)} \leq q \leq q_{\alpha,\gamma}^{(+)}$, with the limits of the pseudo-Brillouin zones given by

$$q_{c,0}^{(\pm)} = \pm\pi[1 - \frac{1}{N_a}] \,, \tag{3.14}$$

for $\bar{N}_{c,0}$ even and

$$q_{c,0}^{(+)} = \pi \,, \qquad q_{c,0}^{(-)} = -\pi[1 - \frac{2}{N_a}] \,, \tag{3.15}$$

or

$$q_{c,0}^{(+)} = \pi[1 - \frac{2}{N_a}] \,, \qquad q_{c,0}^{(-)} = -\pi \,, \tag{3.16}$$

for $\bar{N}_{c,0}$ odd and simply given by

$$q_{\alpha,\gamma}^{(\pm)} = \pm\frac{\pi}{N_a}[d_{\alpha,\gamma} - 1]\,, \tag{3.17}$$

for all the remaining $\alpha, \gamma$ bands.

In the LWS's II (or HWS's II) the situation is somewhat more complex, and has no analogon in the case of the harmonic oscillator. The origin of these states is in the lack of continuous translation symmetry. In these states, which can be interpreted as bound states of $\alpha, 0$ pseudoparticles, we have both $\beta = 1/2$ and $\beta = -1/2$ pseudohole occupancy. The general second quantized representation for all Hubbard-chain eigenstates is [10]

$$|\psi; \{N_{\alpha,\beta}^h\}, \{N_{\alpha,\gamma}\}\rangle = \frac{1}{\sqrt{C}}\prod_{\alpha} A_\alpha \prod_{\gamma=1}^{\infty}\left[[\hat{S}_+^\alpha]^{N^h_{\alpha,\frac{1}{2}}}\prod_{q,q'} a^\dagger_{q,\alpha,-\frac{1}{2}} b^\dagger_{q',\alpha,\gamma}\right]|V\rangle\,, \tag{3.18}$$

where the symbols $\{N_{\alpha,\beta}^h\}$ and $\{N_{\alpha,\gamma}\}$ are abbreviations for the sets $\{N^h_{c,\frac{1}{2}}, N^h_{c,-\frac{1}{2}}, N^h_{s,\frac{1}{2}}, N^h_{s,-\frac{1}{2}}\}$ and $\{N_{c,1}, ..., N_{c,\infty}, N_{s,1}, ..., N_{s,\infty}\}$, respectively, $C = \prod_\alpha (N^h_\alpha!/N^h_{\alpha,-\frac{1}{2}}!)$, $A_\alpha = \prod_\beta \Theta(N^h_{\alpha,\beta} - \sum_{\gamma=1}^{\infty}\gamma N_{\alpha,\gamma})$, and the ladder operators $S^\alpha_+$ are defined in Eq. (3.7). Note that the states (3.18) have a very simple form and present a remarkable similarity with the states (3.6).

As in the harmonic oscillator, the Hubbard model Hamiltonian (and other operators) can be written in terms of the operators $a^\dagger_{q,\alpha,\beta}$ and $b^\dagger_{q,\alpha,\gamma}$ and the energy of the LWS's and HWS's is independent of the $\beta$ quantum number. In general, the non-LWS's (non-HWS's) and the LWS's II (HWS's II) have an energy gap relatively to the corresponding ground state (which is always a LWS's I or HWS's I). In the remaining sections, we present the details of our algebraic solution for the 1D Hubbard model.

## 3.2 Pseudoholes: the $\beta$ quantum number in LWS's I/HWS's I

As was referred above, the description of the non-LWS's, not included in the Bethe-ansatz solution requires the introduction of the $\beta = \pm 1/2$ pseudohole numbers. We start the analysis with the study of the LWS's I. The Bethe-ansatz solution in the (-1,-1) sector (Sec. 2.2) gives for the numbers of $\alpha, 0$ pseudoparticles, $N_{\alpha,0}$, and for the total numbers of permitted orbitals, $d_{\alpha,0}$ (number of states in the respective pseudo-Brillouin zone), the following values [8, 9]

$$N_{c,0} = N\,, \qquad N_{s,0} = \frac{1}{2}\left(N_{c,0} - N_\uparrow + N_\downarrow\right)\,, \tag{3.19}$$

$$d_{c,0} = N_a\,, \qquad d_{s,0} = N_{c,0} - N_{s,0}\,. \tag{3.20}$$

The use of the $SO(4)$ symmetry (Sec. 2.2) allows one to obtain these numbers in the remaining three U(1)⊗U(1) symmetry sectors. The number of pseudoholes in the $\alpha, 0$ band is given by $N^h_\alpha = d_{\alpha,0} - N_{\alpha,0}$. The corresponding results for the LWS's I/HWS's I in the four U(1)⊗U(1) symmetry sectors are listed in Table 3.1. The numbers $N$ and $N_\sigma$ in Table 3.1 are those of the respective $(l_c, l_s)$ sector, and are related to those in different sectors by the particle/hole and spin-up/spin-down symmetries discussed in Sec. 2.2.

Defining $N_e$ as the electron number in a given eta-spin LWS, the respective eigenvalue of $\hat{S}^c_z$ is $S^c_z = -S^c = -\frac{1}{2}(N_a - N_e)$ in terms of electrons, or $S^c_z = -S^c = -\frac{1}{2}N^h_{c,-\frac{1}{2}}$ (see Table 3.1), in terms of pseudoholes. On the other hand, the corresponding HWS has $2N_a - N_e$ electrons and $S^c_z = S^c = \frac{1}{2}(N_a - N_e)$, or, equivalently, $S^c_z = S^c = \frac{1}{2}N^h_{c,\frac{1}{2}}$ (see Table 3.1). Obviously, equivalent results hold for the spin towers. It follows from the results of Table (3.1) that the number of pseudoholes in any

| | $(-1,-1)$ | $(-1,1)$ | $(1,-1)$ | $(1,1)$ |
|---|---|---|---|---|
| $N_{c,0}$ | $N$ | $N$ | $2N_a - N$ | $2N_a - N$ |
| $d_{c,0}$ | $N_a$ | $N_a$ | $N_a$ | $N_a$ |
| $N^h_{c,-\frac{1}{2}}$ | $N_a - N$ | $N_a - N$ | 0 | 0 |
| $N^h_{c,\frac{1}{2}}$ | 0 | 0 | $N - N_a$ | $N - N_a$ |
| $N_{s,0}$ | $N_\downarrow$ | $N_\uparrow$ | $N_a - N_\uparrow$ | $N_a - N_\downarrow$ |
| $d_{s,0}$ | $N_\uparrow$ | $N_\downarrow$ | $N_a - N_\downarrow$ | $N_a - N_\uparrow$ |
| $N^h_{s,-\frac{1}{2}}$ | $N_\uparrow - N_\downarrow$ | 0 | $N_\uparrow - N_\downarrow$ | 0 |
| $N^h_{s,\frac{1}{2}}$ | 0 | $N_\downarrow - N_\uparrow$ | 0 | $N_\downarrow - N_\uparrow$ |

Table 3.1: Values for the total number of pseudoparticles $N_{\alpha,0}$, total number of accessible orbitals $d_{\alpha,0}$, and total number of pseudoholes $N^h_{\alpha,\beta=\pm\frac{1}{2}}$ for LWS's I/HWS's I in the four sectors of symmetry U(1)⊗U(1). The numbers $N$ and $N_\sigma$ are those of the respective $(l_c, l_s)$ sector.

$(l_c, l_s)$ sector is equal to $2|S^\alpha_z|$ —the eigenvalues of $\hat{S}^\alpha_z$—, defined in Sec. 2.2 in terms of electronic operators and in Eq. (3.7) in terms of pseudohole operators. Then, in going from a LWS, belonging to a given $l_\alpha$ sector, to the respective $S_\alpha$ HWS, we

have to apply the ladder operators $S^{\alpha}_{+}$ a $N^{h}_{\alpha}$ number of times, with $N^{h}_{c} = N_a - N_e$ for a eta-spin tower and $N^{h}_{s} = N_{\uparrow} - N_{\downarrow}$ for a spin tower (the numbers $N_{\uparrow}$ and $N_{\downarrow}$ are those for the respective LWS). Hence, as in the isotropic harmonic oscillator, we have in the LWS's I occupancies of $\beta = -1/2$ pseudoholes only. On the other hand, the HWS's I show only $\beta = 1/2$ pseudoholes occupancy. In between we have non-LWS's or non-HWS's whose occupancies refer to mixtures of both $\beta = -1/2$ and $\beta = +1/2$ pseudoholes. The number of pseudoholes is such that it gives the correct values for the $\hat{S}^{\alpha}_{z}$ eigenvalues and the correct number of states for a given $S^{\alpha}$ tower.

## 3.3 Heavy-pseudoparticles: the $\beta$ quantum number in LWS's II/HWS's II

In the LWS's II/HWS's II there is both pseudohole and heavy-pseudoparticle occupancy. In the $(-1,-1)$ sector, the Bethe-ansatz solution gives the following results for the numbers of $\alpha, 0$ pseudoparticles and accessible $d_{\alpha,0}$ orbitals [4, 10]

$$N_{c,0} = N - 2\sum_{\gamma=1}^{\infty}\gamma N_{c,\gamma}\,, \qquad N_{s,0} = N_{\downarrow} - \sum_{\gamma=1}^{\infty}\gamma N_{c,\gamma} - \sum_{\gamma=1}^{\infty}(\gamma+1)N_{s,\gamma}\,, \tag{3.21}$$

and

$$d_{c,0} = N_a\,, \qquad d_{s,0} = N - 2N_{\downarrow} + N_{s,0} + 2\sum_{\gamma=1}^{\infty}\gamma N_{s,\gamma}\,, \tag{3.22}$$

respectively. From the above two equations, it follows that the number of $\alpha, 0$ pseudoholes populating the LWS's II is given by

$$N^{h}_{c} = N_a - N + 2\sum_{\gamma=1}^{\infty}\gamma N_{c,\gamma}\,, \qquad N^{h}_{s} = N - 2N_{\downarrow} + 2\sum_{\gamma=1}^{\infty}\gamma N_{s,\gamma}\,. \tag{3.23}$$

Equation (3.23) shows that the number of holes $N^{h}_{\alpha}$ in the LWS's II is larger than the number of holes in the LWS's I by the addicional term $2\sum_{\gamma=1}^{\infty}\gamma N_{\alpha,\gamma}$. This requires, if we want Eq. (3.7) for $\hat{S}^{\alpha}_{z}$ to give the correct eigenvalues, that half of the pseudoholes in excess, relatively to the respective LWS I, have $\beta = +1/2$. That is, in any LWS/HWS, the numbers of $\beta = \pm 1/2$ pseudoholes must be given by

$$N^h_{c,\beta} = \frac{N^h_c}{2} - \beta[N_a - N]\,, \qquad N^h_{s,\beta} = \frac{N^h_s}{2} - \beta[N_\uparrow - N_\downarrow]\,, \tag{3.24}$$

the total number of $\alpha, 0$ pseudoholes being $N^h_\alpha = \sum_\beta N^h_{\alpha,\beta}$.

Equation (3.24) is a generalization of the pseudohole expressions introduced in the context of LWS's I/HWS's I [9]. It is convenient to introduce the numbers $N^z_\alpha$ such that

$$N^z_\alpha = S^\alpha - |S^\alpha_z| = \frac{1}{2}[\sum_\beta (1 - 2\beta l_\alpha)\hat{N}^h_{\alpha,\beta} - \sum_{\gamma=1}^{\infty} 2\gamma N_{\alpha,\gamma}]\,. \tag{3.25}$$

This number indicates whether a given eigenstate is an LWS (or HWS). The knowledge of all the $N^h_{\alpha,\beta}$ pseudohole and $N_{\alpha,\gamma}$ heavy-pseudoparticle ($\gamma > 0$) numbers provides the knowledge of all pseudoparticle numbers $N_{\alpha,\gamma}$ ($\gamma = 0, 1, 2, 3...$) and $N^z_\alpha$ numbers, the inverse being also true. While the set of $N_{\alpha,\gamma}$ numbers are directly given by the BA solution [4], the $\beta$-dependent pseudohole numbers $N^h_{\alpha,\beta}$ and the numbers $N^z_\alpha$ are not considered by that solution.

It follows from Eq. (3.24) that the electron numbers are exclusive functions of the pseudohole numbers (this had to be so, as required from the form of the $SO(4)$ generators) and read

$$N_\uparrow = \frac{N_a}{2} + \sum_\beta \beta[N^h_{c,\beta} - N^h_{s,\beta}]\,, \qquad N_\downarrow = \frac{N_a}{2} + \sum_\beta \beta[N^h_{c,\beta} + N^h_{s,\beta}]\,. \tag{3.26}$$

The pseudomomentum-number operators

$$\hat{N}^h_{\alpha,\beta}(q) = a^\dagger_{q,\alpha,\beta} a_{q,\alpha,\beta}\,, \qquad \hat{N}_{\alpha,\gamma}(q) = b^\dagger_{q,\alpha,\gamma} b_{q,\alpha,\gamma}\,, \qquad \gamma = 1, 2, ...\,, \tag{3.27}$$

and

$$\hat{N}_{\alpha,0}(q) \equiv 1 - \sum_\beta \hat{N}^h_{\alpha,\beta}(q)\,, \qquad (\gamma = 0)\,, \tag{3.28}$$

play a central role in the generalized theory (see Sec. 4.2). The operator (3.28) has the following alternative representation in terms of $\alpha, 0$ pseudoparticle operators

$$\hat{N}_{\alpha,0}(q) = b^\dagger_{q,\alpha,0} b_{q,\alpha,0}\,. \tag{3.29}$$

The number operators can be expressed in terms of the pseudomomentum distributions as follows

$$\hat{N}^h_{\alpha,\beta} = \sum_q \hat{N}^h_{\alpha,\beta}(q)\,, \qquad \hat{N}_{\alpha,\gamma} = \sum_q \hat{N}_{\alpha,\gamma}(q)\,. \tag{3.30}$$

We emphasize that while all Hamiltonian eigenstates are also eigenstates of the operator $\hat{N}^h_{\alpha,\beta}$ because these numbers are good quantum numbers, this does not hold for the operator $\hat{N}^h_{\alpha,\beta}(q)$; obviously, only the states I are eigenstates of the latter operator. This fact follows directy from the structure of the state (3.18). On the other hand, all Hamiltonian eigenstates are also eigenstates of the pseudoparticle operators $\hat{N}_{\alpha,\gamma}(q)$.

The generalization of the LWS's BA total momentum expression [6, 7, 4], which we denote by $P_{BA}$, to all Hamiltonian eigenstates, requires the addition of an extra term associated with $\eta$ pairing [11, 12]. This is a direct implication of the commutators introduced in Sec. (2.2) and leads to

$$P = P_{BA} + \pi[S^c + S^c_z]\,. \tag{3.31}$$

When this expression provides values of momentum such that $|P| > \pi$, the total momentum is defined as the corresponding value at the first Brillouin zone. In operator form and for sub-canonical ensembles such that $S^\alpha_z \neq 0$, and with $l_\alpha$ given by Eq. (2.14), we have that $N^h_{\alpha,-\frac{l_\alpha}{2}} < N^h_{\alpha,\frac{l_\alpha}{2}}$, and the present representation leads to the following simple expressions for the momentum operator $\hat{P}$ and its eigenvalue $P$

$$\begin{aligned}
\hat{P} &= \sum_{q,\alpha}\sum_{\gamma=0}^{\infty} qC_{\alpha,\gamma}\hat{N}_{\alpha,\gamma}(q) + \pi[\hat{N}^h_{c,\frac{-l_c}{2}} + \sum_{\gamma=1}\hat{N}_{c,\gamma}]\,; \\
P &= \sum_{q,\alpha}\sum_{\gamma=0}^{\infty} qC_{\alpha,\gamma}N_{\alpha,\gamma}(q) + \pi\sum_{\gamma=1}[(1+\gamma)N_{c,\gamma} + N^z_c]\,,
\end{aligned} \tag{3.32}$$

respectively, where $C_{\alpha,0} = 1$ and $C_{c,\gamma} = -1$ for $\gamma > 0$. We note that the momentum term, $\pi\sum_{\gamma=1}[(1+\gamma)N_{c,\gamma} + N^z_c]$, is always a multiple of $\pm\pi$.

The pseudoparticle perturbation theory introduced in the works [13, 14, 15, 16, 17, 18] and developed in a suitable operator basis [8, 9, 19, 20, 21] refers to the Hilbert subspace spanned by the Hamiltonian eigenstates I. At finite values of the magnetic field and chemical potential and at constant electronic numbers the low-energy excitations I are described by pseudoparticle-pseudohole processes relative to the canonical-ensemble GS. The latter state, as well as all excited states I with the same electron numbers, are simple Slater determinants of pseudoparticle $\alpha, 0$ levels [8, 9, 19, 20, 21]. That is, in Eq. (3.18) either $N_{\alpha,\frac{1}{2}} = 0$ for LWS's or $N_{\alpha,-\frac{1}{2}} = 0$ for HWS's.

## 3.4 LWS's and non-LWS's: the criterium

A $S^\alpha$ LWS is such that

$$N^h_{\alpha,\frac{1}{2}} = \sum_{\gamma=1}^{\infty} \gamma N_{\alpha,\gamma} \,, \tag{3.33}$$

whereas for a $S^\alpha$ HWS we have that

$$N^h_{\alpha,-\frac{1}{2}} = \sum_{\gamma=1}^{\infty} \gamma N_{\alpha,\gamma} \,, \tag{3.34}$$

with $N^h_{\alpha,-\frac{1}{2}} \geq N^h_{\alpha,\frac{1}{2}}$ for a LWS and $N^h_{\alpha,\frac{1}{2}} \geq N^h_{\alpha,-\frac{1}{2}}$ for a HWS.

For the particular case of states I, we have that $N_{\alpha,\gamma} = 0$ for all $\gamma = 1, 2, ...$ branches in the former equations. Therefore, the states I are characterized by zero occupancies of the $\alpha, \gamma$ heavy-pseudoparticle bands (with $\gamma > 0$). It then follows from the general Eqs. (3.33) and (3.34) that a $S^\alpha$ LWS I is such that

$$N^h_{\alpha,\frac{1}{2}} = 0 \,, \tag{3.35}$$

whereas for a $S^\alpha$ HWS I, we have that

$$N^h_{\alpha,-\frac{1}{2}} = 0 \,, \tag{3.36}$$

with $N^h_{\alpha,-\frac{1}{2}} \geq 0$ for a LWS I and $N^h_{\alpha,\frac{1}{2}} \geq 0$ for a HWS I. This leads to the simple Slater-determinant form (3.18) found for the states I [9]. These results also confirm that in the case of states I the $\alpha, \beta$ pseudoholes are such that $\beta = \frac{l_\alpha}{2}$ but that this equality does not hold true in the general case. This is because in the case of the states I the Slater determinant (3.18) either involves $\alpha, +\frac{1}{2}$ or $\alpha, -\frac{1}{2}$ pseudoholes only, whereas in the case of the non-LWS's and non-HWS's or in the case of states II (i.e. LWS's or HWS's containing $\alpha, \gamma$ heavy pseudoparticles) the state (3.18) has both $\alpha, +\frac{1}{2}$ and $\alpha, -\frac{1}{2}$ pseudohole occupancies.

In the case of the non-LWS's and non-HWS's, all or some of the off-diagonal generators of the rhs of Eq. (3.18) create new states from a reference BA LWS. The $S^\alpha$ non-LWS's and non-HWS's outside the BA are such that

$$N^h_\alpha - \sum_{\gamma=1}^{\infty} 2\gamma N_{\alpha,\gamma} > |N^h_{\alpha,\frac{1}{2}} - N^h_{\alpha,-\frac{1}{2}}| \,. \tag{3.37}$$

In contrast, in the case of the LWS's II, the $\beta$ flips generated by these operators create a number $\gamma$ of $(\alpha, \frac{+1}{2})$ pseudoholes for each $\alpha, \gamma$ heavy pseudoparticle. Following Eqs. (3.7), (3.8), and (3.25) this is required for the LWS condition $S^\alpha = -S^\alpha_z$.

Therefore, in the latter, cases there is no relation between the quantity $l_\alpha$ defined in Eq. (2.14) and the pseudohole quantum number $\beta$.

## 3.5 The generalized ground state concept

The possible pseudohole and heavy-pseudoparticle numbers are constrained by Eqs. (3.7), (3.8), and (3.25) and together with the number of discrete pseudomomentum values in each band leads to $4^{N_a}$ possible orthonormal Hamiltonian eigenstates of form (3.18), in agreement with the results of Essler *et al.* [5, 6, 7].

The conservation of the pseudohole and heavy-pseudoparticle numbers permits dividing the Hilbert space into subspaces spanned by the set of Hamiltonian eigenstates (3.18) with the same $\{N^h_{\alpha,\beta}\}$ and $\{N_{\alpha,\gamma}\}$ numbers, which correspond to the same sub-canonical ensemble. Obviously, a canonical ensemble (with constant electron numbers $N_\sigma$ and thus with constant values of $N^h_{\alpha,\frac{1}{2}} - N^h_{\alpha,-\frac{1}{2}}$ for both $\alpha = c, s$) is usually realized by several $\{N^h_{\alpha,\beta}\}$, $\{N_{\alpha,\gamma}\}$ sub-canonical ensembles. Let us introduce the generalized ground state (GGS) as the Hamiltonian eigenstate(s) (3.18) of lowest energy in each Hilbert subspace. This type of eigenstate is very useful for the construction of the pseudoparticle perturbation theory of Sec. 4.2. They are of the form

$$|GGS;\{N^h_{\alpha,\beta}\},\{N_{\alpha,\gamma}\}\rangle = \frac{1}{\sqrt{C}}\prod_\alpha A_\alpha \prod_{\gamma=1}^{\infty}\left[[\hat{S}^\alpha_+]^{N^h_{\alpha,\frac{1}{2}}}\prod_{q=q^{(-)}_{\alpha,0}}^{\bar{q}^{(-)}_{F\alpha,0}}\prod_{q=\bar{q}^{(+)}_{F\alpha,0}}^{q^{(+)}_{\alpha,0}}\right.$$
$$\left.\prod_{q'=q^{(-)}_{c,\gamma}}^{q^{(-)}_{Fc,\gamma}}\prod_{q'=q^{(+)}_{Fc,\gamma}}^{q^{(+)}_{c,\gamma}}\prod_{q''=q^{(-)}_{Fs,\gamma}}^{q^{(+)}_{Fs,\gamma}} a^\dagger_{q,\alpha,-\frac{1}{2}} b^\dagger_{q'',c,\gamma} b^\dagger_{q',s,\gamma}\right]|V\rangle\,, \quad (3.38)$$

and when (i) $\alpha = c$, $\gamma > 0$, and $N_{c,\gamma}$ is even or (ii) $\alpha = s$ or $\alpha = c$ and $\gamma = 0$ and $N_{\alpha,\gamma}$ is odd (even) and $I^{\alpha,\gamma}_j$ are integers (half-odd integers) the pseudo-Fermi points are symmetric and given by

$$q^{(\pm)}_{F\alpha,\gamma} = \pm[q_{F\alpha,\gamma} - C_{\alpha,\gamma}\frac{\pi}{N_a}]\,, \quad (3.39)$$

where

$$q_{Fc,\gamma} = \frac{\pi[d_{c,\gamma} - N_{c,\gamma}]}{N_a}\,; \qquad \gamma > 0\,,$$

$$
\begin{aligned}
q_{Fc,0} &= \frac{\pi N_{c,0}}{N_a}\,, \\
q_{Fs,\gamma} &= \frac{\pi N_{s,\gamma}}{N_a}\,.
\end{aligned}
\tag{3.40}
$$

On the other hand, when (i) $\alpha = c$, $\gamma > 0$, and $N_{c,\gamma}$ is odd or (ii) $\alpha = s$ or $\alpha = c$ and $\gamma = 0$ and $N_{\alpha,\gamma}$ is odd (even) and $I_j^{\alpha,\gamma}$ are half-odd integers (integers) we have that

$$
q^{(+)}_{F\alpha,\gamma} = q_{F\alpha,\gamma}\,, \qquad q^{(-)}_{F\alpha,\gamma} = -[q_{F\alpha,\gamma} - C_{\alpha,\gamma}\frac{2\pi}{N_a}]\,,
\tag{3.41}
$$

or

$$
q^{(+)}_{F\alpha,\gamma} = q_{F\alpha,\gamma} - C_{\alpha,\gamma}\frac{2\pi}{N_a}\,, \qquad q^{(-)}_{F\alpha,\gamma} = -q_{F\alpha,\gamma}\,.
\tag{3.42}
$$

The GS associated with a given canonical ensemble is always a state I [9], which is a particular case of the general GGS expression (3.38). It is useful to denote the GS's by $|GS; S^c_z, S^s_z\rangle$, where $S^c_z$ and $S^s_z$ are the eigenvalues of the corresponding canonical ensemble. The GS expression associated with the $(l_c, l_s)$ sector of Hamiltonian symmetry $U(1) \otimes U(1)$ reads

$$
|GS; S^c_z, S^s_z\rangle = \prod_{q=q^{(-)}_{c,0}}^{\bar{q}^{(-)}_{Fc,0}} \prod_{q=\bar{q}^{(+)}_{Fc,0}}^{q^{(+)}_{c,0}} a^{\dagger}_{q,c,\frac{l_c}{2}} \prod_{q=q^{(-)}_{s,0}}^{\bar{q}^{(-)}_{Fs,0}} \prod_{q=\bar{q}^{(+)}_{Fs,0}}^{q^{(+)}_{s,0}} a^{\dagger}_{q,s,\frac{l_s}{2}} |V\rangle\,.
\tag{3.43}
$$

In all sectors of Hamiltonian symmetry there are states I. In the particular case of the SO(4) zero-chemical potential and zero-magnetic field canonical ensemble there is only one state I, the pseudohole and heavy-pseudoparticle vacuum, $|V\rangle$, which is nothing but the SO(4) GS [9]. The same applies to the sectors of Hamiltonian symmetry $SU(2) \otimes U(1)$ and $U(1) \otimes SU(2)$, the GS being always a state I. (In addition, in these sectors there is a large number of excited states I.)

In the case of the two $(l_s)$ $SU(2) \otimes U(1)$ sectors, the GS is both a LWS and HWS of the $\eta$-spin algebra. Therefore, it is empty of $c$ pseudoholes and reads

$$
|GS; 0, S^s_z\rangle = \prod_{q=q^{(-)}_{s,0}}^{\bar{q}^{(-)}_{Fs,0}} \prod_{q=\bar{q}^{(+)}_{Fs,0}}^{q^{(+)}_{s,0}} a^{\dagger}_{q,s,\frac{l_s}{2}} |V\rangle\,.
\tag{3.44}
$$

In the case of the $(l_c)$ $U(1) \otimes SU(2)$ sector the GS is both a LWS and a HWS of the spin algebra and is empty of $s$ pseudoholes. It reads

$$|GS; S^c_z, 0\rangle = \prod_{q=q^{(-)}_{c,0}}^{\bar{q}^{(-)}_{Fc,0}} \prod_{q=\bar{q}^{(+)}_{Fc,0}}^{q^{(+)}_{c,0}} a^{\dagger}_{q,c,\frac{l_c}{2}} |V\rangle \, . \tag{3.45}$$

Finally, the $S^c = S^c_z = 0$ (and $\mu = 0$) and $S^s = S^s_z = 0$ SO(4) ground state is, at the same time, a LWS and HWS of both the $\eta$-spin and spin algebras [8, 9]. Therefore, it is empty of both $c$ and $s$ pseudoholes and it is the vacuum of the pseudohole and heavy-pseudoparticle theory. All the remaining eigenstates can be described by particular cases of the general expression (3.18), being the only difference the values of the momenta $q$ in the product of operators $a^{\dagger}_{\alpha,q,\beta}$ and $b^{\dagger}_{q,\alpha,\gamma}$.

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# Chapter 4

# Pseudoparticle Perturbation Theory

## 4.1 Pseudoparticle Hamiltonian

Using the operational representation for the Hilbert space of the one-dimensional Hubbard model, we develop a generalized perturbation theory whose small parameter is the density of excited pseudoparticles. A similar theory for the LWS-I has been developed previously in the literature [1].

For simplicity, let us denote the general Hamiltonian eigenstates $|\psi; \{N^h_{\alpha,\beta}\}, \{N_{\alpha,\gamma}\}\rangle$ by $|\psi\rangle$ (and the GGS's (3.38) by $|GGS\rangle$). These states are also eigenstates of the $\alpha, \gamma$ pseudomomentum-distribution operators (3.27) such that

$$\hat{N}_{\alpha,\gamma}(q)|\psi\rangle = N_{\alpha,\gamma}(q)|\psi\rangle \, , \tag{4.1}$$

where $N_{\alpha,\gamma}(q)$ represents the eigenvalue of the operator (3.27), which is given by 1 and 0 for occupied and empty values of $q$, respectively.

It follows from the form of the state-generator of the rhs of Eq. (3.18) that all $2S^\alpha + 1$ Hamiltonian eigenstates constructed from the same $S^\alpha = -S^\alpha_z$ LWS by applying onto it $1, 2, ..., 2S^\alpha$ number of times the off-diagonal operator $\hat{S}^\alpha_+$ (3.7) have the same $N_{\alpha,\gamma}(q)$ pseudomomentum distribution.

As in the case of the spatial wave functions, the expression of the energy in terms of the quantum numbers $I^{\alpha,\gamma}_j$ of Eq. (3.11) involves the BA rapidities [2, 3]. These are complex functions of the numbers $I^{\alpha,\gamma}_j$. Following our pseudomomentum definition, Eq. (3.11), in our description they are functions of the pseudomomentum $q$. The real part of the BA rapidities, which we denote by $R_{\alpha,\gamma}(q)$, are in the present basis

eigenvalues of corresponding rapidity operators $\hat{R}_{\alpha,\gamma}(q)$, and obey the eigenvalue equation

$$\hat{R}_{\alpha,\gamma}(q)|\psi\rangle = R_{\alpha,\gamma}(q)|\psi\rangle\,, \tag{4.2}$$

where for the particular case of $R_{c,0}(q)$ we also consider the associate rapidity $K(q)$, which is defined by the following equation

$$R_{c,0}(q) = \frac{\sin K(q)}{u}\,. \tag{4.3}$$

The rapidity $K(q)$ is the eigenvalue of the rapidity operator $\hat{K}(q)$ such that

$$\hat{K}(q)|\psi\rangle = K(q)|\psi\rangle\,. \tag{4.4}$$

The eigenvalues $K(q)$, $R_{c,\gamma}(q)$, and $R_{s,\gamma}(q)$ obey the following non-linear algebraic equations [3, 4]

$$\begin{aligned} K(q) &= q - \frac{2}{N_a}\sum_{\gamma=0}\sum_{q'} N_{s,\gamma}(q')\tan^{-1}\Big(\frac{R_{c,0}(q)-R_{s,\gamma}(q')}{1+\gamma}\Big) \\ &- \frac{2}{N_a}\sum_{\gamma=1}\sum_{q'} N_{c,\gamma}(q')\tan^{-1}\Big(\frac{R_{c,0}(q)-R_{c,\gamma}(q')}{\gamma}\Big)\,, \end{aligned} \tag{4.5}$$

$$\begin{aligned} 2Re\sin^{-1}\Big(u(R_{c,\gamma}(q)+i\gamma)\Big) &= q + \frac{2}{N_a}\sum_{q'} N_{c,0}(q')\tan^{-1}\Big(\frac{R_{c,\gamma}(q)-R_{c,0}(q')}{\gamma}\Big) \\ + \frac{1}{N_a}\sum_{\gamma'=1}\sum_{q'} N_{c,\gamma'}(q')\Theta_{\gamma,\gamma'}\Big(R_{c,\gamma}(q)-R_{c,\gamma'}(q')\Big)\,, \end{aligned} \tag{4.6}$$

and

$$\begin{aligned} 0 &= q - \frac{2}{N_a}\sum_{q'} N_{c,0}(q')\tan^{-1}\Big(\frac{R_{s,\gamma}(q)-R_{c,0}(q')}{1+\gamma}\Big) \\ &+ \frac{1}{N_a}\sum_{\gamma'=0}\sum_{q'} N_{s,\gamma'}(q')\Theta_{1+\gamma,1+\gamma'}\Big(R_{s,\gamma}(q)-R_{s,\gamma'}(q')\Big)\,, \end{aligned} \tag{4.7}$$

where

$$\Theta_{\gamma,\gamma'}\Big(x\Big) = \Theta_{\gamma',\gamma}\Big(x\Big) = \delta_{\gamma,\gamma'}\{2\tan^{-1}\Big(\frac{x}{2\gamma}\Big) + \sum_{l=1}^{\gamma-1} 4\tan^{-1}\Big(\frac{x}{2l}\Big)\}$$

$$+ \quad (1-\delta_{\gamma,\gamma'})\{2\tan^{-1}\Big(\frac{x}{|\gamma-\gamma'|}\Big)+2\tan^{-1}\Big(\frac{x}{\gamma+\gamma'}\Big)$$

$$+ \quad \sum_{l=1}^{\frac{\gamma+\gamma'-|\gamma-\gamma'|}{2}-1} 4\tan^{-1}\Big(\frac{x}{|\gamma-\gamma'|+2l}\Big)\}\,. \tag{4.8}$$

The limits of the pseudo-Brillouin zones, $q^{(\pm)}_{\alpha,\gamma}$, associated with the pseudomomentum summations are given in Eqs. (3.14)-(3.17). Although the integral Eqs. (4.5-4.7) are coupled, note that each of these equations defines the rapidity associated with one of the $\alpha,\gamma$ bands in terms of other rapidities.

The key point is that the eigenvalue $N_{\alpha,\gamma}(q)$ is common to the whole tower of $2S^\alpha+1$ Hamiltonian eigenstates constructed from the same $S^\alpha$ LWS. Also the associate rapidity eigenvalue $R_{\alpha,\gamma}(q)$ of Eq. (4.2) is common to these $2S^\alpha+1$ Hamiltonian eigenstates. This follows from the fact that rapidity solutions $R_{\alpha,\gamma}(q)$ of Eqs. (4.5), (4.6), and (4.7) are functionals of the $N_{\alpha,\gamma}(q)$ distributions and $\beta$ independent. We thus conclude that the LWS rapidities extracted from the BA provide full information on the non-LWS's rapidity operators.

The rapidity eigenvalues of Eqs. (4.2) and (4.4) are independent of the pseudohole numbers $N^h_{\alpha,\beta}$ and only involve the pseudoparticle distributions $N_{\alpha,\gamma}(q)$. The same holds true for the associate rapidity, pseudohole, and pseudoparticle operators. Since the SO(4) Hamiltonian (2) and other physical quantities turn out to be exclusive functionals of the rapidity operators, in studies involving such quantities it is often more convenient to use the $\alpha,\gamma$ pseudoparticle representation (with $\gamma=0,1,2,3,...$) than the $\alpha,\beta$ pseudohole and $\alpha,\gamma$ heavy-pseudoparticle representation (with $\gamma=1,2,3,...$).

By direct insertion in each of Eqs. (4.5)-(4.7) of the corresponding $q^{(\pm)}_{\alpha,\gamma}$ pseudomomenta we find that the functions $R_{\alpha,\gamma}(q)$ have *for all* eigenstates the following boundary values at the limits of the pseudo-Brillouin zones

$$K(q^{(\pm)}_{c,0})=\pm\pi\,,\qquad R_{c,0}(q^{(\pm)}_{c,0})=0\,, \tag{4.9}$$

for $\alpha=c$ and $\gamma=0$ and

$$R_{\alpha,\gamma}(q^{(\pm)}_{\alpha,\gamma})=\pm\infty\,, \tag{4.10}$$

for the remaining choices of the quantum numbers $\alpha,\gamma$.

It is useful to consider the rapidity functions $K^{(0)}(q)$ and $R^{(0)}_{\alpha,\gamma}(q)$ which are the GGS eigenvalues such that

$$\hat{K}(q)|GGS\rangle = K^{(0)}(q)|GGS\rangle\,, \tag{4.11}$$

and

$$\hat{R}_{\alpha,\gamma}(q)|GGS\rangle = R^{(0)}_{\alpha,\gamma}(q)|GGS\rangle\,. \tag{4.12}$$

These are defined by Eqs. (4.5-4.7) with the pseudomomentum distribution given by its GGS value, which we denote by $N^{(0)}_{\alpha,\gamma}(q)$ and is such that

$$\hat{N}_{\alpha,\gamma}(q)|GGS\rangle = N^{(0)}_{\alpha,\gamma}(q)|GGS\rangle\,. \tag{4.13}$$

Following the GGS expression (3.38), $N^{(0)}_{\alpha,0}(q)$ and $N^{(0)}_{s,\gamma}(q)$ have the simple free particle/hole Fermi-like form

$$\begin{aligned} N^{(0)}_{\alpha,\gamma}(q) &= \Theta\Big(C_{\alpha,\gamma}(q^{(+)}_{F\alpha,\gamma} - q)\Big)\,, \qquad 0 < q < q^{(+)}_{\alpha,\gamma} \\ &= \Theta\Big(C_{\alpha,\gamma}(q - q^{(-)}_{F\alpha,\gamma})\Big)\,, \qquad q^{(-)}_{\alpha,\gamma} < q < 0\,. \end{aligned} \tag{4.14}$$

For the particular case of a GS, these distributions read

$$\begin{aligned} N^{(0)}_{\alpha,0}(q) &= \Theta\Big(q^{(+)}_{F\alpha,0} - q\Big)\,, \qquad 0 < q < q^{(+)}_{\alpha,0} \\ &= \Theta\Big(q - q^{(-)}_{F\alpha,0}\Big)\,, \qquad q^{(-)}_{\alpha,0} < q < 0\,, \\ N^{(0)}_{\alpha,\gamma}(q) &= 0\,, \qquad\qquad \gamma > 0\,. \end{aligned} \tag{4.15}$$

In Appendix A we study the rapidity solutions of Eqs. (4.5)-(4.7) both for GGS's and for Hamiltonian eigenstates differing from a GGS by a small density of excited pseudoparticles. In equations (A.7) and (A.8) the parameters $Q^{(\pm)}$ and $r^{(\pm)}_{\alpha,\gamma}$ are defined combining the two equations

$$Q^{(\pm)} = K^{(0)}(q^{(\pm)}_{Fc,0})\,, \qquad r^{(\pm)}_{\alpha,\gamma} = R^{(0)}_{\alpha,\gamma}(q^{(\pm)}_{F\alpha,\gamma})\,, \tag{4.16}$$

with equations (A.4) and (A.5). For later use, it is convenient to introduce the associate parameters

$$Q = K^{(0)}(q_{Fc,0})\,, \qquad r_{\alpha,\gamma} = R^{(0)}_{\alpha,\gamma}(q_{F\alpha,\gamma})\,. \tag{4.17}$$

In the thermodynamic limit, we can take the pseudomomentum continuum limit $q_j \to q$ and the real part of the rapidities become functions of $q$, which we have

called here $R_{\alpha,\gamma}(q)$. In that limit, the BA system of algebraic equations are replaced by the system of infinite coupled integral equations presented in Appendix A.

We have mentioned that the BA solution is most naturally expressed in the pseudoparticle basis. One consequence of this is the simple expression for the Hamiltonian (2.13) in that basis. From the SO(4) symmetry we know that the SO(4) energy is the same for all eigenstates of a given SO(4) tower. Thus, it suffices to know the SO(4) energy for the tower's LWS, which is given by the Bethe ansatz. In the pseudoparticle basis, where the non-LWS's/HWS's are characterized by the $\beta$ quantum number, the SO(4) Hamiltonian is written, as it should be, in terms of the pseudoparticle numbers

$$\begin{aligned}\hat{H}_{SO(4)} &= -2t\sum_{q}\hat{N}_{c,0}(q)\cos[\hat{K}(q)] + 2t\sum_{q,\gamma=1}\hat{N}_{c,\gamma}(q)\sum_{j=\pm 1}\sqrt{1-[u(\hat{R}_{c,\gamma}(q)+ji\gamma)]^2} \\ &+ U[\frac{N_a}{4}-\frac{\hat{N}_{c,0}}{2}-\sum_{\gamma=1}\gamma\hat{N}_{c,\gamma}]\,. \end{aligned} \tag{4.18}$$

Contrary to the SO(4) term, the chemical potencial and the Zeeman term are $\beta$ sensitive, because the respective terms in the Hamiltonian (2.13) do not commute with the ladder operators of the SO(4) algebra. Thus, the inclusion in the Hamiltoninan (4.18) of a chemical potential and a Zeeman terms must be written in terms of pseudoholes, and reads

$$\hat{H} = \hat{H}_{SO(4)} + 2\mu\sum_{\beta}\beta\hat{N}^h_{c,\beta} + 2\mu_0 H\sum_{\beta}\beta\hat{N}^h_{s,\beta}\,. \tag{4.19}$$

This is the pseudoparticle expression of the Hamiltonian (2.13) at all energy scales. The Hamiltonian (4.19) then implies that all energy eigenvalues of a given tower read $E = E_{SO(4)} + 2\mu(S^c + S^c_z) + 2\mu_0 H(S^s + S^s_z)$. Despite its simple appearance, the Hamiltonian (4.18) describes a many-pseudoparticle problem, the reason being that the expression for the rapidity operator in terms of the operators $\hat{N}_{\alpha,\gamma}(q)$ contains many-pseudoparticle interacting terms.

Unsurprisingly, it is difficult to solve the BA operator Eqs. (4.5), (4.6), and (4.7) directly and to obtain the explicit expression for the rapidity operators in terms of the pseudomomentum distribution operators (3.27). In contrast, it is easier to calculate their normal-ordered expression in terms of the normal-ordered operators. The rapidity operators $\hat{R}_{\alpha,\gamma}(q)$ contain all information about the many-pseudoparticle interactions of the quantum-liquid Hamiltonian. There are two fundamental prop-

erties which imply the central role that the rapidity operators of Eqs. (4.11) and (4.12) have in the present quantum problem:

(a) As we find in Sec. 4.2, each of the normal-ordered rapidity operators $: \hat{R}_{\alpha}(q) :$ (relative to the suitable GGS or GS) can be written exclusively in terms of the pseudomomentum distribution operators (3.27).

(b) The normal-ordered version of the SO(4) Hamiltonian (4.18) can be written, exclusively, in terms of the pseudomomentum distribution operators (3.27), but all the corresponding many-pseudoparticle interaction terms can be written in terms of the rapidity operators $: \hat{R}_{\alpha,\gamma}(q) :$. It follows that the rapidity operators commute with the Hamiltonian.

In the ensuing section, we introduce the pseudoparticle perturbation theory which leads to the normal-ordered expressions for the Hamiltonian and rapidity operators. Despite the non-interacting form of the Hamiltonian eigenstates (3.18), the normal-ordered Hamiltonian includes pseudoparticle interaction terms and is, therefore, a many-pseudoparticle operator. However, we find in Sec. 4.2 that these pseudoparticle interactions have a pure forward-scattering, zero-momentum transfer, character.

## 4.2 Pseudoparticle perturbation theory

We will be mostly interested in GS - GGS transitions followed by pseudoparticle - pseudohole excitations involving a small density of $\alpha, \gamma$ pseudoparticles relative to both the GS and GGS distributions. Let us then introduce the normal-ordered pseudomomentum distribution operator

$$: \hat{N}_{\alpha,\gamma}(q) := \hat{N}_{\alpha,\gamma}(q) - N^{(0)}_{\alpha,\gamma}(q)\,. \tag{4.20}$$

When we choose $N^{(0)}_{\alpha,\gamma}(q)$ to be the GS pseudomomentum distribution (4.15) we have

$$: \hat{N}_{\alpha,\gamma}(q) := \hat{N}_{\alpha,\gamma}(q)\,, \qquad\qquad \gamma > 0\,. \tag{4.21}$$

The normal-ordered distribution (4.20) obeys the eigenvalue equation

$$: \hat{N}_{\alpha,\gamma}(q) : |\psi\rangle = \delta N_{\alpha,\gamma}(q)|\psi\rangle\,. \tag{4.22}$$

We also consider the normal-ordered rapidity operator

$$: \hat{R}_{\alpha,\gamma}(q) := \hat{R}_{\alpha,\gamma}(q) - R^{(0)}_{\alpha,\gamma}(q)\,, \tag{4.23}$$

where $R^0_{\alpha,\gamma}(q)$ is the GGS eigenvalue of Eq. (4.12).

In the pseudoparticle basis, the normal-ordered rapidity operators $: \hat{R}_{\alpha,\gamma}(q) :$ contain an infinite number of terms, as we shall demonstrate below. The first of these terms is linear in the pseudomomentum distribution operator $: \hat{N}_{\alpha,\gamma}(q) :$, (4.20), whereas the remaining terms consist of products of two, three,.....,infinite, of these operators. The number of $: \hat{N}_{\alpha,\gamma}(q) :$ operators which appears in these products equals the order of the scattering in the corresponding rapidity term.

A remarkable property is that in the pseudoparticle basis the seemingly "non-perturbative" quantum liquids become perturbative: while the two-electron forward scattering amplitudes and vertices diverge, the two-pseudoparticle $f$ functions (given by Eq. (4.50) below) are finite.

By "perturbative" we also mean here the following: at each point of parameter space (canonical ensemble), the excited eigenstates are of form (3.18) and correspond to quantum-number configurations involving a density of excited pseudoholes and heavy pseudoparticles relative to the GS configuration (3.43) and (4.15). We introduce the following density

$$n'_{ex} = \sum_{\alpha,\beta} n^{\alpha,\beta}_{ex} + \sum_{\alpha,\gamma=1} n^{\alpha,\gamma}_{ex} \, , \tag{4.24}$$

which is kept small. Here

$$n^{\alpha,\beta}_{ex} = \frac{1}{N_a} \sum_q [1 - N^{h,(0)}_{\alpha,\beta}(q)] \delta N_{\alpha,\beta}(q) \, , \tag{4.25}$$

and

$$n^{\alpha,\gamma}_{ex} = \frac{1}{N_a} \sum_q N_{\alpha,\gamma}(q) \, , \tag{4.26}$$

define the densities of excited $\alpha, \beta$ pseudoholes and $\alpha, \gamma$ heavy pseudoparticles, respectively, associated with the Hamiltonian eigenstate $|\psi\rangle$.

In Eq. (4.25), $N^{h,(0)}_{\alpha,\beta}(q)$ is the GS pseudohole distribution which reads

$$\begin{aligned} N^{h,(0)}_{\alpha,-\frac{1}{2}}(q) &= 1 - N^{(0)}_{\alpha,0}(q) \, , \\ N^{h,(0)}_{\alpha,+\frac{1}{2}}(q) &= 0 \, , \end{aligned} \tag{4.27}$$

if the GS is a $S^\alpha$ LWS and

$$
\begin{aligned}
N^{h,(0)}_{\alpha,-\frac{1}{2}}(q) &= 0\,, \\
N^{h,(0)}_{\alpha,+\frac{1}{2}}(q) &= 1 - N^{(0)}_{\alpha,0}(q)\,,
\end{aligned}
\tag{4.28}
$$

if the GS is a $S^\alpha$ HWS, where $N^{(0)}_{\alpha,0}(q)$ is the $\alpha, 0$ pseudoparticle GS distribution (4.15). Our perturbation theory refers to general GS transitions to Hamiltonian eigenstates $|\psi\rangle$ involving (a) a GS - GGS transition and (b) a Landau-liquid pseudoparticle-pseudohole excitation around the GGS. Therefore, the initial state is a GS and we have assumed the GS distribution (4.15) for the $\alpha, \gamma$ heavy pseudoparticles. Following Eq. (4.15), we thus have that $N_{\alpha,\gamma}(q) = \delta N_{\alpha,\gamma}(q)$ in the rhs of Eq. (4.26).

The expectation values of the SO(4) Hamiltonian (4.18) in the final states $|\psi\rangle$ are functions of the density of excited pseudoparticles only. This density is given by

$$
n_{ex} = \sum_{\alpha,\gamma=0} n^{\alpha,\gamma}_{ex}\,,
\tag{4.29}
$$

where $n^{\alpha,\gamma}_{ex}$ is given by

$$
n^{\alpha,0}_{ex} = \frac{1}{N_a}\sum_q [1 - N^{(0)}_{\alpha,0}(q)]\delta N_{\alpha,0}(q)\,,
\tag{4.30}
$$

for $\gamma = 0$ and by (4.26) otherwise. The density (4.29) is small provided the density (4.24) is also small. This then implies that all the densities $n^{\alpha,\gamma}_{ex}$ are small and that we can expand the expectation values in these densities. The perturbative character of the quantum liquid rests on the fact that the evaluation of the expectation values up to the $n^{th}$ order in the densities (4.29) requires considering only the corresponding operator terms of scattering orders less than or equal to $n$. This follows from the linearity of the density of excited $\alpha, \gamma$ pseudoparticles, which are the elementary "particles" of the quantum liquid, in

$$
\delta N_{\alpha,\gamma}(q) = \langle\psi| : \hat{N}_{\alpha,\gamma}(q) : |\psi\rangle\,,
\tag{4.31}
$$

and from the form of (4.26) and (4.30). The perturbative character of the quantum liquid implies, for example, that, to second order in the density of excited pseudoparticles, the energy involves only one- and two-pseudoparticle Hamiltonian terms, as in the case of the quasiparticle terms of a Fermi-liquid energy functional [5, 6].

### 4.2.1 Pseudoparticle bands and $f$-functions

We will develop our perturbation theory considering the two cases where (i) the operator normal-ordering is relative to the initial GS and (ii) that ordering refers to the GGS associated with a GS - GGS transition. In the following we consider the general case of normal ordering relative to a GGS. Later on we will specify when that ordering refers either to a GS (which is a particular case of a GGS) or to a (non-GS) GGS.

The expressions for the rapidity operators $:\hat{R}_{\alpha,\gamma}(q):$ corresponds to expanding the expressions of the operators $:\hat{R}_{\alpha,\gamma}(q):$ in terms of increasing pseudoparticle scattering order. It is convenient to define these expressions in terms of the operators $:\hat{X}_{\alpha,\gamma}(q):$. These are related to the rapidity operators as follows

$$:\hat{R}_{\alpha,\gamma}(q):=R^0_{\alpha,\gamma}(q+:\hat{X}_{\alpha,\gamma}(q):)-R^0_{\alpha,\gamma}(q)\,, \tag{4.32}$$

where $R^{(0)}_{\alpha,\gamma}(q)$ is the suitable $\hat{R}_{\alpha,\gamma}(q)$ GGS eigenvalue of Eq. (4.12).

The operators $:\hat{X}_{\alpha,\gamma}(q):$ contain the same information as the rapidity operators, and involve, exclusively, the two-pseudoparticle phase shifts $\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q')$ that we define below. In Appendix A we introduce (4.32) in the BA equations (4.5-4.7) and expand in the scattering order. This leads to

$$:\hat{X}_{\alpha,\gamma}(q):=\sum_{j=1}^{\infty}\hat{X}^{(j)}_{\alpha,\gamma}(q)\,, \tag{4.33}$$

where $j$ gives the scattering order of the operator term $\hat{X}^{(j)}_{\alpha,\gamma}(q)$. For the first-order term we find

$$\hat{X}^{(1)}_{\alpha,\gamma}(q)=\frac{2\pi}{N_a}\sum_{q',\alpha',\gamma'}\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q'):\hat{N}_{\alpha',\gamma'}(q'):\,, \tag{4.34}$$

where the phase-shift expressions are given below. While the expressions for the phase shifts $\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q')$ are specific to each model because they involve the spectral parameters, the *form* of the operator term $\hat{X}^{(1)}_{\alpha,\gamma}(q)$ (4.34) is universal and refers to all the solvable electronic multicomponent quantum liquids.

The phase shifts $\tilde{\Phi}_{\alpha,\gamma,\alpha'\gamma'}$ are given by

$$\tilde{\Phi}_{c,0;c,0}(k,k')=\bar{\Phi}_{c,0;c,0}\left(\frac{\sin k}{u},\frac{\sin k'}{u}\right)\,, \tag{4.35}$$

$$\tilde{\Phi}_{c,0;\alpha,\gamma}(k,r')=\bar{\Phi}_{c,0;\alpha,\gamma}\left(\frac{\sin k}{u},r'\right)\,, \tag{4.36}$$

$$\tilde{\Phi}_{\alpha,\gamma;c,0}(r,k') = \bar{\Phi}_{\alpha,\gamma;c,0}\left(r,\frac{\sin k'}{u}\right) , \tag{4.37}$$

$$\tilde{\Phi}_{\alpha,\gamma;\alpha,\gamma'}(r,r') = \bar{\Phi}_{\alpha,\gamma;\alpha,\gamma'}(r,r') , \tag{4.38}$$

where the phase shifts $\bar{\Phi}_{\alpha,\gamma;\alpha',\gamma'}$ are defined by the integral equations (A.31)-(A.39) of Appendix A.

The two-pseudparticle phase shifts can be defined in terms of the phase shifts $\bar{\Phi}_{\alpha,\gamma;\alpha',\gamma'}$ as follows

$$\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q') = \bar{\Phi}_{\alpha,\gamma;\alpha',\gamma'}\left(R^{(0)}_{\alpha,\gamma}(q),R^{(0)}_{\alpha,\gamma}(q')\right) . \tag{4.39}$$

The quantity $\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q')$ represents the shift in the phase of the $\alpha',\gamma'$ pseudoparticle of pseudomomentum $q'$ due to a zero-momentum forward-scattering collision with the $\alpha,\gamma$ pseudoparticle of pseudomomentum $q$.

In Appendix B, we use the Hamiltonian expression (4.18) in terms of the rapidity operators to derive the expression for the normal-ordered Hamiltonian. We find that in normal order relative to the suitable GGS (or GS), the Hamiltonian $\hat{H}_{SO(4)}$, Eq. (4.18), can be written as

$$:\hat{H}_{SO(4)}: = \sum_{j=1}^{\infty}\hat{H}^{(j)} . \tag{4.40}$$

For example, the first and second pseudoparticle-scattering order terms read

$$\hat{H}^{(1)} = \sum_{q,\alpha,\gamma}\epsilon^0_{\alpha,\gamma}(q):\hat{N}_{\alpha,\gamma}(q): , \tag{4.41}$$

and

$$\hat{H}^{(2)} = \frac{1}{N_a}\sum_{q,\alpha,\gamma}\sum_{q',\alpha',\gamma'}\frac{1}{2}f_{\alpha,\gamma;\alpha',\gamma'}(q,q'):\hat{N}_{\alpha,\gamma}(q)::\hat{N}_{\alpha',\gamma'}(q'): , \tag{4.42}$$

respectively. All the remaining higher-order operator terms of expressions (4.33) and (4.40) can be obtained by combining the rapidity equations (4.5), (4.6), and (4.7) and the Hamiltonian expression (4.18).

In Appendix B, it is shown that the pseudoparticle bands $\epsilon^0_{\alpha,\gamma}(q)$ can be expressed in terms of the phase shifts (4.39), with the result

$$\epsilon^0_{c,0}(q) \;=\; -\frac{U}{2} - 2t\cos K^{(0)}(q) + 2t\int_{Q^{(-)}}^{Q^{(+)}} dk\tilde{\Phi}_{c,0;c,0}\left(k,K^{(0)}(q)\right)\sin k , \tag{4.43}$$

$$\epsilon^0_{c,\gamma}(q) = -\gamma U + 4tRe\sqrt{1-u^2[R^{(0)}_{c,\gamma}(q)+i\gamma]^2} + 2t\int_{Q^{(-)}}^{Q^{(+)}} dk\widetilde{\Phi}_{c,0;c,\gamma}\left(k, R^{(0)}_{c,\gamma}(q)\right)\sin k\,, \quad (4.44)$$

and

$$\epsilon^0_{s,\gamma}(q) = 2t\int_{Q^{(-)}}^{Q^{(+)}} dk\widetilde{\Phi}_{c,0;s,\gamma}\left(k, R^{(0)}_{s,\gamma}(q)\right)\sin k\,. \quad (4.45)$$

At the pseudo-Brillouin zones the band expressions have the following values

$$\epsilon^0_{\alpha,\gamma}(q^{(\pm)}_{alpha,\gamma}) = 0\,, \quad (4.46)$$

and the associate group velocities, $v_{\alpha,\gamma}(q)$, are given by

$$v_{\alpha,\gamma}(q) = \frac{d\epsilon^0_{\alpha,\gamma}(q)}{dq}\,. \quad (4.47)$$

The two-pseudoparticle forward-scattering phase shifts $\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q')$ defined by Eq. (4.39) and "light" velocities

$$v_{\alpha,\gamma} \equiv v_{\alpha,\gamma}(q_{F\alpha,\gamma})\,, \quad (4.48)$$

play an important role in the physical quantities when the conformal regime is approached [7, 8, 9].

All $\hat{X}^{(j)}_{\alpha,\gamma}(q)$ terms of the rhs of Eq. (4.33) are such that both the $f$ functions on the rhs of Eq. (4.42) and all the remaining higher order coefficients associated with the operators $\hat{H}^{(j)}$ of order $j > 1$ have universal forms in terms of the two-pseudoparticle phase shifts and pseudomomentum derivatives of the bands and coefficients of order $< j$. This follows from the fact that the $S$-matrix for $j$-pseudoparticle scattering factorizes into two-pseudoparticle scattering matrices, as in the case of the usual BA $S$-matrix [10]. For example, we show in Appendix B that although the second-order term $\hat{H}^{(2)}$ of Eq. (4.42) involves an integral over the second-order function $\hat{X}^{(2)}_{\alpha,\gamma}(q)$ (see Eq. (B.12) of Appendix B ), this function is such that $\hat{H}^{(2)}$ can be written exclusively in terms of the first-order functions (4.34)

$$\hat{H}^{(2)} = \sum_{q,\alpha,\gamma} v_{\alpha,\gamma}(q)\hat{X}^{(1)}_{\alpha,\gamma}(q) : \hat{N}_{\alpha,\gamma}(q) : + \frac{N_a}{2\pi}\sum_{\alpha,\gamma}\theta(N_{\alpha,\gamma})\frac{|v_{\alpha,\gamma}|}{2}\sum_{j=\pm 1}[\hat{X}^{(1)}_{\alpha,\gamma}(jq_{F\alpha,\gamma})]^2\,, \quad (4.49)$$

where $|v_{\alpha,\gamma}| = C_{\alpha,\gamma} v_{\alpha,\gamma}$, $\theta(x) = 1$ for $x > 0$, and $\theta(x) = 0$ for $x \leq 0$ and the "Landau" $f$ functions, $f_{\alpha,\gamma;\gamma',\alpha'}(q,q')$, are found in that Appendix to have universal form

$$\begin{aligned} & f_{\alpha,\gamma;\alpha',\gamma'}(q,q') = 2\pi v_{\alpha,\gamma}(q)\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q') + 2\pi v_{\alpha',\gamma'}(q')\Phi_{\alpha',\gamma';\alpha,\gamma}(q',q) \\ + \; & 2\pi \sum_{j=\pm 1} \sum_{\alpha''} \sum_{\gamma''=0}^{\infty} \theta(N_{\alpha'',\gamma''}) C_{\alpha'',\gamma''} v_{\alpha'',\gamma''} \Phi_{\alpha'',\gamma'';\alpha,\gamma}(j q_{F\alpha'',\gamma''}, q) \\ & \Phi_{\alpha'',\gamma'';\alpha',\gamma'}(j q_{F\alpha'',\gamma''}, q') \,, \end{aligned} \tag{4.50}$$

where the pseudoparticle group velocities are given by Eqs. (4.47) and (4.48).

We can also write the expression of $\hat{H}^{(j)}$ for higher scattering orders $j > 2$. The main feature here is that for all sub-canonical ensembles, energy scales, and pseudoparticle scattering orders, the Landau-liquid terms of that Hamiltonian involve only zero-momentum forward-scattering.

### 4.2.2 Energy-gap equations

Let us consider that the normal-ordering of the Hamiltonian (4.40) above refers to the initial GS. In this case, and in contrast to the low-energy Landau theory [1, 7, 11, 12, 13], this Hamiltonian describes finite-energy transitions involving a small density of excited pseudoparticles.

Since the relevant finite-energy excitations involve a topological GS - GGS transition (to be discussed in Chapter 5), it is convenient to define the normal ordering relative to the suitable final GGS of energy

$$\omega_0 = E_{GGS} - E_{GS} \,. \tag{4.51}$$

In this case the Hamiltonian acts directly on the Hilbert subspace of the final GGS where all states have the same choices concerning the integer or half-odd integer character of the numbers $I_j^{\alpha,\gamma}$ of Eq. (3.11).

Normal-ordering relative to the GGS implies separating the problem (4.40) into (a) a finite-energy term associated with the GS - GGS transitions and (b) a low $(\omega - \omega_0)$ energy theory associated with the Landau-liquid pseudoparticle-pseudohole processes around the final GGS. In most cases the excitation energy (4.51) associated with the GS - GGS transitions is finite. The finite energies are the energy gaps of the states II and (or) non-LWS's and non-HWS's relative to the initial GS.

At finite values of $S_z^c$ and $S_z^s$ the low-energy Hilbert space is entirely spanned by states I [1, 11, 14]. We note that, for these states, fixing the electron numbers fixes

the pseudohole numbers [11] and the $\alpha, \gamma$ bands are empty for $\gamma > 0$. Therefore, if we fix the electronic numbers we have that at energy scales smaller than the gaps (4.51) for the states II and non-LWS's and non-HWS's only Landau-liquid excitations (b) are allowed. This justifies the Landau-liquid character of the problem at low energies [1, 7, 11, 15, 16]. Obviously, if we change the electron numbers, there occur at low energy GS - GS transitions which are particular cases of the above GS - GGS transitions (a). Understanding these GS - GS transitions permits one to express the electron operators in terms of the pseudohole operators and topological momentum shifts (Chapter 5).

Let us evaluate the general $\omega_0$ expression for GS - GGS transitions such that the final sub-canonical ensemble is characterized by vanishing or by small values of $N^h_{\alpha,-\frac{l_\alpha}{2}}/N^h_\alpha$. Here, $l_\alpha = \pm 1$ is defined by Eq. (2.14). We also assume that both the initial GS and final GGS correspond to canonical ensembles such that $S^\alpha_z \neq 0$ and belonging the same sector of parameter space, i.e. with the same $l_\alpha$ numbers. We note that since GS's are always $S^\alpha$ LWS's I or HWS's I there are neither $\alpha, -\frac{l_\alpha}{2}$ pseudoholes [see Eqs. (3.35) and (3.36)] nor $\alpha, \gamma$ heavy pseudoparticles ($\gamma > 0$) in the initial GS, and that $N^z_\alpha = 0$ [see Eq. (3.25)] for that state. From Eqs. (4.40)-(4.42), we find for the GS - GGS gap

$$\omega_0 = \sum_\alpha \epsilon^0_{\alpha,0}(q_{F\alpha,0})\Delta N_{\alpha,0} + \sum_{\gamma=1} \epsilon^0_{s,\gamma}(0) N_{s,\gamma} + 2\mu \Delta S^c_z + 2\mu_0 H \Delta S^s_z \, . \tag{4.52}$$

Inserting in Eqs. (3.24) both the pseudohole expressions (3.23) and the expressions $S^c_z = -\frac{1}{2}[N_a - N]$ and $S^s_z = -\frac{1}{2}[N_\uparrow - N_\downarrow]$, we find, after use of Eq. (3.25), the following general expressions for $\Delta N_{c,0}$ and $\Delta N_{s,0}$

$$\begin{aligned} \Delta N_{c,0} &= -2l_c \Delta S^c_z - 2N^z_c - \sum_{\gamma=1} 2\gamma N_{c,\gamma} = \\ &- [N^h_{c,-\frac{l_c}{2}} - \Delta N^h_{c,\frac{l_c}{2}}] - 2N^z_c - \sum_{\gamma=1} 2\gamma N_{c,\gamma} \, , \end{aligned} \tag{4.53}$$

and

$$\begin{aligned} \Delta N_{s,0} = &- \sum_\alpha [l_\alpha \Delta S^\alpha_z + N^z_\alpha] - \sum_{\gamma=1} \gamma N_{c,\gamma} - \sum_{\gamma=1} (1+\gamma) N_{s,\gamma} \\ = &- \frac{1}{2} \sum_\alpha [N^h_{\alpha,-\frac{l_\alpha}{2}} - \Delta N^h_{\alpha,\frac{l_\alpha}{2}} + 2N^z_\alpha] \\ &- \sum_{\gamma=1} \gamma N_{c,\gamma} - \sum_{\gamma=1} (1+\gamma) N_{s,\gamma} \, . \end{aligned} \tag{4.54}$$

Using these and Eq. (3.25) in the rhs of Eq. (4.52) leads to the gap expression (B.10) of Appendix B.

On the other hand, generalization of the results contained in the work [12] for the chemical-potential and magnetic-field expressions to all sectors of parameter space leads to

$$|\mu| = -\epsilon^0_{c,0}(q_{Fc,0}) - \frac{\epsilon^0_{s,0}(q_{Fs,0})}{2}\,, \qquad 2\mu_0|H| = -\epsilon^0_{s,0}(q_{Fs,0})\,. \tag{4.55}$$

From the use of Eqs. (4.53) and (4.54) in the gap equation (4.52), we can rewrite Eq. (B.10) as follows

$$\omega_0 = 2|\mu|N^h_{c,-\frac{l_c}{2}} + 2\mu_0|H|[N^h_{s,-\frac{l_s}{2}} + \sum_{\gamma=1}^{\infty} N_{s,\gamma}] + \sum_{\gamma=1}\epsilon^0_{s,\gamma}(0)N_{s,\gamma}\,, \tag{4.56}$$

which is the general expression for the gap for GS - GGS transitions. It follows from Eqs. (3.25) and (3.7) that the gap expression (4.56) can be rewritten as

$$\omega_0 = 2|\mu|\Big(\sum_{\gamma=1}\gamma N_{c,\gamma} + N^z_c\Big) + 2\mu_0|H|\Big(\sum_{\gamma=1}(1+\gamma)N_{s,\gamma} + N^z_s\Big) + \sum_{\gamma=1}\epsilon^0_{s,\gamma}(0)N_{s,\gamma}\,. \tag{4.57}$$

For GS - GGS transitions to pure LWS's or HWS's II, the use of Eq. (3.25) leads to

$$N^z_\alpha = 0\,, \tag{4.58}$$

for both $\alpha = c, s$. It follows that for such transitions the gap is given by expression (4.57) with $N^z_c = 0$ and $N^z_s = 0$. Therefore, the single ($\gamma > 0$) $\alpha, \gamma$ heavy-pseudoparticle gap is $2\gamma|\mu|$ and $2(1+\gamma)\mu_0|H| + \epsilon^0_{s,\gamma}(0)$ for $c$ and $s$, respectively.

Given a final sub-canonical ensemble we can write

$$:\hat{H} := \hat{H}_0 + \hat{H}_{Landau}\,, \tag{4.59}$$

where $\hat{H}_0$ has eigenvalue $\omega_0$ and corresponds to the GS - GGS transition (a) and $\hat{H}_{Landau}$ is normal-ordered relative to the GGS and is of the form

$$\hat{H}_{Landau} = \hat{H}^{(1)}_L + \hat{H}^{(2)}_L\,, \tag{4.60}$$

where

$$\hat{H}^{(1)}_L = \sum_{q,\alpha,\gamma}\epsilon_{\alpha,\gamma}(q) :\hat{N}_{\alpha,\gamma}(q):\,, \tag{4.61}$$

$$\epsilon_{\alpha,0}(q) = \epsilon^{(0)}_{\alpha,0}(q) - \epsilon^{(0)}_{\alpha,0}(q_{F\alpha,0})\,, \qquad \epsilon_{\alpha,\gamma}(q) = \epsilon^{(0)}_{\alpha,\gamma}(q) - \delta_{\alpha,s}\epsilon^{(0)}_{\alpha,\gamma}(0)\,, \tag{4.62}$$

and $\hat{H}^{(2)}$ is given in Eq. (4.42). The Hamiltonian (4.60) describes the Landau-liquid excitations (b) relative to the GGS. Here (4.60) are the Landau-liquid Hamiltonian terms which are relevant at low energy ($\omega - \omega_0$). Therefore, the corresponding second-order Hamiltonian is suitable to study the physics at low positive energy above the gap, *i.e.*, small ($\omega - \omega_0$).

In general, the different final GGS's of the Hilbert subspace where a given initial GS is transformed upon excitations involving a small density of pseudoparticles have different energies (4.56)-(4.57). This implies that the study of the quantum-liquid physics at energy-scale $\omega_0$ involves, in general, transitions to one sub-cannonical ensemble only. However, if two or several possible final GGS's had the same energy gap $\omega_0$, the physics would involve the Hilbert subspace spanned by all Hamiltonian eigenstates associated with the corresponding different sub-canonical ensembles.

For sub-canonical ensembles such that $S^{\alpha}_{z} \neq 0$ and characterized by small values of $N^{h}_{\alpha,-\frac{l_\alpha}{2}}/N^{h}_{\alpha}$ (where $l_\alpha$ is given in Eq. (2.14)), the gap expression (4.56) leads directly to

$$\hat{H}_0 = 2|\mu|\hat{N}^{h}_{c,-\frac{l_c}{2}} + 2\mu_0|H|[\hat{N}^{h}_{s,-\frac{l_s}{2}} + \sum_{\gamma=1}^{\infty}\hat{N}_{s,\gamma}] + \sum_{\gamma=1}\epsilon^{(0)}_{s,\gamma}(0)\hat{N}_{s,\gamma}\,. \tag{4.63}$$

There is a remarkable similarity between the general Hamiltonian (4.59) and its version in the Hilbert subspace spanned by the states I [1, 11, 14]. Moreover, in the case that the GGS is the GS it self, the gap (4.56)-(4.57) vanishes and the Hamiltonian (4.59) reduces to the above low-energy Hamiltonian. In this case it refers to Landau-liquid $\alpha, 0$ pseudoparticle-pseudohole excitations around the GS.

# Appendix A

# Normal-ordered rapidity operator expressions

Following the discussion of Sec. 4.2, the perturbative character of the system implies the equivalence between expanding in the pseudoparticle scattering order and/or in the pseudomomentum deviations (4.31). In this Appendix we give a short description of the calculation of the normal-ordered operator expansion for the pseudoparticle rapidities (4.33). We focus our study on the evaluation of the functions $X^{(1)}_{\alpha,\gamma}(q)$ and $X^{(2)}_{\alpha,\gamma}(q)$ and associate functions $Q^{(1)}_{\alpha,\gamma}(q)$ and $Q^{(2)}_{\alpha,\gamma}(q)$ (eigenvalues of the operators $\hat{X}^{(1)}_{\alpha}(q)$ and $\hat{X}^{(2)}_{\alpha}(q)$ and $\hat{Q}^{(1)}_{\alpha}(q)$ and $\hat{Q}^{(2)}_{\alpha}(q)$, respectively).

We evaluate here the first-order and second-order terms of the eigenvalues of the operator (4.33). Equation (4.22) then allows the straightforward calculation of the corresponding operator expressions. All the quantities are given in the limit established by Eq. (4.24).

In the thermodynamic limit, Eqs. (4.5)-(4.7) lead to the following equations

$$K(q) = q - \frac{1}{\pi}\int_{q^{(-)}_{s,0}}^{q^{(+)}_{s,0}} dq' N_{s,0}(q') \tan^{-1}(R_{c,0}(q) - R_{s,0}(q')) \tag{A.1}$$

$$\begin{aligned} q &= 2Re \sin^{-1}\Big(u(R_{c,\gamma}(q) + i\gamma)\Big) \\ &- \frac{1}{\pi}\int_{q^{(-)}_{c,0}}^{q^{(+)}_{c,0}} dq' N_{c,0}(q') \tan^{-1}\Big(\frac{R_{c,\gamma}(q) - R_{c,0}(q')}{\gamma}\Big) \end{aligned} \tag{A.2}$$

and

$$
\begin{aligned}
0 &= q - \frac{1}{\pi}\int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} dq' N_{c,0}(q')\tan^{-1}\Big(\frac{R_{s,\gamma}(q)-R_{c,0}(q')}{1+\gamma}\Big) \\
&+ \frac{1}{2\pi}\int_{q_{s,0}^{(-)}}^{q_{s,0}^{(+)}} dq' N_{s,0}(q')\Theta_{1+\gamma,1}\Big(R_{s,\gamma}(q)-R_{s,0}(q')\Big)\,. \qquad \text{(A.3)}
\end{aligned}
$$

In what follows, it is useful to define the GGS rapidities $K^{(0)}(q)$ and $R^{(0)}_{\alpha,\gamma}(q)$ in terms of their inverse functions $2\pi\rho_{\alpha,\gamma}(r)$ as

$$
q = \int_0^{K^{(0)}(q)} dk 2\pi\rho_{c,0}(k)\,, \qquad \text{(A.4)}
$$

$$
q = \int_0^{R^{(0)}_{\alpha,\gamma}(q)} dr 2\pi\rho_{\alpha,\gamma}(r)\,. \qquad \text{(A.5)}
$$

We start by considering the GGS eigenstate rapidities of Eqs. (4.11) and (4.12). If we insert in Eqs. (4.5)-(4.7) the GGS distributions (4.14), after some algebra we find that the functions of the rhs of Eqs. (A.4) and (A.5) defining the inverse of these GGS rapidities are solutions of the following integral equations

$$
2\pi\rho_{c,0}(k) = 1 + \frac{\cos k}{u}\int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr \frac{2\pi\rho_{s,0}(r)}{\pi\left[1+(r-\frac{\sin k}{u})^2\right]}\,, \qquad \text{(A.6)}
$$

$$
2\pi\rho_{c,\gamma}(r) = 2Re\Big(\frac{u}{\sqrt{1-u^2[r+i\gamma]^2}}\Big) - \int_{Q^{(-)}}^{Q^{(+)}} dk \frac{2\pi\rho_{c,0}(k)}{\pi\gamma\left[1+(\frac{\frac{\sin k}{u}-r}{\gamma})^2\right]}\,, \qquad \text{(A.7)}
$$

and

$$
2\pi\rho_{s,\gamma}(r) = \int_{Q^{(-)}}^{Q^{(+)}} dk \frac{2\pi\rho_{c,0}(k)}{\pi(1+\gamma)\left[1+(\frac{\frac{\sin k}{u}-r}{1+\gamma})^2\right]} - \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} \frac{dr'}{2\pi}\Theta^{[1]}_{1,1+\gamma}(r-r')2\pi\rho_{s,0}(r')\,, \qquad \text{(A.8)}
$$

where

$$
\begin{aligned}
\Theta^{[1]}_{\gamma,\gamma'}\Big(x\Big) &= \Theta^{[1]}_{\gamma',\gamma}\Big(x\Big) = \frac{d\Theta_{\gamma,\gamma'}\Big(x\Big)}{dx} \\
&= \delta_{\gamma,\gamma'}\{\frac{1}{\gamma[1+(\frac{x}{2\gamma})^2]} + \sum_{l=1}^{\gamma-1}\frac{2}{l[1+(\frac{x}{2l})^2]}\}
\end{aligned}
$$

$$+ \quad (1-\delta_{\gamma,\gamma'})\{\frac{2}{|\gamma-\gamma'|[1+(\frac{x}{|\gamma-\gamma'|})^2]}+\frac{2}{(\gamma+\gamma')[1+(\frac{x}{\gamma+\gamma'})^2]}$$

$$+ \quad \sum_{l=1}^{\frac{\gamma+\gamma'-|\gamma-\gamma'|}{2}-1}\frac{4}{(|\gamma-\gamma'|+2l)[1+(\frac{x}{|\gamma-\gamma'|+2l})^2]}\}\,, \tag{A.9}$$

is the derivative of the function (4.8) and the parameters $Q^{(\pm)}$ and $r^{(\pm)}_{\alpha,\gamma}$ are defined combining Eqs. (A.4), (A.5), and (4.16).

Let us now consider small deviations from a GGS or GS. The eigenvalue form of Eq. (4.32) is

$$\delta K(q) = K^{(0)}(q+\delta X_{c,0}(q)) - K^{(0)}(q)\,, \tag{A.10}$$

for $\alpha = c$ and $\gamma = 0$ and

$$\delta R_{\alpha,\gamma}(q) = R^0_{\alpha,\gamma}(q+\delta X_{\alpha,\gamma}(q)) - R^0_{\alpha,\gamma}(q)\,, \tag{A.11}$$

for all remaining values of the quantum numbers $\alpha$ and $\gamma$. Here $\delta K(q)$, $\delta R_{\alpha,\gamma}(q)$, and $\delta X_{\alpha,\gamma}(q)$ are the eigenvalues of the operators $:\hat{K}(q):$, $:\hat{R}_{\alpha,\gamma}(q):$, and $:\hat{X}_{\alpha,\gamma}(q):$, respectively. From Eq. (4.33) $\delta X_{\alpha,\gamma}(q)$ can be written as

$$\delta X_{\alpha,\gamma}(q) = X^{(1)}_{\alpha,\gamma}(q) + X^{(2)}_{\alpha,\gamma}(q) + \ldots\,, \tag{A.12}$$

where $X^{(i)}_{\alpha,\gamma}(q)$ is the eigenvalue of the operator $\hat{X}^{(i)}_{\alpha,\gamma}(q)$. Expanding the $\delta R_{\alpha,\gamma}(q)$ expressions (A.10) and (A.11) we find

$$K(q) = \sum_{i=0}^{\infty} K^{(i)}(q)\,, \tag{A.13}$$

and

$$R_{\alpha,\gamma}(q) = \sum_{i=0}^{\infty} R^{(i)}_{\alpha,\gamma}(q)\,, \tag{A.14}$$

respectively, [and $\delta K(q) = \sum_{i=1}^{\infty} K^{(i)}(q)$ and $\delta R_{\alpha,\gamma}(q) = \sum_{i=1}^{\infty} R^{(i)}_{\alpha,\gamma}(q)$] where the zero-order GGS functions $K^{(0)}(q)$ and $R^{(0)}_{\alpha,\gamma}(q)$ are defined by Eqs. Eqs. (A.4) and (A.5). From the resulting equations we can obtain all derivatives of the GGS functions $K^{(0)}(q)$ and $R^{(0)}_{\alpha,\gamma}(q)$ with respect to $q$. The terms of the rhs of Eqs. (A.13) and (A.14) involve these derivatives. For instance, the first-order and second-order terms read

$$K^{(1)}(q) = \frac{dK^{(0)}(q)}{dq} X^{(1)}_{c,0}(q)\,, \tag{A.15}$$

$$R^{(1)}_{\alpha,\gamma}(q) = \frac{dR^{(0)}_{\alpha,\gamma}(q)}{dq} X^{(1)}_{\alpha,\gamma}(q)\,, \tag{A.16}$$

and

$$K^{(2)}(q) = \frac{dK^{(0)}(q)}{dq} X^{(2)}_{c,0}(q) + \frac{1}{2}\frac{d^2K^{(0)}(q)}{dq^2}[X^{(1)}_{c,0}(q)]^2\,, \tag{A.17}$$

$$R^{(2)}_{\alpha,\gamma}(q) = \frac{dR^{(0)}_{\alpha,\gamma}(q)}{dq} X^{(2)}_{\alpha,\gamma}(q) + \frac{1}{2}\frac{d^2R^{(0)}_{\alpha,\gamma}(q)}{dq^2}[X^{(1)}_{\alpha,\gamma}(q)]^2\,, \tag{A.18}$$

respectively, and involve the first and second derivatives.

From Eqs. (A.1)-(A.3) [with $N_{\alpha,\gamma}(q')$ given by the GGS distribution (75)] we find that the first derivatives $\frac{dK^{(0)}_{\alpha}(q)}{dq}$ and $\frac{dR^{(0)}_{\alpha,\gamma}(q)}{dq}$ can be expressed in terms of the functions (A.6)-(A.8) as follows

$$\frac{dK^{(0)}(q)}{dq} = \frac{1}{2\pi\rho_{c,0}(K^{(0)}(q))}\,, \tag{A.19}$$

and

$$\frac{dR^{(0)}_{\alpha,\gamma}(q)}{dq} = \frac{1}{2\pi\rho_{c,\gamma}(R^{(0)}_{\alpha,\gamma}(q))}\,. \tag{A.20}$$

The second derivatives $\frac{d^2K^{(0)}(q)}{dq^2}$ and $\frac{d^2R^{(0)}_{\alpha,\gamma}(q)}{dq^2}$ then read

$$\frac{d^2K^{(0)}(q)}{dq^2} = -\frac{1}{[2\pi\rho_{c,0}(K^{(0)}(q))]^3} 2\pi \frac{d\rho_{c,0}(k)}{dk}|_{k=K^{(0)}(q)}\,, \tag{A.21}$$

and

$$\frac{d^2R^{(0)}_{\alpha,\gamma}(q)}{dq^2} = -\frac{1}{[2\pi\rho_{c,\gamma}(R^{(0)}_{\alpha,\gamma}(q))]^3} 2\pi \frac{d\rho_{\alpha,\gamma}(r)}{dr}|_{r=R^{(0)}_{\alpha,\gamma}(q)}\,. \tag{A.22}$$

By introducing both the distributions

$$N_{\alpha,\gamma}(q) = N^{(0)}_{\alpha,\gamma}(q) + \delta N_{\alpha,\gamma}(q)\,, \tag{A.23}$$

and the first-order and second-order functions (A.15)-(A.22) into Eqs. (A.1)-(A.3), we find after expanding to second order that for $j = 1$ and $j = 2$ the functions $X^{(j)}_{\alpha,\gamma}(q)$ can be written as

$$X^{(j)}_{\alpha,\gamma}(q) = Q^{(j)}_{\alpha,\gamma}(q) + Y^{(j)}_{\alpha,\gamma}(q)\,, \tag{A.24}$$

where $Y^{(j)}_{\alpha,\gamma}(q)$ is even in $q$

$$Y^{(j)}_{\alpha,\gamma}(q) = Y^{(j)}_{\alpha,\gamma}(-q)\,, \tag{A.25}$$

and does not contribute to the physical quantities to second scattering order (and to second order in the density of excited pseudoparticles). Up to this order only $\hat{Q}^{(j)}_{\alpha,\gamma}(q)$ contributes.

To derive this result we have expanded the expression for the even functions $Y^{(j)}_{\alpha,\gamma}(q)$ for $j = 1$ and $j = 2$ to second order in the density of excited pseudoparticles. Following the perturbative character of the quantum liquid in the pseudoparticle basis, the obtained expression is exact up to $j = 2$ pseudoparticle scattering order. Moreover, we find that the even function $Y^{(1)}_{\alpha,\gamma}(q)$ does not contribute to the physical quantities up to that order and can, therefore, be omitted.

Let us introduce the functions $\bar{Q}^{(1)}_{\alpha,\gamma}(r)$ such that

$$Q^{(1)}_{\alpha,\gamma}(q) = \bar{Q}^{(1)}_{\alpha,\gamma}(R^{(0)}_{\alpha,\gamma}(q))\,, \tag{A.26}$$

for all values of $\alpha$ and $\gamma$, with $R^{(0)}_{c,0}(q) = \frac{\sin K^{(0)}(q)}{u}$. It is also useful to define the function $\widetilde{Q}^{(1)}(k)$ such that

$$\widetilde{Q}^{(1)}(k) = \bar{Q}^{(1)}_{c,0}(\frac{\sin k}{u})\,. \tag{A.27}$$

By introducing both the distributions (A.23) and the first-order functions defined in Eq. (A.26) into Eqs. (A.1)-(A.3), we find after expanding to first order that the functions $\bar{Q}^{(1)}_{\alpha,\gamma}(r)$ are defined by the following system of coupled integral equations

$$\begin{aligned}
\bar{Q}^{(1)}_{c,0}(r) &= -\sum_{\gamma=0}\int_{q^{(-)}_{s,\gamma}}^{q^{(+)}_{s,\gamma}} dq\delta N_{s,\gamma}(q)\frac{1}{\pi}\tan^{-1}\Big(\frac{r - R^{(0)}_{s,\gamma}(q)}{1+\gamma}\Big) \\
&- \sum_{\gamma=1}\int_{q^{(-)}_{c,\gamma}}^{q^{(+)}_{c,\gamma}} dq\delta N_{c,\gamma}(q)\frac{1}{\pi}\tan^{-1}\Big(\frac{r - R^{(0)}_{c,\gamma}(q)}{\gamma}\Big) \\
&+ \int_{r^{(-)}_{s,0}}^{r^{(+)}_{s,0}} dr'\frac{\bar{Q}^{(1)}_{s,0}(r')}{\pi\left[1+(r-r')^2\right]}\,,
\end{aligned} \tag{A.28}$$

$$\begin{aligned}
\bar{Q}^{(1)}_{c,\gamma}(r) &= \int_{q^{(-)}_{c,0}}^{q^{(+)}_{c,0}} dq\delta N_{c,0}(q)\frac{1}{\pi}\tan^{-1}\Big(\frac{r - R^{(0)}_{c,0}(q)}{\gamma}\Big) \\
&+ \sum_{\gamma'=1}\int_{q^{(-)}_{c,\gamma'}}^{q^{(+)}_{c,\gamma'}} dq\delta N_{c,\gamma'}(q)\frac{1}{2\pi}\Theta_{\gamma,\gamma'}\Big(r - R^{(0)}_{c,\gamma'}(q)\Big)
\end{aligned}$$

$$- \int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}} dr' \frac{\bar{Q}_{c,0}^{(1)}(r')}{\pi\gamma\left[1+(\frac{r-r'}{\gamma})^2\right]}\,, \tag{A.29}$$

and

$$\begin{aligned}
\bar{Q}_{s,\gamma}^{(1)}(r) &= -\int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} dq\delta N_{c,0}(q)\frac{1}{\pi}\tan^{-1}\Big(\frac{r-R_{c,0}^{(0)}(q)}{1+\gamma}\Big) \\
&+ \sum_{\gamma'=0}\int_{q_{s,\gamma'}^{(-)}}^{q_{s,\gamma'}^{(+)}} dq\delta N_{s,\gamma'}(q)\frac{1}{2\pi}\Theta_{1+\gamma,1+\gamma'}\Big(r-R_{s,\gamma'}^{(0)}(q)\Big) \\
&+ \int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}} dr' \frac{\bar{Q}_{c,0}^{(1)}(r')}{\pi(1+\gamma)\left[1+(\frac{r-r'}{1+\gamma})^2\right]} \\
&- \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr'\bar{Q}_{s,0}^{(1)}(r')\frac{1}{2\pi}\Theta_{1+\gamma,1}^{[1]}\Big(r-r'\Big)\,.
\end{aligned} \tag{A.30}$$

(The use of Eq. (A.28) in Eqs. (A.29) and (A.30) allows the expression of both $\bar{Q}_{c,\gamma}^{(1)}(r)$ and $\bar{Q}_{s,\gamma}^{(1)}(r)$ in terms of free terms and integrals involving $\bar{Q}_{s,0}^{(1)}(r)$.) Combining Eqs. (A.28)-(A.30) with Eqs. (A.26) and (A.27) leads to Eq. (4.34) with the phase shifts defined below. Note that at first order we can either consider the function $\hat{X}_{\alpha,\gamma}^{(1)}(q)$ or the associate function $\hat{Q}_{\alpha,\gamma}^{(1)}(q)$ of Eq. (A.24). Both functions are of the form (4.34). However, the general expression for the phase shifts associated with the function $\hat{X}_{\alpha,\gamma}^{(1)}(q)$ of Eq. (4.34) have extra terms. These arise from the function $\hat{Y}_{\alpha,\gamma}^{(1)}(q)$ of the rhs of Eq. (A.24). If we expand the physical quantities involving the phase shifts to first (and second) order in the density of excited pseudoparticles these extra terms lead to vanishing contributions. For instance, expression (4.34) is identical if we use in it either choice for the phase shift expression. For simplicity, we omit here the phase-shift extra terms associated with the function $\hat{Y}_{\alpha,\gamma}^{(1)}(q)$. We find that the phase shifts associated with the function $\hat{Q}_{\alpha,\gamma}^{(1)}(q)$ are defined by the following coupled integral equations

$$\bar{\Phi}_{c,0;c,0}\,(r,r') = \frac{1}{\pi}\int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr''\frac{\bar{\Phi}_{s,0;c,0}\,(r'',r')}{1+(r-r'')^2}\,, \tag{A.31}$$

$$\bar{\Phi}_{c,0;c,\gamma}\,(r,r') = -\frac{1}{\pi}\tan^{-1}(\frac{r-r'}{\gamma}) + \frac{1}{\pi}\int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr''\frac{\bar{\Phi}_{s,0;c,\gamma}\,(r'',r')}{1+(r-r'')^2}\,, \tag{A.32}$$

$$\bar{\Phi}_{c,0;s,\gamma}\,(r,r') = -\frac{1}{\pi}\tan^{-1}(\frac{r-r'}{1+\gamma}) + \frac{1}{\pi}\int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr''\frac{\bar{\Phi}_{s,0;s,\gamma}\,(r'',r')}{1+(r-r'')^2}\,, \tag{A.33}$$

$$\bar{\Phi}_{c,\gamma;c,0}\left(r,r'\right)=\frac{1}{\pi}\tan^{-1}(\frac{r-r'}{\gamma})-\frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\bar{\Phi}_{c,0;c,0}\left(r'',r'\right)}{\gamma[1+(\frac{r-r''}{\gamma})^2]}\,, \tag{A.34}$$

$$\bar{\Phi}_{c,\gamma;c,\gamma'}\left(r,r'\right)=\frac{1}{2\pi}\Theta_{\gamma,\gamma'}\Big(r-r'\Big)-\frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\bar{\Phi}_{c,0;c,\gamma'}\left(r'',r'\right)}{\gamma[1+(\frac{r-r''}{\gamma})^2]}\,, \tag{A.35}$$

$$\bar{\Phi}_{c,\gamma;s,\gamma'}\left(r,r'\right)=-\frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\bar{\Phi}_{c,0;s,\gamma'}\left(r'',r'\right)}{\gamma[1+(\frac{r-r''}{\gamma})^2]}\,, \tag{A.36}$$

$$\begin{aligned}\bar{\Phi}_{s,\gamma;c,0}\left(r,r'\right) &= -\frac{1}{\pi}\tan^{-1}(\frac{r-r'}{1+\gamma})+\frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\bar{\Phi}_{c,0;c;0}\left(r'',r'\right)}{(1+\gamma)[1+(\frac{r-r''}{1+\gamma})^2]}\\ &- \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}}dr''\bar{\Phi}_{s,0;c,0}\left(r'',r'\right)\frac{\Theta_{1+\gamma,1}^{[1]}\Big(r-r''\Big)}{2\pi}\,,\end{aligned} \tag{A.37}$$

$$\begin{aligned}\bar{\Phi}_{s,\gamma;c,\gamma'}\left(r,r'\right) &= \frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\bar{\Phi}_{c,0;c;\gamma'}\left(r'',r'\right)}{(1+\gamma)[1+(\frac{r-r''}{1+\gamma})^2]}\\ &- \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}}dr''\bar{\Phi}_{s,0;c,\gamma'}\left(r'',r'\right)\frac{\Theta_{1+\gamma,1}^{[1]}\Big(r-r''\Big)}{2\pi}\,,\end{aligned} \tag{A.38}$$

$$\begin{aligned}\bar{\Phi}_{s,\gamma;s,\gamma'}\left(r,r'\right) &= \frac{\Theta_{1+\gamma,1+\gamma'}\Big(r-r'\Big)}{2\pi}+\frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\bar{\Phi}_{c,0;s;\gamma'}\left(r'',r'\right)}{(1+\gamma)[1+(\frac{r-r''}{1+\gamma})^2]}\\ &- \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}}dr''\bar{\Phi}_{s,0;s,\gamma'}\left(r'',r'\right)\frac{\Theta_{1+\gamma,1}^{[1]}\Big(r-r''\Big)}{2\pi}\,.\end{aligned} \tag{A.39}$$

For $\gamma=0$ Eqs. (A.37) and (A.39) can be rewritten as

$$\bar{\Phi}_{s,0;c,0}\left(r,r'\right)=-\frac{1}{\pi}\tan^{-1}(r-r')+\frac{1}{\pi}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dy''G(y,y'')\bar{\Phi}_{s,0;c,0}\left(y'',x'\right)\,, \tag{A.40}$$

and

$$\begin{aligned}\bar{\Phi}_{s,0;s,0}\left(r,r'\right) &= \frac{1}{\pi}\tan^{-1}(\frac{r-r'}{2})-\frac{1}{\pi^2}\int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}}dr''\frac{\tan^{-1}(r''-r')}{1+(r-r'')^2}\\ &+ \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}}dr''G(r,r'')\bar{\Phi}_{s,0;s,0}\left(r'',r'\right)\,,\end{aligned} \tag{A.41}$$

and the kernel $G(r,r')$ reads [7]

$$G(r,r') = -\frac{1}{2\pi}\left[\frac{1}{1+((r-r')/2)^2}\right]\left[1-\frac{1}{2}\left(t(r)+t(r')+\frac{l(r)-l(r')}{r-r'}\right)\right], \quad \text{(A.42)}$$

with

$$t(r) = \frac{1}{\pi}\left[\tan^{-1}(r+r_{c,0}^{(+)}) - \tan^{-1}(r+r_{c,0}^{(-)})\right], \quad \text{(A.43)}$$

and

$$l(r) = \frac{1}{\pi}\left[\ln(1+(r+r_{c,0}^{(+)})^2) - \ln(1+(r+r_{c,0}^{(-)})^2)\right]. \quad \text{(A.44)}$$

In order to evaluate the second-order functions $Q_{\alpha,\gamma}^{(2)}(q)$ of the rhs of Eq. (A.24) for $j=2$ we introduce the functions (A.15)-(A.18) and distributions (A.23) in Eqs. (A.1)-(A.3). Expanding to second order we find after some algebra

$$Q_{\alpha,\gamma}^{(2)}(q) = Q_{\alpha,\gamma}^{(2,*)}(q) + \frac{1}{2}\frac{d}{dq}[[Q_{\alpha,\gamma}^{(1)}(q)]^2], \quad \text{(A.45)}$$

where

$$Q_{\alpha,\gamma}^{(2,*)}(q) = \widetilde{Q}_{\alpha,\gamma}^{(2,*)}(R_{\alpha,\gamma}^{(0)}(q)). \quad \text{(A.46)}$$

It is also useful to define the function $\widetilde{Q}^{(2,*)}(k)$ such that

$$\widetilde{Q}^{(2,*)}(k) = \bar{Q}_{c,0}^{(2,*)}(\frac{\sin k}{u}). \quad \text{(A.47)}$$

The functions $\bar{Q}_{\alpha,\gamma}^{(2,*)}(r)$ are defined by the following system of coupled integral equations

$$\begin{aligned}
\bar{Q}_{c,0}^{(2,*)}(r) &= \sum_{\gamma=0}\int_{q_{s,\gamma}^{(-)}}^{q_{s,\gamma}^{(+)}} dq\delta N_{s,\gamma}(q)\frac{Q_{s,\gamma}^{(1)}(q)}{2\pi\rho_{s,\gamma}\Big(R_{s,\gamma}^{(0)}(q)\Big)}\frac{1}{\pi(1+\gamma)\left[1+(\frac{r-R_{s,\gamma}^{(0)}(q)}{1+\gamma})^2\right]} \\
&+ \sum_{\gamma=1}\int_{q_{c,\gamma}^{(-)}}^{q_{c,\gamma}^{(+)}} dq\delta N_{c,\gamma}(q)\frac{Q_{c,\gamma}^{(1)}(q)}{2\pi\rho_{c,\gamma}\Big(R_{c,\gamma}^{(0)}(q)\Big)}\frac{1}{\pi\gamma\left[1+(\frac{r-R_{c,\gamma}^{(0)}(q)}{\gamma})^2\right]} \\
&+ \sum_{\gamma=0}\frac{1}{2\pi\rho_{s,\gamma}\Big(r_{s,\gamma}\Big)}\sum_{j=\pm1}\frac{[Q_{s,\gamma}^{(1)}(jq_{Fs,\gamma})]^2}{2\pi(1+\gamma)\left[1+(\frac{r-jr_{s,\gamma}}{1+\gamma})^2\right]} \\
&+ \sum_{\gamma=1}\frac{1}{2\pi\rho_{c,\gamma}\Big(r_{c,\gamma}\Big)}\sum_{j=\pm1}\frac{[Q_{c,\gamma}^{(1)}(jq_{Fc,\gamma})]^2}{2\pi\gamma\left[1+(\frac{r-jr_{c,\gamma}}{\gamma})^2\right]}
\end{aligned}$$

$$+ \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr' \frac{\bar{Q}_{s,0}^{(2,*)}(r')}{\pi\left[1+(r-r')^2\right]}\,, \tag{A.48}$$

$$\begin{aligned}
\bar{Q}_{c,\gamma}^{(2,*)}(r) &= -\int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} dq\delta N_{c,0}(q)\frac{\cos K^{(0)}(q)}{u}\frac{Q_{c,0}^{(1)}(q)}{2\pi\rho_{c,0}\Big(k^{(0)}(q)\Big)}\frac{1}{\pi\gamma\left[1+(\frac{r-R_{c,0}^{(0)}(q)}{\gamma})^2\right]} \\
&- \sum_{\gamma'=1}\int_{q_{c,\gamma'}^{(-)}}^{q_{c,\gamma'}^{(+)}} dq\delta N_{c,\gamma'}(q)\frac{Q_{c,\gamma'}^{(1)}(q)}{2\pi\rho_{c,\gamma'}\Big(R_{c,\gamma'}^{(0)}(q)\Big)}\frac{1}{2\pi}\Theta_{\gamma,\gamma'}^{[1]}\Big(r-R_{c,\gamma'}^{(0)}(q)\Big) \\
&- \frac{\cos Q}{u}\frac{1}{2\pi\rho_{c,0}\Big(Q\Big)}\sum_{j=\pm 1}\frac{[Q_{c,0}^{(1)}(jq_{Fc,0})]^2}{2\pi\gamma\left[1+(\frac{r-jr_{c,0}}{\gamma})^2\right]} \\
&- \sum_{\gamma'=1}\frac{1}{2\pi\rho_{c,\gamma'}\Big(r_{c,\gamma'}\Big)}\frac{1}{2}\sum_{j=\pm 1}[Q_{c,\gamma'}^{(1)}(jq_{Fc,\gamma'})]^2\frac{1}{2\pi}\Theta_{\gamma,\gamma'}^{[1]}\Big(r-jr_{c,\gamma'}\Big) \\
&- \int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}} dr'\frac{\bar{Q}_{c,0}^{(2,*)}(r')}{\pi\gamma\left[1+(\frac{r-r'}{\gamma})^2\right]}\,,
\end{aligned} \tag{A.49}$$

and

$$\begin{aligned}
\bar{Q}_{s,\gamma}^{(2,*)}(r) &= \int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} dq\delta N_{c,0}(q)\frac{\cos K^{(0)}(q)}{u}\frac{Q_{c,0}^{(1)}(q)}{2\pi\rho_{c,0}\Big(k^{(0)}(q)\Big)}\frac{1}{\pi(1+\gamma)\left[1+(\frac{r-R_{c,0}^{(0)}(q)}{1+\gamma})^2\right]} \\
&- \sum_{\gamma'=0}\int_{q_{s,\gamma'}^{(-)}}^{q_{s,\gamma'}^{(+)}} dq\delta N_{s,\gamma'}(q)\frac{Q_{s,\gamma'}^{(1)}(q)}{2\pi\rho_{s,\gamma'}\Big(R_{s,\gamma'}^{(0)}(q)\Big)}\frac{1}{2\pi}\Theta_{1+\gamma,1+\gamma'}^{[1]}\Big(r-R_{s,\gamma'}^{(0)}(q)\Big) \\
&+ \frac{\cos Q}{u}\frac{1}{2\pi\rho_{c,0}\Big(Q\Big)}\sum_{j=\pm 1}\frac{[Q_{c,0}^{(1)}(jq_{Fc,0})]^2}{2\pi(1+\gamma)\left[1+(\frac{r-jr_{c,0}}{1+\gamma})^2\right]} \\
&- \sum_{\gamma'=0}\frac{1}{2\pi\rho_{s,\gamma'}\Big(r_{s,\gamma'}\Big)}\frac{1}{2}\sum_{j=\pm 1}[Q_{s,\gamma'}^{(1)}(jq_{Fs,\gamma'})]^2\frac{1}{2\pi}\Theta_{1+\gamma,1+\gamma'}^{[1]}\Big(r-jr_{s,\gamma'}\Big) \\
&+ \int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}} dr'\frac{\bar{Q}_{c,0}^{(2,*)}(r')}{\pi(1+\gamma)\left[1+(\frac{r-r'}{1+\gamma})^2\right]} \\
&- \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr'\bar{Q}_{s,0}^{(2,*)}(r')\frac{1}{2\pi}\Theta_{1+\gamma,1}^{[1]}\Big(r-r'\Big)\,.
\end{aligned} \tag{A.50}$$

As for the first-order case, the use of either the function $Q_{\alpha,\gamma}^{(2)}(q)$ defined by Eqs. (A.45)-(A.47) or of the full function $X_{\alpha,\gamma}^{(2)}(q)$ of Eq. (A.24) for $j=2$ leads to the same results for the physical quantities up to second order in the density of excited pseudoparticles.

Note that the free terms of Eqs. (A.48)-(A.50) involve the first-order functions only. This implies that the unique solutions of these integral equations can be expressed in terms of the first-order functions. Therefore, following Eqs. (4.34) and (A.24) the second-order functions can also be expressed in terms of the pseudoparticle phase shifts.

# Appendix B

# Normal-ordered Hamiltonian expression

In order to derive the first-order and second-order Hamiltonian terms of Eqs. (4.41) and (4.42), we again consider eigenvalues and deviations. The energy associated with the Hamiltonian (4.18) reads

$$\begin{aligned} E_{SO(4)} &= -\frac{2tN_a}{2\pi}\int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} N_{c,0}(q)\cos K(q) \\ &+ \frac{4tN_a}{2\pi}\sum_{\gamma=1}\int_{q_{c,\gamma}^{(-)}}^{q_{c,\gamma}^{(+)}} N_{c,\gamma}(q) Re\sqrt{1-[u(R_{c,\gamma}(q)+i\gamma)]^2} \\ &+ U[\frac{N_a}{4}-\frac{N_{c,0}}{2}-\sum_{\gamma=1}\gamma N_{c,\gamma}]\,. \end{aligned} \tag{B.1}$$

To caculate the bands (4.43)-(4.45) we introduce in this energy Eqs. (A.15), (A.16), and (A.23) and expand the obtained expression to first order in the deviations with the result

$$\begin{aligned} \Delta E_{SO(4)}^{(1)} &= \frac{N_a}{2\pi}\{\int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} \delta N_{c,0}(q)[-2t\cos K^{(0)}(q)-\frac{U}{2}] \\ &+ \sum_{\gamma=1}\int_{q_{c,\gamma}^{(-)}}^{q_{c,\gamma}^{(+)}} \delta N_{c,\gamma}(q)[4tRe\sqrt{1-[u(R_{c,\gamma}^{(0)}(q)+i\gamma)]^2}-\gamma U] \\ &+ 2t\int_{Q^{(-)}}^{Q^{(+)}} dk\widetilde{Q}^{(1)}(k)\sin k \\ &- 4t\sum_{\gamma=1}\int_{r_{c,\gamma}^{(-)}}^{r_{c,\gamma}^{(+)}} dr\bar{Q}_{c,\gamma}^{(1)}(r)Re\Big(\frac{u^2[r+i\gamma]}{\sqrt{1-u^2[r+i\gamma]^2}}\Big)\}\,, \end{aligned} \tag{B.2}$$

where the functions $\widetilde{Q}^{(1)}(k)$ and $\bar{Q}^{(1)}_{c,\gamma}(r)$ are defined by Eqs. (A.27)-(A.29). The use of Eqs. (A.24), (A.26), (A.27), and (4.34) in (B.2) leads after some straightforward algebra to

$$\Delta E^{(1)}_{SO(4)} = \sum_{q,\alpha,\gamma} \epsilon^0_{\alpha,\gamma}(q)\delta\hat{N}_{\alpha,\gamma}(q)\,, \tag{B.3}$$

with the bands given by Eqs. (4.43)-(4.45) in terms of the phase shifts (A.31)-(A.39).

An equivalent representation for the band energies is

$$\epsilon^0_{c,0}(q) = -\frac{U}{2} - 2t\cos K^{(0)}(q) - \int_{r^{(-)}_{s,0}}^{r^{(+)}_{s,0}} dr 2t\eta_{s,0}(r)\frac{1}{\pi}\tan^{-1}\left(r - R^{(0)}_{c,0}(q)\right)\,, \tag{B.4}$$

$$\begin{aligned}\epsilon^0_{c,\gamma}(q) &= -\gamma U + 4tRe\sqrt{1-u^2[R^{(0)}_{c,\gamma}(q)+i\gamma]^2} \\ &- \int_{Q^{(-)}}^{Q^{(+)}} dk\frac{1}{\pi}\tan^{-1}\left(\frac{\frac{\sin k}{u} - R^{(0)}_{c,\gamma}(q)}{\gamma}\right) 2t\eta_{c,0}(k)\,,\end{aligned} \tag{B.5}$$

and

$$\begin{aligned}\epsilon^0_{s,\gamma}(q) &= -2t\int_{Q^{(-)}}^{Q^{(+)}} dk\frac{1}{\pi}\tan^{-1}\left(\frac{\frac{\sin k}{u} - R^{(0)}_{s,\gamma}(q)}{1+\gamma}\right)\sin k \\ &+ \int_{r^{(-)}_{s,0}}^{r^{(+)}_{s,0}} dr 2t\eta_{s,0}(r)\frac{1}{2\pi}\Theta_{1,1+\gamma}\Big(r - R^{(0)}_{s,\gamma}(q)\Big) \\ &- \int_{r^{(-)}_{c,0}}^{r^{(+)}_{c,0}} dr'\frac{\tan^{-1}\left(\frac{r'-R^{(0)}_{s,\gamma}(q)}{1+\gamma}\right)}{\pi^2[1+(r-r')^2]}\,,\end{aligned} \tag{B.6}$$

where the functions $2t\eta_{c,0}(k)$ and $2t\eta_{\alpha,\gamma}(r)$ are defined by the integral equations

$$2t\eta_{c,0}(k) = 2t\sin k + \frac{\cos k}{u}\int_{r^{(-)}_{s,0}}^{r^{(+)}_{s,0}} dr\frac{2t\eta_{s,0}(r)}{\pi\left[1+(r-\frac{\sin k}{u})^2\right]}\,, \tag{B.7}$$

$$\begin{aligned}2t\eta_{c,\gamma}(r) &= -4tRe\Big(\frac{u^2[r+i\gamma]}{\sqrt{1-u^2[r+i\gamma]^2}}\Big) \\ &+ \int_{Q^{(-)}}^{Q^{(+)}} dk\frac{2t\eta_{c,0}(k)}{\pi\gamma\left[1+(\frac{\frac{\sin k}{u}-r}{\gamma})^2\right]}\,,\end{aligned} \tag{B.8}$$

and

$$
\begin{aligned}
2t\eta_{s,\gamma}(r) &= 2t\int_{Q^{(-)}}^{Q^{(+)}} dk \frac{\sin k}{\pi(1+\gamma)\left[1+(\frac{\frac{\sin k}{u}-r}{1+\gamma})^2\right]} \\
&- \int_{r_{s,0}^{(-)}}^{r_{s,0}^{(+)}} dr' 2t\eta_{s,0}(r')\frac{1}{2\pi}[\Theta^{(1)}_{1,1+\gamma}\Big(r'-r\Big) \\
&- \int_{r_{c,0}^{(-)}}^{r_{c,0}^{(+)}} dr'' \frac{1}{\pi^2(1+\gamma)\left[1+(\frac{r-r''}{1+\gamma})^2\right][1+(r'-r'')^2]}] \, . \qquad \text{(B.9)}
\end{aligned}
$$

The gap expressions (4.56) and (4.57) can be rewritten in terms of pseudoparticle bands as

$$
\begin{aligned}
\omega_0 = &- 2\epsilon^0_{c,0}(q_{Fc,0})N^h_{c,\frac{-l_c}{2}} - \epsilon^0_{s,0}(q_{Fs,0})\sum_{\alpha} N^h_{\alpha,\frac{-l_\alpha}{2}} \\
&- \sum_{\gamma=1}[\epsilon^0_{s,0}(q_{Fs,0}) - \epsilon^0_{s,\gamma}(0)]N_{s,\gamma} \, , \qquad \text{(B.10)}
\end{aligned}
$$

and

$$
\begin{aligned}
\omega_0 = &- [2\epsilon^0_{c,0}(q_{Fc,0}) + \epsilon^0_{s,0}(q_{Fs,0})]\Big(\sum_{\gamma=1}\gamma N_{c,\gamma} + N^z_c\Big) \\
&- \epsilon^0_{s,0}(q_{Fs,0})\Big(\sum_{\gamma=1}[1+\gamma]N_{s,\gamma} + N^z_s\Big) + \sum_{\gamma=1}\epsilon^0_{s,\gamma}(0)N_{s,\gamma} \, , \qquad \text{(B.11)}
\end{aligned}
$$

respectively. In order to derive the expression for the second-order Hamiltonian (4.42) and associate $f$ functions (4.50) we expand the energy (B.1) to second-order with the result

$$
\begin{aligned}
\Delta E^{(2)}_{SO(4)} &= \frac{N_a}{2\pi}\{\int_{q_{c,0}^{(-)}}^{q_{c,0}^{(+)}} dq \delta N_{c,0}(q)\frac{2t\sin K^{(0)}(q)}{2\pi\rho_{c,0}\Big(K^{(0)}(q)\Big)}Q^{(1)}_{c,0}(q) \\
&- \sum_{\gamma=1}\int_{q_{c,\gamma}^{(-)}}^{q_{c,\gamma}^{(+)}} dq \delta N_{c,\gamma}(q)\frac{Q^{(1)}_{c,\gamma}(q)}{2\pi\rho_{c,\gamma}\Big(R^{(0)}_{c,\gamma}(q)\Big)}4tRe\Big(\frac{u^2[R^{(0)}_{c,\gamma}(q)+i\gamma]}{\sqrt{1-u^2[R^{(0)}_{c,\gamma}(q)+i\gamma]^2}}\Big) \\
&+ \frac{2t\sin Q}{2\pi\rho_{c,0}(Q)}\frac{1}{2}\sum_{j=\pm 1}[Q^{(1)}_{c,0}(jq_{Fc,0})]^2 \\
&- \sum_{\gamma=1}\frac{1}{2}\sum_{j=\pm 1}\frac{[Q^{(1)}_{c,\gamma}(jq_{c,\gamma})]^2}{2\pi\rho_{c,\gamma}(r_{c,\gamma})}4tRe\Big(\frac{u^2[r_{c,\gamma}+i\gamma]}{\sqrt{1-u^2[r_{c,\gamma}+i\gamma]^2}}\Big) \\
&+ \int_{Q^{(-)}}^{Q^{(+)}} dk \widetilde{Q}^{(2,*)}(k) 2t\sin k
\end{aligned}
$$

$$- \sum_{\gamma=1} \int_{r_{c,\gamma}^{(-)}}^{r_{c,\gamma}^{(+)}} dr \bar{Q}_{c,\gamma}^{(2,*)}(r) 4tRe\Big(\frac{u^2[r+i\gamma]}{\sqrt{1-u^2[r+i\gamma]^2}}\Big)\Big\}\,. \tag{B.12}$$

Inserting the suitable functions in the rhs of Eq. (B.12), performing some integrations by using symmetry properties of the kernels of the integral equation (A.28)-(A.30) and (A.48)-(A.50), and replacing deviations by pseudomomentum normal-ordered operators (4.20) we find after some algebra expression (4.49). Note that replacing in Eq. (4.49) the function $X_{\alpha,\gamma}^{(1)}(q)$ by the associate function $Q_{\alpha,\gamma}^{(1)}(q)$ leads to the same result. By the use of Eq. (4.34) expression (4.42) can be rewritten in terms of the $f$ functions (4.50) as given in the rhs of Eq. (4.42).

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# Chapter 5

# Excitations and Finite-Size Effects

## 5.1 Introduction

In this Chapter we introduce the quasiparticle concept for the 1D Hubbard Model. Exception made to Secs. 5.4 and 5.5, we deal in this Chapter with LWS's I/HWS's I only. As we shall see, these quasiparticles have not exactly the same physical meaning as in Fermi-liquid theory [1, 2, 3, 4, 5]. In the latter theory, the quasiparticle concept is used to describe low-energy excitations at constant or variable electronic and magnetization densities, $n$ and $m$, respectively. The quasiparticle in a Fermi-liquid is related to the electronic operators trought a factor $Z$ –the renormalization factor. The value of $Z$ is determined by the electronic correlations.

In our Landau-liquid description of the Hubbard chain the quasiparticles do not describe the elementary excitations at constant $n$ and $m$. These are described by the $\alpha$ pseudoholes and by the $\alpha, \gamma$ heavy-pseudoparticles, introduced in Chapter 3. In contrast, excitations that change $n$ and $m$ are described by composite objects of pseudoholes, that we call (in this restricted Fermi-liquid sense) quasiparticles. Due to the non-perturbative character of the one-dimensional many-body problem [6, 7, 8], the renormalization factor that connects the quasiparticle and electronic operators vanishes as the Fermi points are approached [9].

The quasiparticle operator is defined as the generator of a ground-state–ground-state transition involving the addition or removal of one electron to or from the many-body ground state. We find that the quasiparticle momentum equals the expected electronic momentum $k = \pm k_{F\sigma}$. It is the combined momenta (i) from the addition or removal of pseudoparticles and (ii) from the global pseudomomentum shifts of $\pm\pi/N_a$ which leads to this final result. This type of pseudomomentum shifts

are also present in excitations connecting the ground state and LWS's II (or HWS's II). We will illustrate the importance of these momentum shifts [10, 11] in the limits $n = 1$ and $U/4t^2 \gg 1$, where the model is closely related to the anti-ferromagnetic Heisenberg chain.

## 5.2 Ground-state – ground-state topological excitations

The quasiparticle operator, $\tilde{c}^{\dagger}_{k_{F\sigma},\sigma}$, creates one quasiparticle with spin projection $\sigma$ and momentum $k_{F\sigma}$. As in Fermi liquid theory, such operator is the generator of the following ground-state–ground-state transition

$$\tilde{c}^{\dagger}_{k_{F\sigma},\sigma}|GS; N_{\sigma}, N_{-\sigma}\rangle = |GS; N_{\sigma}+1, N_{-\sigma}\rangle \, . \tag{5.1}$$

The quasiparticle operator defines a one-to-one correspondence between the addition of one electron to the system and the creation of one quasiparticle. The momentum of the ground states $|GS; N_{\sigma}, N_{-\sigma}\rangle$ associated with canonical ensembles of U(1)⊗U(1) symmetryis given in Table 5.1. Since we are studying ground-state–ground-state transitions, $\alpha, \gamma > 1$ heavy-pseudoparticles are not involved.

| | $(-1,-1)$ | $(-1,1)$ | $(1,-1)$ | $(1,1)$ |
|---|---|---|---|---|
| (A) $P$ | $\pm 2k_F$ | $\pm 2k_F$ | $\pm[2\pi - 2k_F]$ | $\pm[2\pi - 2k_F]$ |
| (B) $P$ | $\pm k_{F\uparrow}$ | $\pm k_{F\uparrow}$ | $\pm k_{F\uparrow}$ | $\pm k_{F\uparrow}$ |
| (C) $P$ | $\pm k_{F\downarrow}$ | $\pm k_{F\downarrow}$ | $\pm k_{F\downarrow}$ | $\pm k_{F\downarrow}$ |
| (D) $P$ | 0 | 0 | 0 | 0 |

Table 5.1: Values of the ground-state momentum in the four $(l, l')$ sectors of Hamiltonian symmetry $U(1)\otimes U(1)$. The different momentum values correspond to the following parities of the numbers $\bar{N}_{s,0}$ and $N_{s,0}$, respectively: (A) even, even; (B) even, odd; (C) odd, even; and (D) odd, odd. In the case of the $(1, \pm 1)$ sectors, if $k_{F\sigma} > \pi$ then $\pm k_{F\sigma}$ should be replaced by the first-Brillouin-zone momenta $\pm[2\pi - k_{F\sigma}]$.

The study of the ground-state momentum (3.32) confirms that the relative momentum of ground states differing in the number of $\sigma$ electrons by one equals the $U = 0$ Fermi points, ie $\Delta P = \pm k_{F\sigma}$.

It is interesting to study the expression of the $\sigma$ quasiparticle and quasihole operators in the $\alpha,\beta$ pseudohole basis for all sectors of Hamiltonian symmetry. Since we are discussing the problem of addition or removal of one particle, the boundary conditions (3.12) and (3.13) play a crucial role. When we add or remove one electron from the many-body system we have to consider the transitions between states with integer and half-integer quantum numbers $I_j^{\alpha,0}$. The transition between two ground states differing in the number of electrons by one is then associated with two different processes: a backflow in the Hilbert space of the $\alpha,\beta$ pseudoholes with a shift of all the pseudomomenta by $\pm\frac{\pi}{N_a}$ and the creation and (or) annihilation of one pair of $c$ and $s$ pseudoholes at the pseudo-Fermi points (or at the limit of the pseudo-Brillouin zone for the $s$ pseudohole).

The backflow associated with a shift of all the pseudomomenta by $\pm\frac{\pi}{N_a}$ is described by a topological unitary operator such that

$$V_\alpha^{\pm} a^\dagger_{q,\alpha,\beta} V_\alpha^{\mp} = a^\dagger_{q\mp\frac{\pi}{N_a},\alpha,\beta}\,. \tag{5.2}$$

Obviously, the pseudohole vacuum $|V\rangle$ is invariant under this operator, this is $V_\alpha^{\pm}|V\rangle = |V\rangle$. It is simple to find that $V_\alpha^{\pm}$ reads

$$V_\alpha^{\pm} = \exp\left\{-\sum_{q,\beta} a^\dagger_{q\pm\frac{\pi}{N_a},\alpha,\beta} a_{q,\alpha,\beta}\right\}\,. \tag{5.3}$$

The structure of this operator reveals that the pseudomomentum of all pseudoholes are translated by $\pm\pi/N_a$. Adding all pseudohole contributions gives a large momentum. This large-momentum excitation induced by the operator (5.3) is the $\alpha$ topological momentum shift. Note that in the present case of the Hilbert subspace spanned by the states I of the $(l,l')$ sector only the value $\beta=\frac{l}{2}$ for $\alpha=c$ and the value $\beta=\frac{l'}{2}$ for $\alpha=s$ contributes to the $\beta$ summation of Eq. (5.3)

In addition to the topological momentum shift, the quasiparticle or quasihole excitation includes creation and (or) annihilation of pseudoholes. The changes in the pseudohole and pseudoparticle numbers and the corresponding changes in the values of $S^c$, $S^c_z$, $S^s$, and $S^s_z$ are given in Tables 5.2 and 5.3 for the ground-state – ground-state transitions $(N_\uparrow,N_\downarrow)\rightarrow(N_\uparrow\pm 1,N_\downarrow)$ and $(N_\uparrow,N_\downarrow)\rightarrow(N_\uparrow,N_\downarrow\pm 1)$, respectively.

We consider below the expressions for the quasiparticles $\tilde{c}^\dagger_{k_{F\uparrow},\uparrow}$ and $\tilde{c}^\dagger_{k_{F\downarrow},\downarrow}$ associated with the transitions $(N_\uparrow,N_\downarrow)\rightarrow(N_\uparrow+1,N_\downarrow)$ and $(N_\uparrow,N_\downarrow)\rightarrow(N_\uparrow,N_\downarrow+1)$, respectively, and the quasiholes $\tilde{c}_{k_{F\uparrow},\uparrow}$ and $\tilde{c}_{k_{F\downarrow},\downarrow}$ associated with the transitions $(N_\uparrow,N_\downarrow)\rightarrow(N_\uparrow-1,N_\downarrow)$ and $(N_\uparrow,N_\downarrow)\rightarrow(N_\uparrow,N_\downarrow-1)$, respectively.

| | $(-1,-1)$ | $(-1,1)$ | $(1,-1)$ | $(1,1)$ |
|---|---|---|---|---|
| $\Delta N_c^h$ | $\mp 1$ | $\mp 1$ | $\pm 1$ | $\pm 1$ |
| $\Delta N_c$ | $\pm 1$ | $\pm 1$ | $\mp 1$ | $\mp 1$ |
| $\Delta N_c^*$ | 0 | 0 | 0 | 0 |
| $\Delta N_s^h$ | $\pm 1$ | $\mp 1$ | $\pm 1$ | $\mp 1$ |
| $\Delta N_s$ | 0 | $\pm 1$ | $\mp 1$ | 0 |
| $\Delta N_s^*$ | $\pm 1$ | 0 | 0 | $\mp 1$ |
| $\Delta S^c$ | $\mp 1/2$ | $\mp 1/2$ | $\pm 1/2$ | $\pm 1/2$ |
| $\Delta S_z^c$ | $\pm 1/2$ | $\pm 1/2$ | $\pm 1/2$ | $\pm 1/2$ |
| $\Delta S^s$ | $\pm 1/2$ | $\mp 1/2$ | $\pm 1/2$ | $\mp 1/2$ |
| $\Delta S_z^s$ | $\mp 1/2$ | $\mp 1/2$ | $\mp 1/2$ | $\mp 1/2$ |

Table 5.2: Changes in the numbers of pseudoholes, pseudoparticles, pseudoparticle orbitals, and in the values of $S^c$, $S_z^c$, $S^s$, and $S_z^s$ in the ground-state–ground-state transition $(N_\uparrow, N_\downarrow) \rightarrow (N_\uparrow \pm 1, N_\downarrow)$.

We emphasize that because the initial ground state for the above two quasiparticles and two quasiholes is the same, the $\sigma$ quasiparticle and $\sigma$ quasihole momenta differ by $\pm\frac{2\pi}{N_a}$. Therefore, the corresponding quasiparticle and quasihole expressions are not related by an adjunt transformation. On the other hand, the operators $\tilde{c}^\dagger_{\pm k_{F\sigma},\sigma}$ and $\tilde{c}_{\pm k_{F\sigma},\sigma}$ associated with the transitions $(N_\sigma, N_{-\sigma}) \rightarrow (N_\sigma + 1, N_{-\sigma})$ and $(N_\sigma+1, N_{-\sigma}) \rightarrow (N_\sigma, N_{-\sigma})$ are obviously related by such transformation. In this case the initial (final) ground state of the electrons (holes) is the final (initial) ground state of the holes (electrons). Moreover, let us consider the set of four operators $\tilde{c}^\dagger_{\pm k_{F\uparrow},\uparrow}$, $\tilde{c}_{\pm k_{F\uparrow},\uparrow}$, $\tilde{c}^\dagger_{\pm k_{F\downarrow},\downarrow}$, and $\tilde{c}_{\pm k_{F\downarrow},\downarrow}$ such that the creation operators act on the same initial ground state $(N_\uparrow, N_\downarrow)$ transforming it in the ground states $(N_\uparrow + 1, N_\downarrow)$ and $(N_\uparrow, N_\downarrow + 1)$, respectively, and the hole operators act on the corresponding latter states giving rise to the original ground state. Let us consider the reduced Hilbert subspace spanned by these three ground states. If we combine that with the electron and hole expressions introduced below, it is easy to show that the corresponding quasiparticle and quasihole operators $\tilde{c}^\dagger_{\pm k_{F\uparrow},\uparrow}$, $\tilde{c}_{\pm k_{F\uparrow},\uparrow}$, $\tilde{c}^\dagger_{\pm k_{F\downarrow},\downarrow}$, and $\tilde{c}_{\pm k_{F\downarrow},\downarrow}$ obey the usual anticommutation relations.

The two electrons and two holes refer to the same initial ground state. The pseudo-Fermi points and pseudohole-Fermi points of the expressions below refer to that initial ground state. On the other hand, $s$ pseudohole creation and annihilation

| | $(-1,-1)$ | $(-1,1)$ | $(1,-1)$ | $(1,1)$ |
|---|---|---|---|---|
| $\Delta N_c^h$ | $\mp 1$ | $\mp 1$ | $\pm 1$ | $\pm 1$ |
| $\Delta N_c$ | $\pm 1$ | $\pm 1$ | $\mp 1$ | $\mp 1$ |
| $\Delta N_c^*$ | 0 | 0 | 0 | 0 |
| $\Delta N_s^h$ | $\mp 1$ | $\pm 1$ | $\mp 1$ | $\pm 1$ |
| $\Delta N_s$ | $\pm 1$ | 0 | 0 | $\mp 1$ |
| $\Delta N_s^*$ | 0 | $\pm 1$ | $\mp 1$ | 0 |
| $\Delta S^c$ | $\mp 1/2$ | $\mp 1/2$ | $\pm 1/2$ | $\pm 1/2$ |
| $\Delta S_z^c$ | $\pm 1/2$ | $\pm 1/2$ | $\pm 1/2$ | $\pm 1/2$ |
| $\Delta S^s$ | $\mp 1/2$ | $\pm 1/2$ | $\mp 1/2$ | $\pm 1/2$ |
| $\Delta S_z^s$ | $\pm 1/2$ | $\pm 1/2$ | $\pm 1/2$ | $\pm 1/2$ |

Table 5.3: Changes in the numbers of pseudoholes, pseudoparticles, pseudoparticle orbitals, and in the values of $S^c$, $S_z^c$, $S^s$, and $S_z^s$ in the ground-state – ground-state transition $(N_\uparrow, N_\downarrow) \rightarrow (N_\uparrow, N_\downarrow \pm 1)$.

operators at the limits of the pseudo-Brillouin zones refer to the final and initial ground states, respectively. In the case of the $(l, l')$ sectors of Hamiltonian symmetry $U(1) \otimes U(1)$ we consider that the initial and final ground states belong the same sector of parameter space. In the case of the $(l')$ sectors of Hamiltonian symmetry $SU(2) \otimes U(1)$ [or $(l)$ sectors of Hamiltonian symmetry $U(1) \otimes SU(2)$] we consider that the initial and final ground states belong to sectors of parameter space characterized by the same value of $(l')$ [or $(l)$]. We present below the electron and hole expressions found for different initial ground states in the nine sectors of parameter space. It is useful to introduce the pseudohole-Fermi point $\bar{q}_{F\alpha}^{(\pm)}$ such that $\bar{q}_{F\alpha}^{(\pm)} = q_{F\alpha}^{(\pm)} \pm 2\pi/N_a$

For initial ground states in the $(-1,-1)$ sector of Hamiltonian symmetry $U(1) \otimes U(1)$ we find

$$\tilde{c}^\dagger_{\pm k_{F\uparrow},\uparrow} = a_{\bar{q}^{(\pm)}_{Fc},c,-\frac{1}{2}} V_s^{\pm} a^\dagger_{q_s^{(\pm)},s,-\frac{1}{2}}\,, \qquad \tilde{c}^\dagger_{\pm k_{F\downarrow},\downarrow} = V_c^{\pm} a_{\bar{q}^{(\pm)}_{Fc},c.-\frac{1}{2}} a_{\bar{q}^{(\pm)}_{Fs},s,-\frac{1}{2}}\,, \tag{5.4}$$

for the electrons and

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = a^\dagger_{q^{(\pm)}_{Fc},c,-\frac{1}{2}} V_s^{\mp} a_{q_s^{(\pm)},s,-\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^\dagger_{q^{(\pm)}_{Fc},c,-\frac{1}{2}} a^\dagger_{q^{(\pm)}_{Fs},s,-\frac{1}{2}}\,, \tag{5.5}$$

for the holes.

For the $(-1,1)$ sector we find

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = V_c^{\pm} a_{\bar{q}^{(\pm)}_{Fc},c,-\frac{1}{2}} a_{\bar{q}^{(\pm)}_{Fs},s,\frac{1}{2}}\,, \qquad \tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = a_{\bar{q}^{(\pm)}_{Fc},c,-\frac{1}{2}} V_s^{\pm} a^{\dagger}_{q^{(\pm)}_s,s,\frac{1}{2}}\,, \tag{5.6}$$

for the electrons and

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,-\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = a^{\dagger}_{q^{(\pm)}_{Fc},c,-\frac{1}{2}} V_s^{\mp} a_{q^{(\pm)}_s,s,\frac{1}{2}}\,, \tag{5.7}$$

for the holes.

In the $(1,-1)$ sector the result is

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,-\frac{1}{2}}\,, \qquad \tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} V_s^{\mp} a_{q^{(\pm)}_s,s,-\frac{1}{2}}\,, \tag{5.8}$$

for the electrons and

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = V_c^{\pm} a_{\bar{q}^{(\pm)}_{Fc},c,\frac{1}{2}} a_{\bar{q}^{(\pm)}_{Fs},s,-\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = a_{\bar{q}^{(\pm)}_{Fc},c,\frac{1}{2}} V_s^{\pm} a^{\dagger}_{q^{(\pm)}_s,s,-\frac{1}{2}}\,, \tag{5.9}$$

for the holes.

The expressions for the $(1,1)$ sector are

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} V_s^{\mp} a^{\dagger}_{q^{(\pm)}_s,s,\frac{1}{2}}\,, \qquad \tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,\frac{1}{2}}\,, \tag{5.10}$$

for the electrons and

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = a_{\bar{q}^{(\pm)}_{Fc},c,\frac{1}{2}} V_s^{\pm} a_{q^{(\pm)}_s,s,\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_c^{\pm} a_{\bar{q}^{(\pm)}_{Fc},c,\frac{1}{2}} a_{\bar{q}^{(\pm)}_{Fs},s,\frac{1}{2}}\,, \tag{5.11}$$

for the holes.

According to Eqs. (5.4)-(5.11) the $\sigma$ quasiparticles and quasiholes are many-pseudohole objects which recombine the colors $c$ and $s$ (charge and spin in the limit $m = n_{\uparrow} - n_{\downarrow} \to 0$) giving rise to spin projection $\uparrow$ and $\downarrow$ and have Fermi surfaces at $\pm k_{F\sigma}$.

Similar expressions can be derived for the sectors of parameter space where the Hamiltonian (4.19) has higher symmetry. We start by considering the sectors of Hamiltonian symmetry $SU(2) \otimes U(1)$ where

$$q_{Fc}^{(+)} = -q_{Fc}^{(-)} = q_c^{(+)} = -q_c^{(-)} = \pi[1 - \frac{1}{N_a}]\,. \tag{5.12}$$

For ground states of the $l' = -1$ sector of Hamiltonian symmetry $SU(2) \otimes U(1)$ the electrons read

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,\frac{1}{2}} a^{\dagger}_{q_{Fs}^{(\pm)},s,-\frac{1}{2}}\,, \qquad \tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = a^{\dagger}_{q_{Fc}^{(\pm)},c,\frac{1}{2}} V_s^{\mp} a_{q_s^{(\pm)},s,-\frac{1}{2}}\,, \tag{5.13}$$

and the holes read

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = a^{\dagger}_{q_{Fc}^{(\pm)},c,-\frac{1}{2}} V_s^{\mp} a_{q_s^{(\pm)},s,-\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,-\frac{1}{2}} a^{\dagger}_{q_{Fs}^{(\pm)},s,-\frac{1}{2}}\,. \tag{5.14}$$

For the $l' = 1$ sector of Hamiltonian symmetry $SU(2) \otimes U(1)$ the electrons read

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = a^{\dagger}_{q_{Fc}^{(\pm)},c,\frac{1}{2}} V_s^{\mp} a^{\dagger}_{q_s^{(\pm)},s,\frac{1}{2}}\,, \qquad \tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,\frac{1}{2}} a^{\dagger}_{q_{Fs}^{(\pm)},s,\frac{1}{2}}\,, \tag{5.15}$$

and the holes read

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,-\frac{1}{2}} a^{\dagger}_{q_{Fs}^{(\pm)},s,\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_s^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,-\frac{1}{2}} a_{q_s^{(\pm)},s,\frac{1}{2}}\,. \tag{5.16}$$

In the sectors of Hamiltonian symmetry $U(1) \otimes SU(2)$ we have that

$$q_{Fs}^{(+)} = -q_{Fs}^{(-)} = q_s^{(+)} = -q_s^{(-)} = \pi[\frac{n}{2} - \frac{1}{N_a}]\,. \tag{5.17}$$

In the case of the $l = -1$ sector of Hamiltonian symmetry $U(1) \otimes SU(2)$ the up-spin electron and hole read

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = V_c^{\pm} a_{\bar{q}_{Fc}^{(\pm)},c,-\frac{1}{2}} a^{\dagger}_{q_s^{(\pm)},s,\frac{-1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,-\frac{1}{2}} a^{\dagger}_{q_s^{(\pm)},s,\frac{1}{2}}\,, \tag{5.18}$$

and the down-spin electron and hole read

$$\tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = V_c^{\pm} a_{\bar{q}_{Fc}^{(\pm)},c,-\frac{1}{2}} a^{\dagger}_{\bar{q}_s^{(\pm)},s,\frac{1}{2}}\,, \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q_{Fc}^{(\pm)},c,-\frac{1}{2}} a^{\dagger}_{q_s^{(\pm)},s,-\frac{1}{2}}\,. \tag{5.19}$$

For the $l = 1$ sector of Hamiltonian symmetry $U(1) \otimes SU(2)$ the up-spin electron and hole read

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{s},s,-\frac{1}{2}} , \qquad \tilde{c}_{\pm k_{F\uparrow},\uparrow} = V_c^{\pm} a_{\bar{q}^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{s},s,\frac{1}{2}} , \tag{5.20}$$

and the down-spin electron and hole read

$$\tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{s},s,\frac{1}{2}} , \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_c^{\pm} a_{\bar{q}^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{s},s,\frac{-1}{2}} . \tag{5.21}$$

Finally, for the $SO(4)$ initial ground state both Eq. (49) and the following equation

$$q^{(+)}_{Fs} = -q^{(-)}_{Fs} = q^{(+)}_{s} = -q^{(-)}_{s} = \pi[\frac{1}{2} - \frac{1}{N_a}] , \tag{5.22}$$

hold true and we find for the electrons

$$\tilde{c}^{\dagger}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,-\frac{1}{2}} , \qquad \tilde{c}^{\dagger}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,\frac{1}{2}} , \tag{5.23}$$

and for the holes

$$\tilde{c}_{\pm k_{F\uparrow},\uparrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,-\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,\frac{1}{2}} , \qquad \tilde{c}_{\pm k_{F\downarrow},\downarrow} = V_c^{\mp} a^{\dagger}_{q^{(\pm)}_{Fc},c,-\frac{1}{2}} a^{\dagger}_{q^{(\pm)}_{Fs},s,-\frac{1}{2}} . \tag{5.24}$$

Equations (5.23)-(5.24) reveal that removing or adding electrons from the $SO(4)$ ground state always involves creation of pseudoholes. Furthermore, while in the case of the $(l, l')$ sectors the initial and final ground states belong in general to the same sector, in the case of the SO(4) ground state each of the four possible transitions associated with adding one up-spin or one down-spin quasiparticle or quasihole leads to four ground states belonging to a different $(l, l')$ sector. If the initial ground state belongs to the $(l')$ $SU(2) \otimes U(1)$ sector [or to the $(l)$ $U(1) \otimes SU(2)$ sector] then two of the final ground states belong to the $(1, l')$ [or to the $(l, 1)$] sector and the remaining two ground states to the $(-1, l')$ [or to the $(l, -1)$] sector.

## 5.3 Low-energy excitations and symmetry

Given a ground state with electron numbers $(N_\sigma, N_{-\sigma})$, we find in this section that the set of all pseudoholes of different type which constitute, in pairs, the $\uparrow$ and $\downarrow$ electrons and $\uparrow$ and $\downarrow$ holes associated with the ground-state transitions $(N_\uparrow, N_\downarrow) \rightarrow$

$(N_\uparrow \pm 1, N_\downarrow)$ and $(N_\uparrow, N_\downarrow) \rightarrow (N_\uparrow, N_\downarrow \pm 1)$ transform as the symmetry group of the Hamiltonian (4.19) in the corresponding sector of parameter space.

Equations (3.7) tell us that the values of $S^c$ and $S^c_z$ are fully determined by the number of $c, \beta$ pseudoholes whereas the number of $s, \beta$ pseudoholes determines the values of $S^s$ and $S^s_z$. In addition, note that the quasiparticle and quasihole operators (5.4)-(5.11), (5.13)-(5.16), (5.18)-(5.21), and (5.23)-(5.24) involve always a change in the number of $c$ and $s$ pseudoholes by one. Moreover, when acting on the suitable ground state these operators change the values of $S^c$ and $S^c_z$ by $\pm 1/2$ and $\pm sgn(S^c_z)1/2$, respectively, and the values of $S^s$ and $S^s_z$ by $\pm 1/2$ and $\pm sgn(S^s_z)1/2$, respectively. (The corresponding changes in the pseudohole numbers and in the values of $S^c$, $S^c_z$, $S^s$, and $S^s_z$ are shown in Tables 5.2 and 5.3.) The analysis of the changes in the pseudohole numbers could lead to the conclusion that the $c, \pm\frac{1}{2}$ pseudoholes have quantum numbers $(S^c = 1/2; S^s = 0; S^c_z = \pm 1/2; S^s_z = 0)$ and that the $s, \mp\frac{1}{2}$ pseudoholes have quantum numbers $(S^c = 0; S^s = 1/2; S^c_z = 0; S^s_z = \pm 1/2)$. If this was true the $c$ and corresponding $\beta$ pseudohole quantum numbers could be identified with $S^c$ and $S^c_z$ for $S^c = 1/2$ and $S^c_z = \pm 1/2$, respectively, and the $s$ and corresponding $\beta$ pseudohole quantum numbers could be identified with $S^s$ and $S^s_z$ for $S^s = 1/2$ and $S^s_z = \pm 1/2$, respectively. (Note that $S^\alpha$ and $S^\alpha_z$ do not refer to the whole many-electron sustem but to a single electron) However, this is not in general true. This holds true in the particular case of zero-momentum number operators. On the other hand, the above identities are also true for finite-momentum operators for $c, \pm\frac{1}{2}$ in the limit of zero chemical potential and for $s, \pm\frac{1}{2}$ in the limit of zero magnetic field, as we find below.

In order to confirm that the above equivalences are not in general true for finite-momentum fluctuations, we consider the $\alpha$-pseudohole fluctuation operator [12, 13]

$$\rho_\alpha(k) = -\sum_{q,\beta} \beta a^\dagger_{q,\alpha,\beta} a_{q+k,\alpha,\beta} \,, \tag{5.25}$$

and the $S^c_z$- (charge) and $S^s_z$- (spin) fluctuation operators

$$\rho_{S^c_z}(k) = \sum_{k',\sigma} \left[ \frac{1}{2}\delta_{k,o} - c^\dagger_{k'+k,\sigma} c_{k',\sigma} \right] , \tag{5.26}$$

and

$$\rho_{S^s_z}(k) = \sum_{k',\sigma} \sigma c^\dagger_{k'+k,\sigma} c_{k',\sigma} \,, \tag{5.27}$$

respectively. From Eqs. (3.7) and (3.26) we find

$$\rho_c(0) = \rho_{S_z^c}(0) = N_a - N_\uparrow - N_\downarrow \, , \tag{5.28}$$

and

$$\rho_s(0) = \rho_{S_z^s}(0) = N_\uparrow - N_\downarrow \, . \tag{5.29}$$

We then conclude that at zero momentum the above equivalences hold true. The electron numbers $N_\uparrow$ and $N_\downarrow$ are good quantum numbers of the many-electron system. Since the exact Hamiltonian eigenstates are simple Slater determinants of $\alpha, \beta$-pseudohole levels, the numbers of $\alpha, \beta$ pseudoholes are thus required to be also good quantum numbers. They are such that Eqs. (5.28) and (5.29) are obeyed.

On the other hand, the conservation of electron and pseudohole numbers does not require the finite-momentum $c$ and $s$ fluctuations being bare finite-momentum charge and spin fluctuations, respectively. For simplicity, we consider the smallest momentum values, $k \pm \frac{2\pi}{N_a}$. We emphasize that for $k = \pm\frac{2\pi}{N_a}$, acting the operator $\rho_\alpha(k)$ onto a ground state of general form (3.43) generates a sinlge-pair $\alpha$-pseudoparticle-pseudohole excitation where the $\alpha, \beta$ pseudohole at $q = \bar{q}_{F\alpha}^{(\pm)}$ moves to $q = q_{F\alpha}^{(\pm)}$. If in $c, \beta$ the color $c$ was eta spin and $\beta = S_z^c$ and in $s, \beta$ the color $s$ was spin and $\beta = S_z^s$, we should have that $\rho_c(\pm\frac{2\pi}{N_a}) = \rho_{S_z^c}(\pm\frac{2\pi}{N_a})$ and $\rho_s(\pm\frac{2\pi}{N_a}) = \rho_{S_z^s}(\pm\frac{2\pi}{N_a})$, respectively. However, the results of the works [12, 13] show that this is not true for the sectors of Hamiltonian symmetry $U(1) \otimes U(1)$. Altough the pseudohole summations of Eqs. (3.7) and (3.26) give $S^c$, $S^s$, $S_z^c$, and $S_z^s$ this does not require each $c$ pseudohole having $\eta$ spin 1/2 and spin 0 and each $s$ pseudohole having $\eta$ spin 0 and spin 1/2. Also, the fact that the quasiparticle or quasihole of Eqs. $(5.4) - (5.11)$, $(50) - (5.16)$, $(5.18) - (58)$, and $(5.23) - (5.24)$ has $S^c = 1/2; S^s = 1/2; S_z^c = sgn(S_z^c)1/2; S_z^s = sgn(S_z^s)1/2$ does not tell how these values are destributed by the corresponding $c$ pseudohole, $s$ pseudohole, and topological momentum shifts.

The studies of the works [12, 13] reveal that for finite values of the chemical potential and magnetic field there is a $c$ and $s$ separation of the low-energy and small-momentum excitations but that the orthogonal modes $c$ and $s$ are not in general charge and spin, respectively [12, 13]. On the other hand, these studies have found that in the limit of zero chemical potential the finite-momentum $c$ fluctuations become real charge excitations and that in the limit of zero magnetic field the finite-momentum $s$ fluctuations become real spin excitations. In the latter limit the $c$ excitations are also real charge excitations and the $c$ and $s$ low-energy separation

becomes the usual charge and spin separation [6, 7, 8].

It follows that in the case of the SO(4) canonical ensemble the set of pseudoholes involved in the description of the two electron and two hole operators (5.23)-(5.24), which are the $c, +\frac{1}{2}$; $c, -\frac{1}{2}$; $s, +\frac{1}{2}$; and $s, -\frac{1}{2}$ pseudoholes at the pseudo-Fermi points, transform in the $S^c = 1/2$ and $S^s = 1/2$ representation of the SO(4) group. Moreover, it can be shown from the changes in the BA quantum numbers and from the study of the pseudohole energies that the $S^c = 1/2$ and $S^s = 1/2$ elementary excitations studied Essler *et al.* [14] are simple combinations of one of the ground-state – ground-state transitions generated by the operators (5.23)-(5.24) with a single pseudoparticle-pseudohole process relative to the final ground state. In addition, the usual half-filling holons and zero-magnetization spinons can be shown to be limiting cases of our pseudohole excitations. For instance, the $(S^c = 1/2; S^s = 0; S^c_z = 1/2; S^s_z = 0)$ anti holon and $(S^c = 1/2; S^s = 0; S^c_z = -1/2; S^s_z = 0)$ holon excitations [14] are at lowest energy generated from the SO(4) ground state by the operators $V_c^- a^\dagger_{q^{(\pm)}_{Fc},c,\frac{1}{2}}$ and $V_c^+ a^\dagger_{q^{(\pm)}_{Fc},c,-\frac{1}{2}}$, respectively. Also at lowest energy, the two $(S^c = 0; S^s = 1/2; S^c_z = 0; S^s_z = 1/2)$ and $(S^c = 0; S^s = 1/2; S^c_z = 0; S^s_z = -1/2)$ spinons [14] are generated from that ground state by the operators $a^\dagger_{q^{(\pm)}_{Fs},s,-\frac{1}{2}}$ and $a^\dagger_{q^{(\pm)}_{Fs},s,\frac{1}{2}}$, respectively. The full spectrum of these excitations is obtained by adding to these generators a suitable single pseudoparticle-pseudohole-pair operator.

Since the $SO(4)$ symmetry only allows Hamiltonian eigenstates with integer values of $S^c_z + S^s_z$, the holon – spinon pairs of Eqs. (5.23)-(5.24) cannot be separated. This also holds true in the general case, the electron being constituted by one $c$ pseudohole, one $s$ pseudohole, and one many-pseudohole topological momentum shift of large momentum, as confirmed by Eqs. (5.4)-(5.11), (5.13)-(5.16), and (5.18)-(5.21). Also in this case the fact that only Hamiltonian eigenstates with integer values of $S^c_z + S^s_z$ are allowed prevents these three excitations from being separated.

As for the SO(4) ground state, we can relate the symmetry of the Hamiltonian (4.19) in a given canonical ensemble by looking at the pseudohole contents of the corresponding two electrons and two holes of Eqs. (5.4)-(5.11), (5.13)-(5.16), and (5.18)-(5.21). For instance, Eqs. (5.4)-(5.11) show that in the $(l, l')$ sectors of Hamiltonian symmetry $U(1) \otimes U(1)$ the two electrons and two holes involve one pair of the same type of pseudoholes, namely the corresponding $c, \frac{l}{2}$ and $s, \frac{l'}{2}$ pseudoholes. Each of these transforms in the representation of the group $U(1)$ and, therefore, the set of two pseudoholes transforms in the representation of the group $U(1) \otimes U(1)$.

In the case of the $(l')$ sectors of Hamiltonian symmetry $SU(2) \otimes U(1)$ $c$ is $\eta$ spin

and the corresponding quantum number $\beta$ is $S_z^c$ and Eqs. (5.13)-(5.16) confirm that the two electrons and holes involve either one $c, \frac{1}{2}$ pseudohole or one $c, -\frac{1}{2}$ pseudohole combined with one $s, \frac{l'}{2}$ pseudohole. The $c, \frac{1}{2}$ and $c, -\frac{1}{2}$ pseudoholes transform in the $S^c = 1/2$ representation of the $\eta$-spin $SU(2)$ group, whereas the $s, \frac{l'}{2}$ pseudohole transforms in the representation of the $U(1)$ group. Therefore, the set of $c, \frac{1}{2}$; $c, -\frac{1}{2}$; and $s, \frac{l'}{2}$ pseudoholes transforms in the $S^c = 1/2$ representation of the $SU(2) \otimes U(1)$ group.

In the case of the $(l)$ sectors of Hamiltonian symmetry $U(1) \otimes SU(2)$ $s$ is spin and the corresponding quantum number $\beta$ is $\beta = S_z^s$ and Eqs. (5.18)-(5.21) show that the two electrons and two holes are constituted by either one $s, \frac{1}{2}$ or one $s, -\frac{1}{2}$ pseudohole combined with one $c, \frac{l}{2}$ pseudohole. The $s, \frac{1}{2}$ and $s, -\frac{1}{2}$ pseudoholes transform in the $S^s = 1/2$ representation of the spin $SU(2)$ group and the $c, \frac{l}{2}$ pseudohole transforms in the representation of the $U(1)$ group. It follows that the set of the $c, \frac{l}{2}$; $s, \frac{1}{2}$; and $s, -\frac{1}{2}$ pseudoholes transforms in the $S^s = 1/2$ representation of the $U(1) \otimes SU(2)$ group.

## 5.4 Finite-energy topological momentum-shift operators

The simple form of the GGS expression (3.38), GS expressions (3.43)-(3.45), and of the general-Hamiltonian eigenstates (3.18) introduced in Chapter 3 has a deep physical meaning. It reveals that in the present basis these eigenstates of the many-electron quantum problem are "non-interacting" states of simple Slater-determinant form. However, that the numbers $I_j^{\alpha,\gamma}$ of the rhs of Eq. (28) can be integers or half-odd integers for different Hamiltonian eigenstates, makes the problem much more involved than a simple non-interacting case. This change in the integer or half-odd integer character of some of the numbers $I_j^{\alpha,\gamma}$ of two states, shifts *all* the occupied pseudomomenta. As in the case of last section, transition between a GS (46) and *any* eigenstate (3.18) can be separated into two types of excitations: (a) a topological GS – GGS transition which involves the creation or annihilation of pseudoholes and (or) heavy pseudoparticles as well as the occurrence of topological momentum shifts and (b) a *Landau-liquid* excitation associated with pseudoparticle - pseudohole processes relative to the GGS.

The topological transitions (a) are basically superpositions of three kinds of elementary transitions: (i) GS - GS transitions involving changes in the $\sigma$ electron

numbers by one, (ii) single $\beta$ flip processes of $\alpha, \beta$ pseudoholes which lead to non-LWS's and non-HWS's outside the BA, and (iii) creation of single $\alpha, \gamma$ pseudoparticles at constant values of $S^c$, $S^c_z$, $S^s$, and $S^s_z$. While the transitions (i) are gapless, the elementary excitations (ii) and (iii) require a finite amount of energy.

The generators of the excitations (i) were studied in the previous section and in the work [11] and the ones of (ii) involve only topological momentum shifts and $\beta$ flips (which describe either creation of electron pairs or spin flip processes). Consider as an example of a transition (iii) the creation of one $c, \gamma$ pseudoparticle which is found to be the relevant process for the finite-frequency conductivity [15]. (We examine here explicitly topological momentum shifts of occupied bands only, *i.e.* these which generate momentum.) When $\gamma > 0$ is even (or odd) the generator reads $V_c^{\pm 1} G_{c,\gamma}$ (or $G_{c,\gamma} V_s^{\pm 1}$), where the topological-momentum-shift operator was defined above and

$$G_{c,\gamma} = [\hat{S}^c_+]^\gamma \prod_{q=q^{(-)}_{Fc,0}}^{q^{(-)}_{Fc,0}+\frac{2\pi}{Na}(\gamma-1)} \prod_{q^{(+)}_{Fc,0}-\frac{2\pi}{Na}(\gamma-1)}^{q^{(+)}_{Fc,0}} a^\dagger_{q,c,-\frac{1}{2}} b^\dagger_{q'=0,c,\gamma} \, . \tag{5.30}$$

Therefore, such transitions involve one $c$ or $s$ topological momentum shift, the creation of a number $\gamma$ of $c, \frac{1}{2}$ pseudoholes and $\gamma$ of $c, -\frac{1}{2}$ pseudoholes, and the creation of one $c, \gamma$ pseudoparticle at $q = 0$. Similar results hold for the topological momentum shifts associated with the creation of one $s, \gamma$ pseudoparticle. In next section we show the physical importance of this latter momentum shifts.

## 5.5 Momentum shifts at work: the example of spin waves

By use of a simple example, we now show that the topological momentum shifts contribute to the total momentum of a given excitation. We consider 1D Hubbard model at electronic and magnetization densities equal to 1 and 0, respectively, and in the strong coupling regime $U/4t^2 \gg 1$.

It was shown by Ogata *et al.* [16] that in the strong coupling regime the Bethe-ansatz wave function for the Hubbard model decouples into the product of the 1D anti-ferromagnetic Heisenberg model wave function [17] and a Slater determinant of free spinless fermions. At $n = 1$ the spinless fermions have no dynamics and we are left with the antiferromagnetic Heisenberg chain with magnetic coupling given by $4t^2/U$. The correct description of the anti-ferromagnetic chain (2.20) excitation

spectrum at zero magnetic field was given by Faddeev *et al.* [18]. These authors found that the excitation spectrum is two parametric, which leads to a continumn of excitations. The excitation spectrum $E(q_1, q_2)$ and the excitation momentum $\Delta P$ are given by

$$E(q_1, q_2) = \frac{J\pi}{2}[\cos(q_1) + \cos(q_2)]\,, \qquad \Delta P = \pi - q_1 - q_2\,. \tag{5.31}$$

Here $J$ is the antiferromagnetic coupling and $q_1$ and $q_2$ are the momentum of two spin waves (each with spin 1/2). The factor $\pi$ in $\Delta P$ expression refers to the ground-state momentum ($N_\downarrow$ was choosen to be odd and the number of sites $N_a$ was choosen to be even).

The same results can be obtained for the Hubbard chain in the strong-coupling regime. Although the spinless fermions band is full, all the fermions change their momenta by $\pi/N_a$, what recovers the excitation momentum of the Heisenberg chain. For $U/4t^2 \gg 1$ and electronic density $n = 1$, the energy band of the $s, 0$ pseudoparticles is given by [19]

$$\varepsilon^0_{s,0}(q) = -\frac{4t^2}{U}\frac{\pi}{2}\cos(q) \tag{5.32}$$

and the $c, 0$ energy band by

$$\varepsilon^0_{c,0}(q) = -2t\cos(q) + \mathcal{O}(4t^2/U)\,. \tag{5.33}$$

At zero magnetic field the ground state is the pseudohole vacuum, that is the SO(4) ground state. In this case the $s, \gamma$-energy bands collapse to the point $\varepsilon^0_{s,\gamma}(q) = 0$ and $q = 0$. Both the $c, 0$ and the $s, 0$ bands are filled in the ground state and $\varepsilon^0_{s,0}(q_{Fs,0}) = \varepsilon^0_{s,\gamma}(0) = 0$. Thus, creation of the $s, \gamma$ heavy-pseudoparticles costs no energy (excitations involving creation of $c, \gamma$ heavy-pseudoparticles have an energy gap). That is, excitations between the ground state and LWS's II. Let us consider that the initial ground has both $N_\downarrow$ and $N_\uparrow$ odd. From Table 5.1 we see that the ground state has zero momentum. The simplest excitation one can think of is, under these conditions, the creation of one single $s, 1$ heavy pseudoparticle. From the numbers (3.26) and keeping constant $N_\downarrow$ and $N_\uparrow$, we see that the total number of $s, 0$ pseudoholes varies by 2, and that the number of $c, 0$ pseudoparticles remains unchanged (the corresponding number of pseudoholes is zero). ( Equation (3.10) confirms that the $s, 1$ pseudo-Brillouin zone is reduced to the single $q = 0$ point.) Equations (3.12) and (3.13) imply that all $c, 0$ pseudoparticles (spinless fermions

in this limit) change their momenta by $\pi/N_a$. This leads to a finite momentum of $\delta q = \pi$, and the energy and momentum excitation spectra are

$$E(q_1, q_2, q_3) = \varepsilon_{s,1}(q_3) + \frac{4t^2}{U}\frac{\pi}{2}[\cos(q_1) + \cos(q_2)] = \frac{4t^2}{U}\frac{\pi}{2}[\cos(q_1) + \cos(q_2)] \quad (5.34)$$

and

$$\Delta P = \pi + q_3 - q_1 - q_2 = \pi - q_1 - q_2\,, \quad (5.35)$$

respectively. It is obvious that Eqs. (5.34) and (5.35) recover Faddeev's results (5.31) for the Heisenberg chain and that our $s, 0$ pseudoparticles are Faddev's spin-1/2 spin waves, in agreement with the results of Sec. 5.3.

The same excitation spectra, (5.34) and (5.35), are obtained if we take the limit $H = 0^+$ and make a triplet excitation (flip one electron spin). In this limit and for the same parity of the electronic numbers $N_\sigma$ we have just used, the ground state has two holes in the $s, 0$ band, as Eq. (3.10) implies. The ground-state momentum is zero. Due to the electronic spin-flip excitation, the boundary conditions (3.12) and (3.13) adjust in such a way that the final state still has two holes in the $s, 0$ band. The number of $s, 0$ pseudoparticles changes by one, and a momentum shift of $\pi/N_a$ occurs in the $c, 0$ band, what leads, at half-filling, to a finite momentum of $\pi$. We then recover the result that at zero magnetic field the triplet and the singlet excitations are degenerated.

Without the use of the Bethe-ansatz equations, Dias and Lopes dos Santos found equivalent results [10]. For $U = \infty$ they confirmed that all the spin configurations are degenerated. This corresponds, in the pseudoparticle formalism, to $\varepsilon^0_{s,\gamma\geq 0}(q) = 0$. Despite this massive degeneracy, changes in the spin configurations lead to a global momentum shift of $\pi/N_a$ in the $c, 0$ pseudoparticle band. This effect was represented by Dias and Lopes dos Santos as a fictitious magnetic flux through the spinless-fermion ring. This simple representation shows that the change in the pseudomomenta is such that the system minimizes its energy when both the spin configuration changes and one electron is added to or removed from the system.

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# Chapter 6

# Zero-Temperature Transport

## 6.1 Introduction

The transport properties of strongly correlated electron models for low-dimensional conductors has been a subject of experimental and theoretical interest for over twenty years. Low-dimensional conductors show large deviations in their transport properties from the usual single-particle description. This suggests that electronic correlations might play an important role in these systems [1, 2, 3, 4, 5, 6], even if the on-site Coulomb repulsion is small [5].

In this chapter we use the generalized pseudoparticle theory to study the charge and spin currents of the Hubbard chain at finite energy. For that we solve the BA equations with a twist angle for all electronic densities and magnetizations. We express the charge and the spin-diffusion currents in terms of the elementary currents of the charge and spin carriers. It is shown that the latter carriers are the $\alpha, \gamma$ pseudoparticles of the pseudoparticle-perturbation theory (PPT) presented in Chapter 3 and introduced in the work [7]. We evaluate their couplings to charge and spin and define the charge and spin pseudoparticle transport masses. The ratios of these masses over the corresponding static mass provide important information on the role of electronic correlations in the transport of charge and spin in the 1D quantum liquid. Furthermore, we find that the transport of charge and spin can be described by means of pseudoparticle kinetic equations. Our results are a generalization to finite energies of the low-energy results on transport of charge and spin results obtained in earlier works [8, 9]. This is possible by means of the generalized pseudoparticle representation introduced in Chapters 3 and 4.

Recently, the pseudoparticle description of all BA Hamiltonian eigenstates in-

troduced in Chapter 3 [7] has allowed the evaluation of analytical expressions for correlation functions at finite energy [13, 14]. From these results one can obtain expressions for the absorption-band edges of the frequency-dependent electronic conductivity, $\sigma(\omega)$ [15].

## 6.2 Review of fundamental concepts in pseudoparticle theory

Although the pseudoparticle description, introduced in Chapter 3, refers to all Hamiltonian eigenstates [7], in this Chapter we restrict our study to the Hilbert subspace involved in the zero-temperature charge and spin frequency-dependent conductivity [15]. This is spanned by all the Hamiltonian eigenstates contained in the states $\hat{j}^{\zeta}|GS\rangle$, where $|GS\rangle$ denotes the ground state and $\hat{j}^{\zeta}$ are the charge ($\zeta = \rho$) and spin ($\zeta = \sigma_z$) current operators [given by Eqs. (6.15) and (6.16 below, respectively]. Since these current operators commute with the six generators of the $\eta$-spin and spin algebras [16] (Chapter 2.1), our Hilbert subspace is in the present parameter space spanned only by the lowest-weight states (LWS's) of these algebras [17] (Chapter 3). This refers to the Hilbert subspace directly described by the BA solution [7]. [Therefore, following the studies and notations of Chapter 3 [7], we can use the $\alpha, \gamma = 0$ pseudoparticles instead of the $\alpha, \beta$ pseudoholes (with $\beta = \pm\frac{1}{2}$) required for the description of the non-LWS's outside the BA solution.]

The $c, 0$ and $s, 0$ pseudoparticle branches have been called in previous low-energy studies $c$ and $s$ pseudoparticle branches, respectively [8, 9]. They were shown to describe the low-energy excitations of the Hubbard chain and to determine the low-energy behavior of its charge and spin transport properties [8, 9]. (In the limit of low energy the heavy-pseudoparticle branches are empty.) On the other hand, description of the LWS's of the model that have a finite-energy gap, $\omega_0$, relatively to the ground state involves the heavy pseudoparticle branches $c, \gamma > 0$ and $s, \gamma > 0$ (Chapter 3) [7].

A very useful concept in this theory is that of generalized ground state (GGS). In Chapter 3 it was defined as the Hamiltonian eigenstate(s) of lowest energy in the Hilbert subspace associated with a given sub-canonical ensemble. The concept of sub-canonical ensemble follows from the conservation laws of the $\alpha, \gamma$ pseudoparticle numbers, $N_{\alpha,\gamma}$. Each Hamiltonian eigenstate has constant values for these numbers and a sub-canonical ensemble refers to a given choice of constant $N_{\alpha,\gamma}$ numbers.

On the other hand, the concept of GGS has been recently extended [13, 14] as follows (i) filled $\alpha,\gamma$ pseudoparticle seas with compact occupations around $q=0$, i.e. for $q^{(-)}_{F\alpha,\gamma,+1} \leq q \leq q^{(+)}_{F\alpha,\gamma,+1}$, where the pseudo-Fermi points are given by $q^{(\pm)}_{F\alpha,\gamma,+1} = \pm\frac{\pi N_{\alpha,\gamma}}{N_a} + O(1/N_a)$, and (ii) filled $\alpha,\gamma$ pseudoparticle seas with compact occupations for $q^{(-)}_{\alpha,\gamma} \leq q \leq q^{(-)}_{F\alpha,\gamma,-1}$ and for $q^{(+)}_{F\alpha,\gamma,-1} \leq q \leq q^{(-)}_{\alpha,\gamma}$, where the pseudo-Fermi points are given by $q^{(\pm)}_{F\alpha,\gamma,-1} = \pm[q_{\alpha,\gamma} - \frac{\pi N_{\alpha,\gamma}}{N_a}] + O(1/N_a)$. Recent developments on the problem [13, 14, 15], have revealed that the creation of one $\alpha,\gamma$ pseudoparticle from the ground state involves, to leading order, a number $2\gamma$ of electrons. Since the currents are two-electron operators, it follows that the creation of single $\alpha,1$ pseudoparticles from the ground state are the most important contributions to the transport of charge ($\alpha = c$) and spin ($\alpha = s$) at finite energies. On the other hand, since the states $\hat{j}^{\zeta}|GS\rangle$ which define our Hilbert space have zero momentum (relatively to the ground state) and the creation from the ground state of single $\alpha,1$ pseudoparticles of type (ii) is a finite-momentum excitation, for simplicity in this chapter we restrict our study to GGS's of type (i). Therefore, in order to simplify our notation we denote the pseudo-Fermi points $q^{(\pm)}_{F\alpha,\gamma,+1}$ simply by $q^{(\pm)}_{F\alpha,\gamma}$. These are given by $q^{(\pm)}_{F\alpha,\gamma} = \pm q_{F\alpha,\gamma} + O(1/N_a)$ where the pseudo-Fermi momentum (Chapter 3) [7]

$$q_{F\alpha,\gamma} = \frac{\pi N_{\alpha,\gamma}}{N_a}\,, \tag{6.1}$$

appears in several expressions below. Note, however, that the generalization of our results to GGS's of type (ii) is straightfoward. We emphasize that in Chapter 3 the definition of GGS refers to the above choice (i) for the $c,0$ and $s,\gamma$ branches and to the choice (ii) for the $c,\gamma$ branch with $\gamma > 0$. Therefore, in the case of the $c,\gamma > 0$ pseudoparticles our GGS choice differs from the choice of that chapter.

The ground state is a special case of a GGS where there is no $\alpha,\gamma > 0$ heavy-pseudoparticle occupancy [7] and the pseudo-Fermi points (6.1) are of the form

$$q_{Fc,0} = 2k_F\,; \qquad q_{Fs,0} = k_{F\downarrow}\,; \qquad q_{F\alpha,\gamma} = 0 \quad \gamma > 0\,. \tag{6.2}$$

Since the conservation of the electron numbers imposes the following sum rules on the numbers $N_{\alpha,\gamma}$ (Chapter 3) [7]

$$N_{\downarrow} = \sum_{\gamma>0}\gamma N_{c,\gamma} + \sum_{\gamma}(1+\gamma)N_{s,\gamma}\,, \tag{6.3}$$

and

$$N = N_{c,0} + 2\sum_{\gamma>0} \gamma N c,\gamma\,, \tag{6.4}$$

the creation of heavy pseudoparticles from the ground state at constant electron numbers requires the annihilation of $\alpha, 0$ pseudoparticles. It follows from Eqs. (6.3) and (6.4) that the changes $\Delta N_{\alpha,0}$ associated with a corresponding ground-state – GGS transition read

$$\Delta N_{s,0} = -\sum_{\gamma>0} \gamma N_{c,\gamma} - \sum_{\gamma>0} (1+\gamma) N_{s,\gamma}\,, \tag{6.5}$$

and

$$\Delta N_{c,0} = -2\sum_{\gamma>0} \gamma N c,\gamma\,. \tag{6.6}$$

For instance, the creation of one $c,\gamma$ heavy pseudoparticle from the ground state requires the annihilation of a number $2\gamma$ of $c,0$ pseudoparticles and of a number $\gamma$ of $s,0$ pseudoparticles, whereas the creation of one $s,\gamma$ pseudoparticle involves the annihilation of a number $1+\gamma$ of $s,0$ pseudoparticles and conserves the number of $c,0$ pseudoparticles.

## 6.3 Charge and spin currents: solution of the BA Equations

Within linear response theory the charge and spin currents of the 1D Hubbard model can be computed by performing a spin-dependent Peierls-phase substitution [18, 19] in the hopping integral of Hamiltonian (2.10), $t \to te^{\pm i\phi_\sigma/N_a}$, leading to Hamiltonian (2.5).

It has been possible to solve the Hamiltonian (2.10) with the additional hopping phase $e^{\pm i\phi_\sigma/N_a}$ by means of the coordinate BA both with twisted and toroidal boundary conditions, both approaches giving essentially the same results [19, 20]. One obtains the energy spectrum of the model parameterized by a set a numbers $\{k_j, \Lambda_\delta\}$ which are solution of the BA interaction equations given by

$$e^{ik_j N_a} = e^{i\phi_\uparrow} \prod_{\delta=1}^{N_\downarrow} \frac{\sin(k_j) - \Lambda_\delta + iU/4}{\sin(k_j) - \Lambda_\delta - iU/4}\,, \qquad (j = 1, \ldots, N)\,, \tag{6.7}$$

and

$$\prod_{j=1}^{N}\frac{\sin(k_j)-\Lambda_\delta+iU/4}{\sin(k_j)-\Lambda_\delta-iU/4}=e^{i(\phi_\downarrow-\phi_\uparrow)}\prod_{\beta=1,\neq\delta}^{N_\downarrow}\frac{\Lambda_\beta-\Lambda_\delta+iU/2}{\Lambda_\beta-\Lambda_\delta-iU/2}\,,\qquad(\delta=1,\ldots,N_\downarrow)\,. \tag{6.8}$$

These equations reduce to Eqs. (2.36) and (2.37) with $\phi_\uparrow=\phi_\downarrow$.

However, previous studies of the $\phi_\sigma\neq 0$ problem [19, 20] have only considered the real BA rapidities of Eqs. (6.7) and (6.8) which refer to low energy. Here we follow the same steps as Takahashi [21] for the $\phi_\sigma=0$ Eqs. (6.7) and (6.8) and consider both real and complex rapidities. We then arrive to the following $\phi_\sigma\neq 0$ equations which refer to the real part of these rapidities

$$\begin{aligned}k_jN_a &= 2\pi I_j^c+\phi_\uparrow-\sum_\gamma\sum_{j'=1}^{N_{s,\gamma}}2\tan^{-1}\left(\frac{\sin(k_j)/u-R_{s,\gamma,j'}}{(\gamma+1)}\right)\\ &- \sum_{\gamma>0}\sum_{j'=1}^{N_{c,\gamma}}2\tan^{-1}\left(\frac{\sin(k_j)/u-R_{c,\gamma,j'}}{\gamma}\right)\,,\end{aligned} \tag{6.9}$$

$$\begin{aligned}2N_aRe\,\sin^{-1}([R_{c,\gamma,j}+i\gamma]u) &= 2\pi I_j^{c,\gamma}+\gamma(\phi_\uparrow+\phi_\downarrow)\\ &- \sum_{j'=1}^{N_c}2\tan^{-1}\left(\frac{\sin(k_{j'})/u-R_{c,\gamma,j}}{\gamma}\right)\\ &+ \sum_{\gamma'>0}\sum_{j'=1}^{N_{c,\gamma'}}\Theta_{\gamma,\gamma'}(R_{c,\gamma,j}-R_{c,\gamma',j'})\,,\end{aligned} \tag{6.10}$$

and

$$\begin{aligned}&\sum_{j'=1}^{N_c}2\tan^{-1}\left(\frac{R_{s,\gamma,j}-\sin(k'_j)/u}{(1+\gamma)}\right)+(1+\gamma)(\phi_\uparrow-\phi_\downarrow)=\\ &= 2\pi I_j^{s,\gamma}+\sum_{\gamma'}\sum_{j'=1}^{N_{s,\gamma'}}\Theta_{\gamma+1,\gamma'+1}(R_{s,\gamma,j}-R_{s,\gamma',j'})\,.\end{aligned} \tag{6.11}$$

The functions $\Theta_{\gamma,\gamma'}(x)$ [and $\Theta_{\gamma+1,\gamma'+1}(x)$] of Eqs. (6.9), (6.10), and (6.11) are defined by Eq. (4.8). The following definitions for the real part of the rapidities, $\Lambda_\alpha^{n+1}/u=R_{s,\gamma,j}$ (with $n+1=\gamma$ and $\alpha=j$), $\Lambda_\alpha^{'n}/u=R_{c,\gamma,j}$ (with $n=\gamma$ and $\alpha=j$), and $\gamma=1,2,\ldots,\infty$ for the $N_{c,\gamma}$ sums and $\gamma=0,1,2,\ldots,\infty$ for the $N_{s,\gamma}$ sums, allows us to recover Takahashi's formulae for $\phi=0$ [21]. Here and often below we use the

notation $c \equiv c,0$, which allows the $c,\gamma$ sums to run over $1,2,3,\ldots,\infty$. Whether we are using this notation or the previous one will be obvious from the context.

The important numbers $I_j^c$, $I_j^{c,\gamma}$, and $I_j^{s,\gamma}$ which appear when going from Eqs. (6.7) and (6.8) to Eqs. (6.9), (6.10), and (6.11) are the quantum numbers which describe the Hamiltonian eigenstates. As we have seen in Chapter 3, it is convenient to describe the eigenstates of the model in terms of pseudomomentum $\{q_j^{\alpha,\gamma} = 2\pi I_j^{\alpha,\gamma}/N_a\}$ distributions, where $I_j^{c,0} \equiv I_j^c$. The energy and momentum eigenvalues are given by [7]

$$\begin{aligned} E &= -2t\sum_{j=1}^{N_c}\cos(k_j) + \sum_{\gamma>0}\sum_{j=1}^{N_{c,\gamma}} 4tRe\sqrt{1-u^2[R_{c,\gamma,j}-i\gamma]^2} \\ &+ N_a(U/4-\mu) + N(\mu-U/2) - \mu_0 H(N_\uparrow - N_\downarrow), \end{aligned} \tag{6.12}$$

and

$$P = \frac{2\pi}{N_a}\left[\sum_{j=1}^{N_c}(I_j^c + \frac{\phi_\uparrow}{N_a}) + \sum_{\gamma}\sum_{j=1}^{N_{s,\gamma}}(I_j^{s,\gamma} - (\gamma+1)\frac{\phi_{\uparrow-\downarrow}}{N_a}) - \sum_{\gamma>0}\sum_{j=1}^{N_{c,\gamma}}(I_j^{c,\gamma} + \gamma\frac{\phi_{\uparrow+\downarrow}}{N_a})\right] + \pi\sum_{\gamma>0}N_{c,\gamma}\,, \tag{6.13}$$

respectively. Eqs. (6.12) and (6.13) are the eigenvalues of Eqs. (4.19) and (3.32). We emphasize that the rapidity dependence on $\phi_\sigma$ is defined by Eqs. (6.9)-(6.11) and determines the energy-functional (6.12) dependence on $\phi_\sigma$. The corresponding $\phi_\sigma = 0$ expressions recover the rapidity equations (6.9), (6.10), and (6.11).

In the limit of a large system ($N_a \to \infty$, $N/N_a$ fixed), and using the same methods as in Chapters 3 and 4, we can develop a generalization of the low-energy pseudoparticle-Landau-liquid description of the Hubbard model. This generalization refers to energies just above the set of energies $\omega_0$ given by

$$\omega_0 = 2\mu\sum_{\gamma>0}\gamma N_{c,\gamma} + 2\mu_0 H\sum_{\gamma>0}(1+\gamma)N_{s,\gamma} + \sum_{\alpha,\gamma>0}\epsilon^0_{\alpha,\gamma}(0)N_{\alpha,\gamma}\,, \tag{6.14}$$

where the Hamiltonian (4.40) truncated up to second order describes the quantum-problem at $(\omega-\omega_0)$ low energies. Note that the choice $\omega_0 = 0$, which refers to $N_{\alpha,\gamma} = 0$ for $\gamma > 0$, recovers the usual low-energy theory [8, 9]. On the other hand, when $\omega_0 > 0$, in addition to finite occupancy of the usual $c,0 \equiv c$ and $s,0 \equiv s$ pseudoparticle bands, there is finite occupancy for some of the branches of the $c,\gamma$ and $s,\gamma$ heavy-pseudoparticles [7].

In the above thermodynamic limit the rapidity real parts $k_j = k_j(q_j)$, $R_{s,\gamma,j} = R_{s,\gamma,j}(q_j)$, and $R_{c,\gamma,j} = R_{c,\gamma,j}(q_j)$ proliferate on the real axis. As we have done in Chapters 3 and 4, Eqs. (6.9), (6.10), and (6.11) can be rewritten as integral equations with an explicit dependence on the pseudomomentum distribution functions $N_{\alpha,\gamma}(q)$. These are Eqs. (A.7), (A.8), and (A.9) of Appendix A which refer to the case $\phi_\sigma \neq 0$. In that Appendix we derive ground-state normal-ordered expressions for the rapidities and charge and spin currents.

The combination of Eqs. (6.12), (A.7), (A.8), and (A.9) allows the evaluation of several interesting transport quantities. This includes the charge and spin currents and the charge and spin pseudoparticle transport masses. The charge and spin current operators $\hat{j}^\zeta$ (with $\zeta = \rho$ for charge, and $\zeta = \sigma_z$ for spin) are for the 1D Hubbard model given by [8, 9]

$$\hat{j}^\rho = -eit \sum_\sigma \sum_{j=1}^{N_a} (c^\dagger_{j\sigma} c_{j+1\sigma} - c^\dagger_{j+1\sigma} c_{j\sigma}) \,, \tag{6.15}$$

and

$$\hat{j}^{\sigma_z} = -(1/2)it \sum_\sigma \sum_{j=1}^{N_a} \sigma (c^\dagger_{j\sigma} c_{j+1\sigma} - c^\dagger_{j+1\sigma} c_{j\sigma}) \,. \tag{6.16}$$

Importantly, the discrete nature of the model implies that the commutators of the Hamiltonian (2.10) and of the current operators $\hat{j}^\zeta$, Eqs. (6.15) and (6.16), are non zero. It follows that the BA wave function does not diagonalizes simultaneously the Hamiltonian (2.10) and the current operators (6.15) and (6.16). Since the BA solution alone only provides the diagonal part in the Hamiltonian-eigenstate basis of the physical operators [7], we can only evaluate expressions for the diagonal part of the currents which provide the mean values of the charge and spin currents. These refer to all LWS's and are important quantities for they allow us to compute the transport masses of the charge and spin carriers of the system. In addition, our formalism defines the charge and spin carriers. These are found to be the $c$ (i.e., $c, 0$) and $c, \gamma$ pseudoparticles for charge, and the $c$ and $s, \gamma$ pseudoparticles for spin. This follows from Eqs. (A.7)-(A.9) and also from the Boltzmann transport analysis of Sec. 6.5.

We emphasize that combining the generalized pseudoparticle representation of Chapter 3 [7] with a low-energy $(\omega - \omega_0)$ conformal-field theory [13, 14], leads to finite-energy current – current correlation function expressions which are determined by the non-diagonal terms (in the Hamiltonian-eigenstate basis) of the current operators. This is a generalization of the low-energy correlation-function studies of several

authors [10, 11, 22, 23]. However, these expressions cannot be derived within the BA solution alone. Therefore, these studies go beyond the scope of the present thesis and here we consider the diagonal part of the charge and spin current operators only.

The mean value of the current operator $\hat{j}^{\zeta}$ evaluated for the LWS $|m\rangle$ is given by

$$\langle m|\,\hat{j}^{\zeta}|m\rangle = -\left.\frac{d(E_m/N_a)}{d(\phi/N_a)}\right|_{\phi=0}\,, \tag{6.17}$$

where $E_m$ is the energy of the Hamiltonian eigenstate $|m\rangle$ and [19]

$$\begin{aligned} \phi &= \phi_{\uparrow} = \phi_{\downarrow}\,, \qquad \zeta = \rho\,, \\ \phi &= \phi_{\uparrow} = -\phi_{\downarrow}\,, \qquad \zeta = \sigma_z\,. \end{aligned} \tag{6.18}$$

In our basis the LWS's are simply obtained by considering all the possible occupation distributions of the pseudomomenta $q_j = 2\pi I_j^{\alpha,\gamma}/N_a$. Therefore, it is convenient to describe the matrix elements $\langle m|\,\hat{j}^{\zeta}|m\rangle$ in terms of the pseudomomentum occupation distributions $N_{\alpha,\gamma}(q)$. This leads to a functional form for the current mean values. The computation of $\langle m|\,\hat{j}^{\zeta}|m\rangle$ involves the expansion of Eqs. (6.12) and (A.7)-(A.9) up to first order in the flux $\phi$. Writing Eq. (6.12) in the limit of $N_a \to \infty$, expanding it up to first order in the flux $\phi$, and using Eq. (6.17) we obtain

$$\begin{aligned} \langle m|\,\hat{j}^{\zeta}|m\rangle &= -2t\frac{1}{2\pi}\int_{-q_c}^{q_c} dq N_c(q) K^{\phi}(q)\sin(K(q)) \\ &+ \sum_{\gamma>0} 4t\frac{1}{2\pi}\int_{-q_{c,\gamma}}^{q_{c,\gamma}} dq N_{c,\gamma}(q) Re\,\frac{u^2[R_{c,\gamma}(q)-i\gamma]}{\sqrt{1-u^2[R_{c,\gamma}(q)-i\gamma]^2}} R^{\phi}_{c,\gamma}(q)\,, \end{aligned} \tag{6.19}$$

where the important functions $W^{\phi}(q)$ (with $W = K, R_{s,\gamma}$, and $R_{c,\gamma}$) are the derivatives of the rapidity functions defined by Eqs. (A.7) - (A.9) in order to the flux $\phi$ at $\phi = 0$. They obey a set of integral equations obtained from differentiation of Eqs. (A.7) - (A.9).

It is convenient to write $\langle m|\,\hat{j}^{\zeta}|m\rangle$ in normal order relatively to the ground state. To achieve this goal we expand all the rapidities $W(q)$ and the functions $W^{\phi}(q)$ as

$$W(q) = W^0(q) + W^1(q) + \dots\,, \tag{6.20}$$

$$W^{\phi}(q) = W^{0,\phi}(q) + W^{1,\phi}(q) + \dots\,, \tag{6.21}$$

respectively. In these equations the functions $W^0(q)$ and $W^{0,\phi}(q)$ are both referred to the ground state, and the functions $W^1(q)$ and $W^{1,\phi}(q)$ are first-order functionals of the deviations $\delta N_{\alpha,\gamma}(q)$. In Appendix A we show that the above expansions lead to a ground-state normal-ordered representation. To first order in the deviations, the normal-ordered expression for the matrix element (6.19) simply reads

$$\langle m|\,\hat{j}^{\zeta}|m\rangle = \sum_{\alpha}\sum_{\gamma}\int_{-q_{\alpha,\gamma}}^{q_{\alpha,\gamma}} dq\delta N_{\alpha,\gamma}(q) j^{\zeta}_{\alpha,\gamma}(q)\,, \tag{6.22}$$

where the elementary-current spectrum $j^{\zeta}_{\alpha,\gamma}(q)$ is given by

$$j^{\zeta}_{\alpha,\gamma}(q) = \sum_{\alpha'}\sum_{\gamma'}\theta(N_{\alpha',\gamma'})\mathcal{C}^{\zeta}_{\alpha',\gamma'}\left[v_{\alpha,\gamma}(q)\delta_{\alpha,\alpha'}\delta_{\gamma,\gamma'} + F^{1}_{\alpha,\gamma;\alpha',\gamma'}(q)\right]\,. \tag{6.23}$$

Here

$$F^{1}_{\alpha,\gamma;\alpha',\gamma'}(q) = \frac{1}{2\pi}\sum_{j=\pm 1} j f_{\alpha,\gamma;\alpha',\gamma'}(q, jq_{F\alpha',\gamma'})\,, \tag{6.24}$$

and $\mathcal{C}^{\zeta}_{\alpha,\gamma}$ are the coupling constants of the pseudoparticles to charge and spin given by

$$\mathcal{C}^{\zeta}_{\alpha,\gamma} = \delta_{\alpha,c}\delta_{\gamma,0} + \mathcal{K}^{\zeta}_{\alpha,\gamma}\,, \tag{6.25}$$

where

$$\mathcal{K}^{\rho}_{\alpha,\gamma} = \delta_{\alpha,c}2\gamma\,; \qquad \mathcal{K}^{\sigma_z}_{\alpha,\gamma} = -\delta_{\alpha,s}2(1+\gamma)\,. \tag{6.26}$$

As in a Fermi liquid [24, 25], the expressions of the elementary currents (6.23) involve the velocities $v_{\alpha,\gamma}(q)$ and the interactions [or $f$-functions] $f_{\alpha,\gamma;\alpha',\gamma'}(q,q')$. However, the pseudoparticle coupling contants to charge and spin, Eqs. (6.25) and (6.26), are very different from the corresponding couplings of the Fermi-liquid quasiparticles. We emphasize that at low energy Eq. (6.22) recovers the expression already obtained in previous works [8, 9] which only contains the $c \equiv c,0$ and $s \equiv s,0$ elementary currents. The coupling constants (6.25)-(6.26) play an important role in the description of charge and spin transport and are a generalization for $\gamma > 0$ of the couplings introduced previously [8, 9]. They define the $\alpha,\gamma$ pseudoparticles as charge and spin carriers. We emphasize that when $\mathcal{C}^{\zeta}_{\alpha,\gamma} = 0$ the corresponding $\alpha,\gamma$ pseudoparticles do not couple to $\zeta$ (i.e. charge or spin). Therefore, for $\gamma > 0$ the $c,\gamma$ and $s,\gamma$ pseudoparticles do not couple to spin and charge, respectively. This is related to the charge and spin separation of one-dimensional quantum liquids.

Importantly, when $\mathcal{C}^{\zeta}_{\alpha,\gamma} = 0$ the $\alpha,\gamma$ pseudoparticle – pseudohole processes do not contribute to the $\zeta$ correlation functions.

In contrast to the general current expression (6.19), expression (6.22) is only valid for Hamiltonian eigenstates which differ from the ground-state pseudoparticle occupancy by a small density of psudoparticles. This is because in expression (6.22) we are only considering the first-order deviation term.

The velocity term of the current-spectrum expression (6.23) is what we would expect for a non-interacting gas of pseudoparticles and the second term takes account for the dragging effect on a single pseudoparticle due to its interactions with the remaining pseudoparticles. (This is similar to the Fermi-liquid quasiparticle elementary currents [24, 25].) We remind that Eq. (6.23) is valid for finite energies $\omega$ just above the energy $\omega_0$ corresponding to the suitable set of finite $N_{\alpha,\gamma}$ numbers. These numbers characterize the state $|m\rangle$. Therefore, the sum over $\gamma$ is in Eq. (6.23) restricted to the $\alpha,\gamma$ bands that have non-zero occupancy of pseudoparticles, as is imposed by the presence of the step function. Within the PPT, the deviation second-order pseudoparticle energy expansion corresponds to the deviation first-order current expansion (6.22) which refers to small positive values $(\omega-\omega_0)$ of the excitation energy. In contrast to Fermi liquid theory, our PPT is valid for finite energies [just above the energy values $\omega_0$, Eq. (6.14)] because (i) there is only forward scattering among the pseudoparticles at all energy scales and (ii) at low $(\omega-\omega_0)$ energy values only two-pseudoparticle forward-scattering interactions are relevant. (In a Fermi liquid this is only true for $\omega_0 = 0$ and $\omega \rightarrow 0$ [24, 25].) We emphasize that the current expression (6.19) includes all orders of scattering and, therefore, applies to all energies without restrictions.

## 6.4 Pseudoparticle static and transport masses

In previous studies [8, 9] the charge and spin transport masses of the $c,0$ and $s,0$ pseudoparticles were defined and were shown to play an important role in the transport of charge and spin. For instance, they were shown to fully determine the charge and spin stiffnesses [8, 9, 19, 26, 27, 28, 29]. Here we generalize the mass definitions of these studies to $\gamma > 0$ and define the charge and spin transport masses, $m^{\zeta}_{\alpha,\gamma}$, as

$$m^{\zeta}_{\alpha,\gamma} = \frac{q_{F\alpha,\gamma}}{\mathcal{C}^{\zeta}_{\alpha,\gamma} j^{\zeta}_{\alpha,\gamma}} \, , \tag{6.27}$$

where $j^{\zeta}_{\alpha,\gamma} = j^{\zeta}_{\alpha,\gamma}(q_{F\alpha,\gamma})$. These masses contain important physical information. As in a Fermi liquid [24, 25], the ratio

$$r^{\zeta}_{\alpha,\gamma} = m^{\zeta}_{\alpha,\gamma}/m^{*}_{\alpha,\gamma}\,, \tag{6.28}$$

of the transport mass, $m^{\zeta}_{\alpha,\gamma}$, over the static mass, $m^{*}_{\alpha,\gamma}$, provides a measure of the electronic correlation importance in transport. Similarly to the $\gamma = 0$ case [8, 9], the latter is in general defined as

$$m^{*}_{\alpha,\gamma} = \frac{q_{F\alpha,\gamma}}{v_{\alpha,\gamma}}\,. \tag{6.29}$$

In Appendix B we define the mass (6.29) in terms of suitable functions and find some limiting expressions.

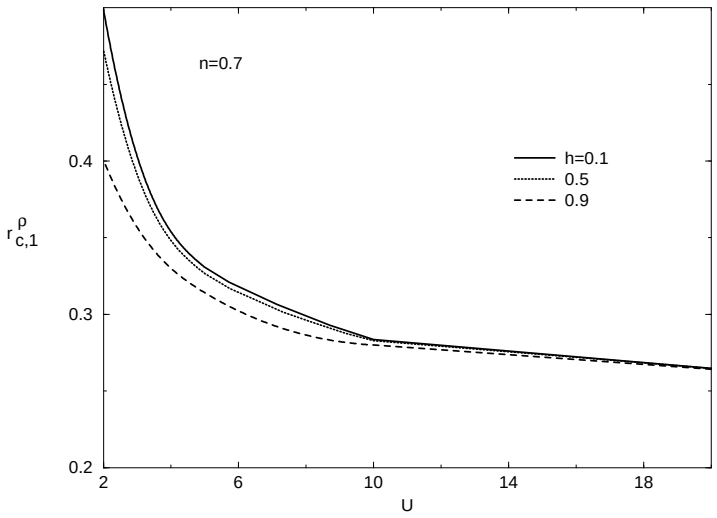



Figure 6.1: The ratio $m^{\rho}_{c,1}/m^{*}_{c,1}$ as function of $U$ at electronic density $n = 0.7$ and for values of the magnetic field $h = H/H_c = 0.1$ (full line), $h = 0.5$ (dashed line) and $h = 0.9$ (dashed-dotted line). For other electronic densities, the plots follow the same trends as for $n = 0.7$.

It can be shown from the transport- and static-mass expressions that the ratio $m^{\zeta}_{\alpha,\gamma}/m^{*}_{\alpha,\gamma}$ involves the Landau parameters

$$F^{i}_{\alpha,\gamma;\alpha',\gamma'} \equiv F^{i}_{\alpha,\gamma;\alpha',\gamma'}(q_{F\alpha,\gamma})\,; \qquad i = 0, 1\,, \tag{6.30}$$

with $F^{i}_{\alpha,\gamma;\alpha',\gamma'}(q)$ given by Eq. (6.24). These parameters can be written as follows

$$F^{i}_{\alpha,\gamma;\alpha',\gamma'} = -\delta_{\alpha,\alpha'}\delta_{\gamma,\gamma'}v_{\alpha,\gamma} + \sum_{\alpha'',\gamma''}\theta(N_{\alpha'',\gamma''})v_{\alpha'',\gamma''}[\xi^{i}_{\alpha'',\gamma'';\alpha,\gamma}\xi^{i}_{\alpha'',\gamma'';\alpha',\gamma'}]\,, \qquad (6.31)$$

where the quantities $\xi^{i}_{\alpha,\gamma;\alpha',\gamma'}$ are given by

$$\xi^{i}_{\alpha,\gamma;\alpha',\gamma'} = \delta_{\alpha,\alpha'}\delta_{\gamma,\gamma'} + \sum_{l=\pm 1} l^{i}\Phi_{\alpha,\gamma;\alpha',\gamma'}(q_{F\alpha,\gamma}, lq_{F\alpha',\gamma'})\,. \qquad (6.32)$$

We find for the ratios $m^{\zeta}_{\alpha,\gamma}/m^{*}_{\alpha,\gamma}$ the following expressions

$$\frac{m^{\zeta}_{\alpha,0}}{m^{*}_{\alpha,0}} = \frac{v_{\alpha,0}}{\mathcal{C}^{\zeta}_{\alpha,\gamma}(\sum_{\alpha',\alpha''}\mathcal{C}^{\zeta}_{\alpha',0}v_{\alpha'',0}\xi^{1}_{\alpha'',0;\alpha,0}\xi^{1}_{\alpha'',0;\alpha',0})}\,, \qquad \gamma = 0\,, \qquad (6.33)$$

and

$$\frac{m^{\zeta}_{\alpha,\gamma}}{m^{*}_{\alpha,\gamma}} = \frac{1}{\mathcal{C}^{\zeta}_{\alpha,\gamma}(\mathcal{C}^{\zeta}_{\alpha,\gamma} + \sum_{\alpha'}\mathcal{C}^{\zeta}_{\alpha',0}\xi^{1}_{\alpha,\gamma;\alpha',0})}\,, \qquad \gamma > 0\,. \qquad (6.34)$$

In the Table 6.1 analytical limiting values for the mass ratios of form (6.28) are listed. Obviously, since for $\gamma > 0$ the $c,\gamma$ and $s,\gamma$ pseudoparticles do not couple to spin and charge, respectively, the ratios $m^{\sigma_z}_{c,\gamma}/m^{*}_{c,\gamma}$ and $m^{\rho}_{s,\gamma}/m^{*}_{s,\gamma}$ are infinite.

| | $H \to H_c$ | $H \to 0$ | $n \to 1$ |
|---|---|---|---|
| $m^{\rho}_{c,\gamma}/m^{*}_{c,\gamma}$ | $\frac{1}{2\gamma(2\gamma-\eta_{\gamma-1})}$ | $\frac{1}{2\gamma(2\gamma+\xi^{1}_{c,\gamma;c,0})}$ | $\frac{1}{4\gamma^2}$ |
| $m^{\rho}_{c,0}/m^{*}_{c,0}$ | $\frac{v_c}{2t\sin(\pi n_{\uparrow})}$ | $\frac{1}{(\xi_0)^2}$ | $\infty$ |
| $m^{\sigma_z}_{s,\gamma}/m^{*}_{s,\gamma}$ | $\frac{1}{2(\gamma+1)(2\gamma+2-\eta_{\gamma})}$ | $\frac{1}{2(\gamma+1)(2\gamma+2+2\xi^{1}_{s,\gamma;s,0})}$ | $\frac{1}{2(\gamma+1)(2\gamma+2+2\xi^{1}_{s,\gamma;s,0}-\xi^{1}_{s,\gamma;c,0})}$ |

Table 6.1: Mass ratios in several limits of physical interest. The function $\eta_{\gamma}$ is defined as $\eta_{\gamma} = 2/(\pi)\tan^{-1}[(\sin(n\pi))/(u[\gamma+1])]$. The equations for the static masses $m^{*}_{\alpha,\gamma}$ are given in Appendix B. In the case $H \to 0$, simple expressions for the parameters $\xi^{1}_{\alpha,\gamma;\alpha',0}$, Eq. (6.32), can be obtained from the results of Appendix D. The ratios $m^{\sigma_z}_{c,\gamma}/m^{*}_{c,\gamma}$ and $m^{\rho}_{s,\gamma}/m^{*}_{s,\gamma}$ are infinite. The dependence on $U$ and $n$ of the parameter $\xi_0$ has been studied by Frahm and Korepin [22, 23].

As was referred previously, it can be shown from the results of Chapter 3 and other studies [7, 13, 14, 15] that the creation of one $\alpha,\gamma$ pseudoparticle from the

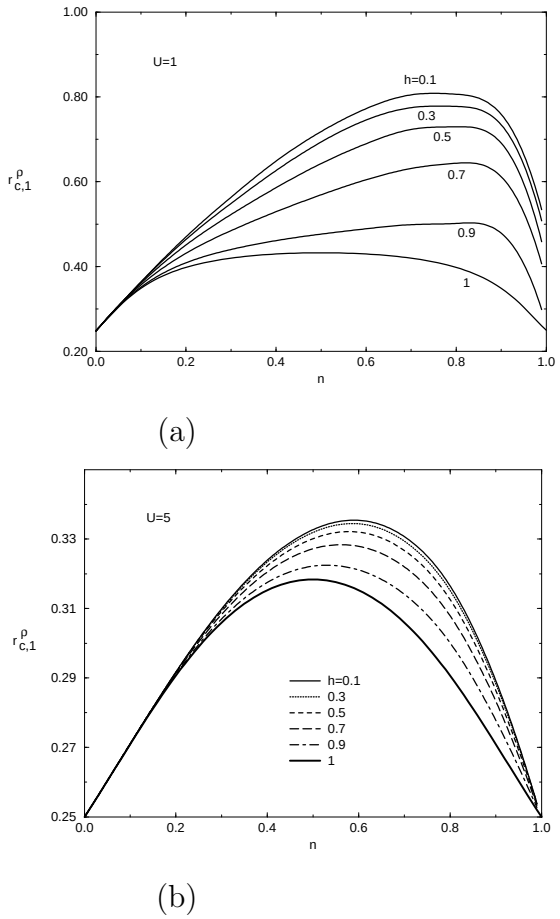
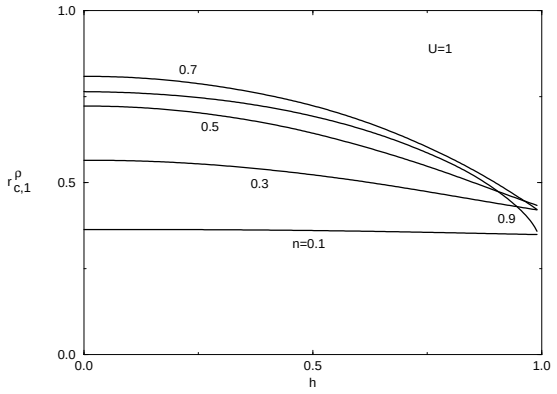
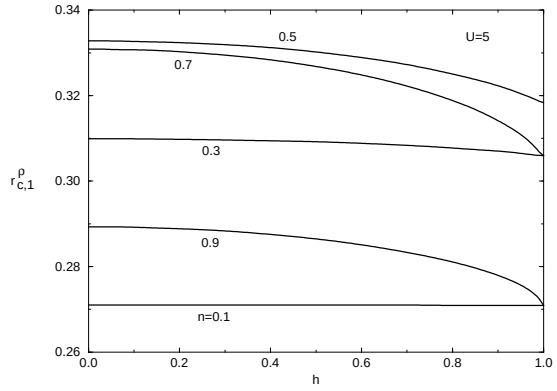



Figure 6.2: The ratio $m^{\rho}_{c,1}/m^{*}_{c,1}$ as function of the electronic density $n$ and for values of the magnetic field $h = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. The onsite Coulomb interaction is (a) $U = 1$ and (b) $U = 5$.

ground state is a finite-energy excitation which, to leading order, involves a number $2\gamma$ of electrons. Therefore, and since the current operators are of two-electron character and couple to charge and spin according to the values of the constants (6.25) and (6.26), at finite energies the $c, 1$ and $s, 1$ heavy pseudoparticles play the major role in charge and spin transport, respectively. On the other hand, the $\alpha, \gamma > 1$ heavy pseudoparticles have a minor role in charge and spin transport. It follows that in the present section we restrict our study to the ratios (6.28) involving $\gamma = 1$ heavy pseudoparticles. We consider the ratios $m^{\rho}_{c,1}/m^{*}_{c,1}$ and $m^{\sigma_z}_{s,1}/m^{*}_{s,1}$. (Note that $m^{\sigma_z}_{c,1}/m^{*}_{c,1} = m^{\rho}_{s,1}/m^{*}_{s,1} = \infty$.) We also consider the case of the $c, 0$ charge-mass ratio which is closely related to the charge stiffness studied in detail by other authors




(a)

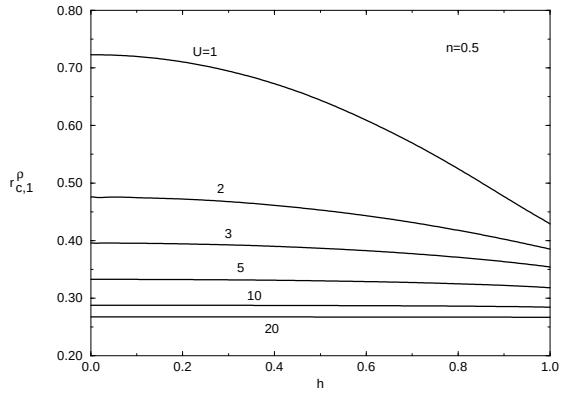



(b)

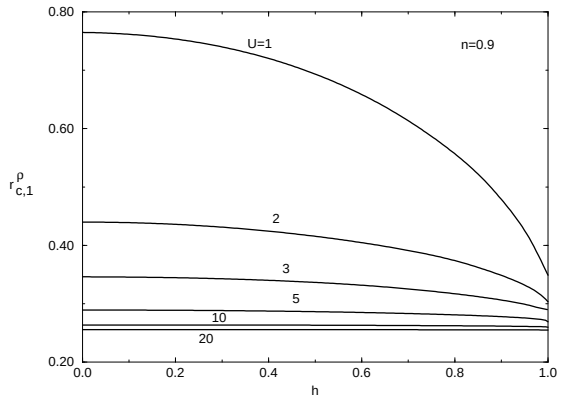
Figure 6.3: The ratio $m^{\rho}_{c,1}/m^{*}_{c,1}$ as function of the the magnetic field $h$ and for values of the electronic density $n = 0.1$, $n = 0.3$, $n = 0.5$, $n = 0.7$, and $n = 0.9$. The onsite Coulomb interaction is (a) $U = 1$ and (b) $U = 5$.

[8, 9]. In Figs. 6.1-6.12 these ratios are plotted as functions of the onsite repulsion $U$ in units of $t$, electronic density $n$, and magnetic field $h = H/H_c$. Note that the ratios of the figures are smaller than one. Moreover, the $\alpha, 1$ mass ratios never achieve the value 1 whereas the $\alpha, 0$ mass ratios tend to one in some limits because of the generalized adiabatic principle [8, 9].

Combined analysis of Figs. 6.1 and 6.2 reveals that the charge-mass ratio for the $c, 1$ pseudoparticle is, for large $U$, fairly independent both of the band filling $n$ and magnetic field $h$. It is a decreasing function of $U$ and as a function of the density, $n$, goes through a maximum for a density which is a decreasing function of $U$. Moreover, figures 6.3 and 6.4 show that this ratio is a decreasing function of the




(a)




(b)

Figure 6.4: The ratio $m^{\rho}_{c,1}/m^{*}_{c,1}$ as function of the the magnetic field $h$ and for values of the onsite Coulomb interaction $U = 1$, $U = 2$, $U = 3$, $U = 5$, $U = 10$, and $U = 20$. The electronic density is (a) $n = 0.5$ and (b) $n = 0.9$.

magnetic field.

In contrast, Figs. 6.5 - 6.8 reveal that the charge-mass ratio for the $c, 0$ pseudoparticle is an increasing function of $U$ and of $h$ and as a function of the density, $n$, goes through a minimum for a density which is a decreasing function of $U$. Note that from Fig. 6.5 the evolution of the $c, 0$ pseudoparticles to free spinless fermions as $U$ increases is clear. This is signaled by the ratio going to one as $U \rightarrow \infty$. This behavior follows from the generalized adiabatic principle [8, 9] and agrees with the well known decoupling of the BA wave function in free spinless fermions (in the low-energy sector [30]) and localized antiferromagnetic spins [31]. Figures 6.7 and 6.8 also reveal that in the fully-polarized ferromagnetic limit, $h \rightarrow 1$, the ratio goes to

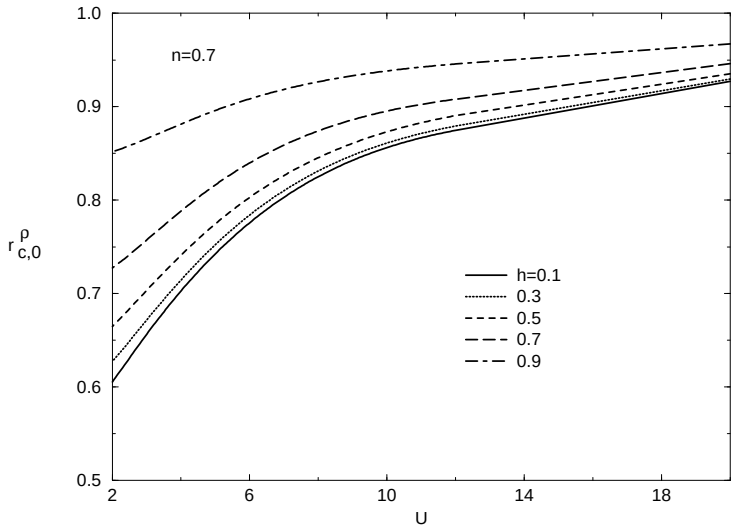


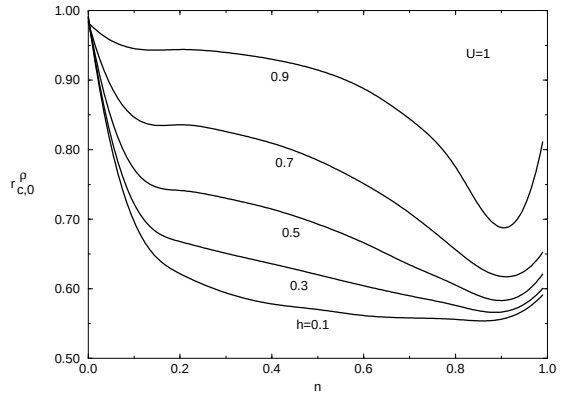

Figure 6.5: The ratio $m^{\rho}_{c,0}/m^{*}_{c,0}$ as function of $U$, for electronic density $n = 0.7$, and for values of the magnetic field $h = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. For other electronic densities, the plots follow the same trends as for $n = 0.7$.

one. This mass-ratio behavior also follows from the generalized adiabatic principle [8, 9] and confirms that in that limit the onsite Coulomb interations play no role in charge transport (they are froozen by the Pauli principle) .

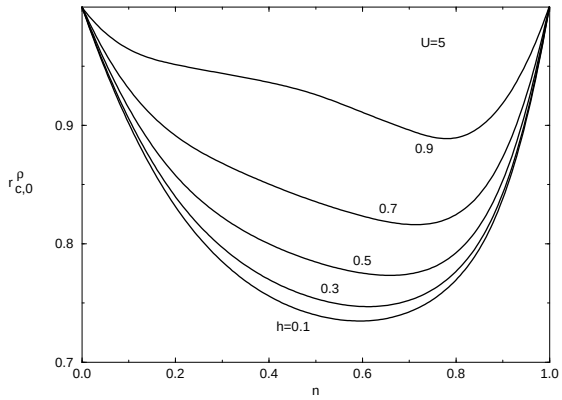
Note that in the large-$U$ Figs. 6.2 - (c) and 6.6 - (c) the ratios $m^{\rho}_{c,1}/m^{*}_{c,1}$ and $m^{\rho}_{c,0}/m^{*}_{c,0}$, respectively, are almost symmetric around the density $n = 0.5$. This implies that for large $U$ the charge transport properties show similarities in the cases of vanishing densities and of densities closed to one.

Figure 6.9 shows that the spin-mass ratio of the $s, 1$ pseudoparticles is a decreasing function of $U$ but that it depends little on $U$ for $U > 6$. For large $U$ this ratio almost does not depend on the density $n$, as revealed by Fig. 6.10 - (c). Figures 6.10 show that, in general, it is an increasing function of $n$ but that for $h \rightarrow 1$ it has a maximum for an intermediate density. In figures 6.11 and 6.12 this spin-mass ratio is plotted as a function of $h$. It is a decreasing function of $h$.

The transport masses are very sensitive to the effects of electronic correlations, as for instance to the metal-insulator transition which occurs at zero temperature when $n \rightarrow 1$ [41]. As a direct result of this transition, $m^{\rho}_{c,0} \rightarrow \infty$ as $n \rightarrow 1$, as was shown and discussed in the works [8, 9]. Moreover, the zero-temperature charge and spin stiffnesses, $D^{\varsigma}$, [8, 9, 19, 26, 27, 28, 29], defined as




(a)

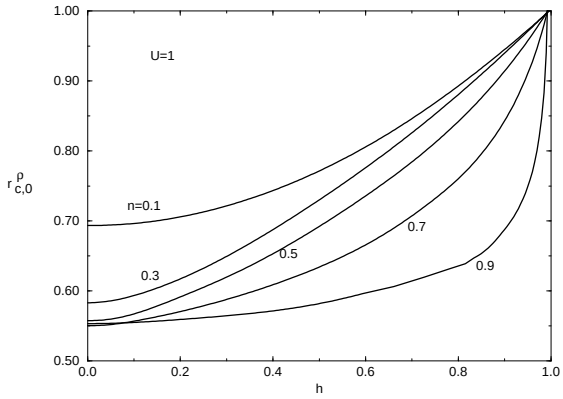



(b)

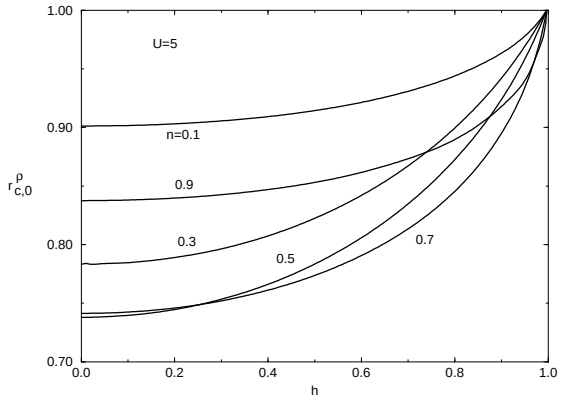
Figure 6.6: The ratio $m^{\rho}_{c,0}/m^{*}_{c,0}$ as function of the electronic density $n$ and for values of the magnetic field $h = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. The onsite Coulomb interaction is (a) $U = 1$ and (b) $U = 5$.

$$D^{\zeta} = \frac{1}{2}\frac{d^2(E_0/N_a)}{d(\phi/N_a)^2}\bigg|_{\phi=0} , \tag{6.35}$$

where $\phi$ is defined for charge $\zeta = \rho$ and spin $\zeta = \sigma_z$ in Eq. (6.18), are such that $2\pi D^{\zeta} = \sum_{\alpha} q_{F\alpha,0}/m^{\zeta}_{\alpha,0}$ [8, 9]. For charge, $m^{\rho}_{s,0} = \infty$, and the latter expression reads $2\pi D^{\rho} = q_{Fc,0}/m^{\rho}_{c,0}$ and is such that $D^{\rho} \rightarrow 0$ as $n \rightarrow 1$, satisfying Kohn criterion [32]. These quantities can be computed within the pseudoparticle formalism by direct evaluation of Eq. (6.35). They can also be obtained by combining a pseudoparticle Boltzmann transport description with linear response theory [8, 9]. In order to confirm the validity and correctness of our formalism, in Appendix C we have recovered




(a)



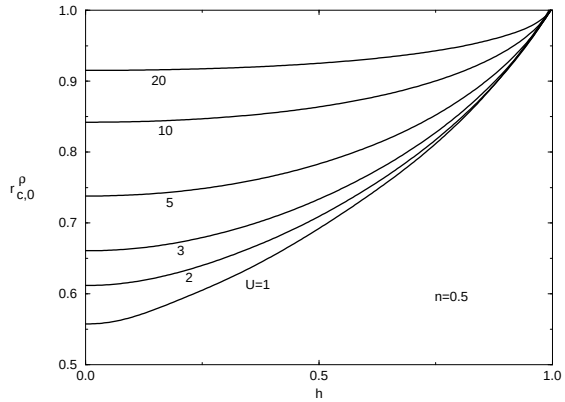

(b)

Figure 6.7: The ratio $m^{\rho}_{c,0}/m^{*}_{c,0}$ as function of the magnetic field $h$ and for values of the electronic density $n = 0.1$, $n = 0.3$, $n = 0.5$, $n = 0.7$, and $n = 0.9$. The onsite Coulomb interaction is (a) $U = 1$ and (b) $U = 5$.

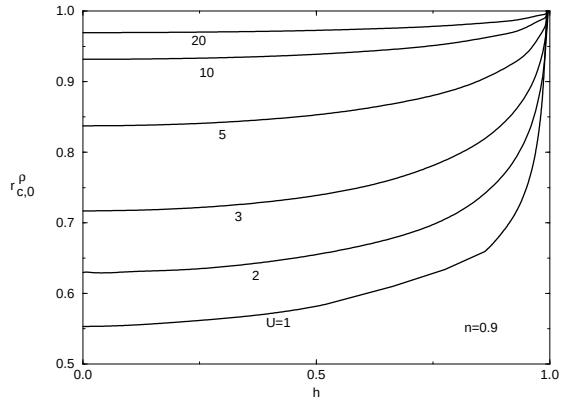
the charge and spin stiffness expressions (135) - (137) of the studies [8, 9] by direct use of Eq. (6.35).

Equations (6.25) and (6.26) show that the Hubbard-chain charge carriers are the $c, \gamma$ pseudoparticles. In contrast to the zero-temperature limit where the $c, 0$ pseudoparticles fully determine the charge stiffness, we expect that the $c, \gamma$ heavy pseudoparticles play an important role in the charge-transport properties at finite temperatures [33, 34, 35].

In Appendix D we present simpler equations to define the pseudoparticle bands and phase shifts in the limit of zero magnetic field. These results show that for $H \rightarrow 0$ and $\gamma > 0$ the bands $\epsilon^{0}_{s,\gamma}(q)$ collapse to a point. This is because both the




(a)




(b)

Figure 6.8: The ratio $m^{\rho}_{c,0}/m^{*}_{c,0}$ as function of the the magnetic field $h$ and for values of the onsite Coulomb interaction $U = 1$, $U = 2$, $U = 3$, $U = 5$, $U = 10$, and $U = 20$. The electronic density is (a) $n = 0.5$ and (b) $n = 0.9$.

bandwidth [see Eq. (D.1)] and the momentum pseudo-Brillouin zone width (in the ground state)

$$\begin{aligned} q_{c,0} &= \pi\,; \qquad q_{c,\gamma} = \pi - 2k_F \quad \gamma > 0\,, \\ q_{s,0} &= k_{F\uparrow}\,; \qquad q_{s,\gamma} = k_{F\uparrow} - k_{F\downarrow} \quad \gamma > 0\,, \end{aligned} \tag{6.36}$$

go to zero as $H \rightarrow 0$. This behavior is also present in the Heisenberg chain and, therefore, in that model the triplet and singlet exitations are degenerated at zero magnetic field [36]. This also holds true for the Hubbard chain at $H = 0$ and in the limit $U \gg 4t$, where the BA wave function factorizes in a spinless-fermion Slater

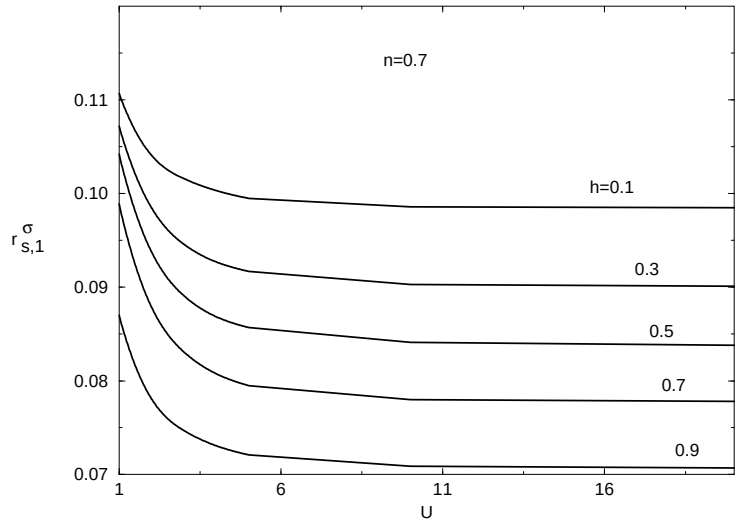


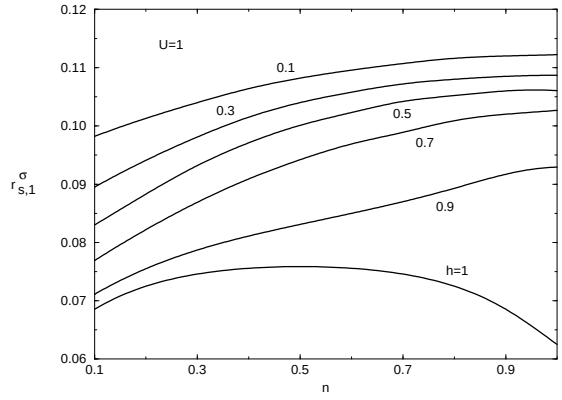

Figure 6.9: The ratio $m^{\sigma_z}_{s,1}/m^*_{s,1}$ as function of $U$, for electronic density $n = 0.7$, and for values of the magnetic field $h = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. For other electronic densities, the plots follow the same trends as for $n = 0.7$.

determinant and in the BA wave function for the 1D antiferromagnetic Heisenberg chain. On the other hand, in the limit $n \rightarrow 1$ the bands $\epsilon^0_{c,\gamma}(q)$ (for $\gamma > 0$) collapse to a point also because both the bandwidth and the momentum pseudo-Brillouin zone width [see Eq. (6.36)] go to zero in that limit.

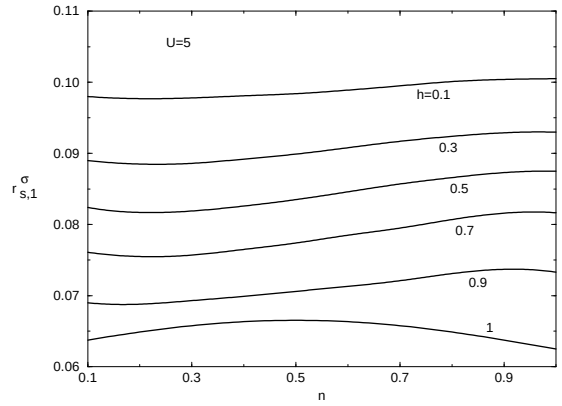
## 6.5 Kinetic equations for the pseudoparticles

In the previous sections the quantum-liquid physics for energies just above the $\omega_0$ values, Eq. (6.14), was described in terms of homogeneous pseudoparticle distributions. The pseudoparticles experience only zero-momentum forward-scattering interactions at all energy scales. This property is absent in Fermi-liquid theory where it holds true only at low excitation energy when the quasiparticles are well defined quantum objects [24, 25, 37, 38]. This unconventional character of integrable models [39, 40] allows us to extend the use of the kinetic equations to energy scales just above the $\omega_0$ energy values, Eq. (6.14), and not only to low energies [8, 9]. The results presented in this section are a generalization of the kinetic-equation low-energy studies [8, 9].

In the final Hilbert subspace of energy $\omega$ relative to the initial ground state




(a)



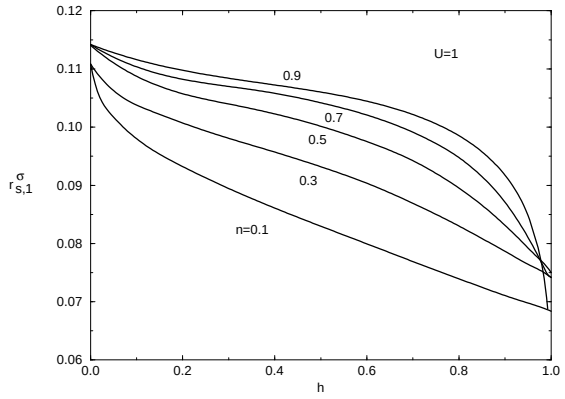

(b)

Figure 6.10: The ratio $m^{\sigma_z}_{s,1}/m^*_{s,1}$ as function of the electronic density $n$ and for values of the magnetic field $h = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. The onsite Coulomb interaction is (a) $U = 1$ and (b) $U = 5$.

the Hubbard model can be mapped onto a continuum field theory of small energy $(\omega - \omega_0)$ [13, 14]. The time coordinate $t$ of such theory is the Fourier transform of the small energy $(\omega - \omega_0)$ which corresponds to a finite energy $\omega$ in the original Hubbard model. The validity of this approach is confirmed by the fact that it fully reproduces the rigorous results of Section 6.3.

Let us consider excitations described by space and time dependent pseudoparticle distribution functions, $N_{\alpha,\gamma}(q, x, t)$, given by

$$N_{\alpha,\gamma}(q, x, t) = N^0_{\alpha,\gamma}(q) + \delta N_{\alpha,\gamma}(q, x, t)\,, \tag{6.37}$$

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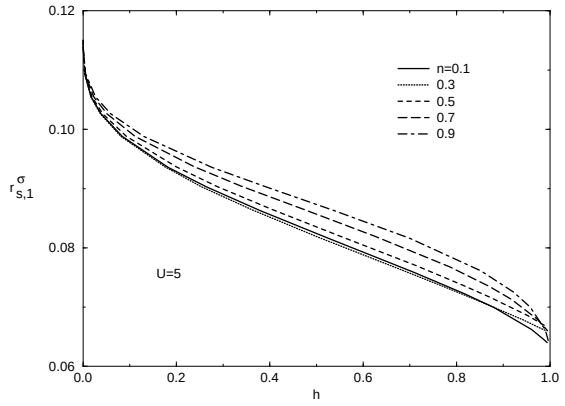


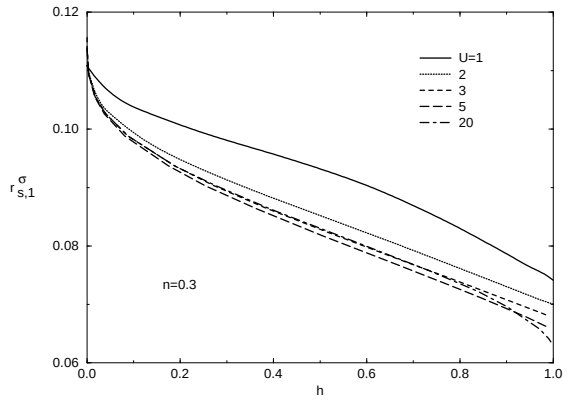

(b)

Figure 6.11: The ratio $m^{\sigma_z}_{s,1}/m^{*}_{s,1}$ as function of the magnetic field $h$ and for values of the electronic density $n = 0.1$, $n = 0.3$, $n = 0.5$, $n = 0.7$, and $n = 0.9$. The onsite Coulomb interaction is (a) $U = 1$ and (b) $U = 5$.

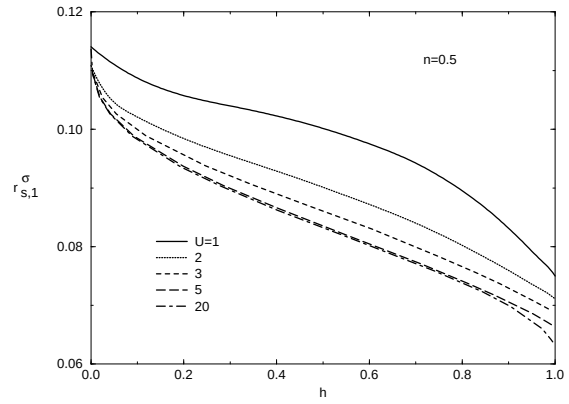
where $N^{0}_{\alpha,\gamma}(q)$ is the ground-state distribution. It follows from the PPT introduced Chapter 3 [7] and discussed in the Chapter 3 that the single-pseudoparticle local energy is given, to first order in the deviations $\delta N_{\alpha,\gamma}(q,x,t)$, by

$$\check{\varepsilon}_{\alpha,\gamma}(q,x,t) = \epsilon_{\alpha,\gamma}(q) + \frac{1}{2\pi}\sum_{\alpha',\gamma'}\int_{-q_{\alpha',\gamma'}}^{q_{\alpha',\gamma'}} dq' \delta N_{\alpha',\gamma'}(q',x,t) f_{\alpha,\gamma;\alpha',\gamma'}(q,q')\,. \qquad (6.38)$$

Let $\mathcal{A}^{\zeta}$ represent the total charge, $\zeta = \rho$, or spin, $\zeta = \sigma_z$. It follows from the relations (6.3) and (6.4) involving the pseudoparticle and electron numbers that $\mathcal{A}^{\zeta}$ depends linearly on the pseudoparticle deviation numbers. Thus, in the case




(a)




(b)

Figure 6.12: The ratio $m^{\sigma_z}_{s,1}/m^{*}_{s,1}$ as function of the the magnetic field $h$ and for values of the onsite Coulomb interaction $U = 1$, $U = 2$, $U = 3$, $U = 5$, $U = 10$, and $U = 20$. The electronic density is (a) $n = 0.3$ and (b) $n = 0.5$.

of inhomogeneous excitations described by Eq. (6.37) the corresponding expectation value at point $x$ and time $t$, $\langle \mathcal{A}^{\zeta}(x,t)\rangle$, can be written as

$$\langle \mathcal{A}^{\zeta}(x,t)\rangle = \langle \mathcal{A}^{\zeta}\rangle_0 + \frac{N_a}{2\pi}\sum_{\alpha',\gamma'}\int_{-q_{\alpha',\gamma'}}^{q_{\alpha',\gamma'}} dq' \delta N_{\alpha',\gamma'}(q',x,t)\mathcal{C}^{\zeta}_{\alpha',\gamma'} \times a^{\zeta}\,, \tag{6.39}$$

where $a^{\rho} = -e$ and $a^{\sigma_z} = 1/2$.

In this"semi-classical" approach the response to a scalar field, $V^{\zeta}(x,t)$, is proportional to the conserved quantity $\mathcal{A}^{\zeta}$. As for low energy [8, 9], in the presence of the inhomogeneous potential the force $\mathcal{F}^{\zeta}(x,t)_{\alpha,\gamma}$ that acts upon the $\alpha,\gamma$ pseudoparticle is given by $\mathcal{F}^{\zeta}_{\alpha,\gamma}(x,t) = -[\partial V^{\zeta}(x,t)/\partial x]\mathcal{C}^{\zeta}_{\alpha,\gamma} \times a^{\zeta}$. It follows that the deviations

$\delta N_{\alpha,\gamma}(q,x,t)$ are determined by the solution of a system of kinetic equations (one equation for each occupied $\alpha,\gamma$ branch) which reads

$$\begin{aligned} 0 &= \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial t} + \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial x}\frac{\partial \breve{\varepsilon}_{\alpha,\gamma}(q,x,t)}{\partial q} - \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial q}\frac{\partial \breve{\varepsilon}_{\alpha,\gamma}(q,x,t)}{\partial x} \\ &- \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial q}\frac{\partial V^{\zeta}(x,t)}{\partial x}\mathcal{C}^{\zeta}_{\alpha,\gamma} \times a^{\zeta}\,. \end{aligned} \tag{6.40}$$

Introducing Eq. (6.37) in Eq. (6.40), expanding to first order in the deviations $\delta N_{\alpha,\gamma}(q,x,t)$, and using Eq. (6.38) we obtain the following set of linearized kinetic equations

$$\begin{aligned} 0 &= \frac{\partial \delta N_{\alpha,\gamma}(q,x,t)}{\partial t} + v_{\alpha,\gamma}(q)\frac{\partial \delta N_{\alpha,\gamma}(q,x,t)}{\partial x} \\ &- \frac{\partial \delta N_{\alpha,\gamma}(q,x,t)}{\partial q}\left\{\frac{\partial V^{\zeta}(x,t)}{\partial x}\mathcal{C}^{\zeta}_{\alpha,\gamma} \times a^{\zeta}\right. \\ &+ \left.\sum_{\alpha',\gamma'}\frac{1}{2\pi}\int_{-q_{\alpha',\gamma'}}^{q_{\alpha',\gamma'}} dq'\frac{\partial \delta N_{\alpha',\gamma'}(q',x,t)}{\partial x} f_{\alpha,\gamma;\alpha',\gamma'}(q,q')\right\}. \end{aligned} \tag{6.41}$$

The conservation law for $\langle \mathcal{A}^{\zeta}(x,t)\rangle$ leads in one dimension to

$$\frac{\partial \langle \mathcal{A}^{\zeta}(x,t)\rangle}{\partial t} + \frac{\langle \mathcal{J}^{\zeta}(x,t)\rangle}{\partial x} = 0\,, \tag{6.42}$$

where $\langle \mathcal{A}^{\zeta}(x,t)\rangle$ is given by Eq. (6.39) and $\langle \mathcal{J}^{\zeta}(x,t)\rangle$ is the associate current. Multiplying Eq. (6.41) by $\mathcal{C}^{\zeta}_{\alpha,\gamma} \times a^{\zeta}$, summing over $\alpha$ and $\gamma$, and integrating over $q$ we find for $V^{\zeta}(x,t) = 0$ and by comparing the result with Eq. (6.42) that the current spectrum $j^{\zeta}_{\alpha,\gamma}(q)$ is given by $a^{\zeta}$ times expression (6.23). (This expression has been derived from the solution of the BA equations with $a^{\zeta} = 1$.)

This agreement confirms the validity of the above low-$(\omega - \omega_0)$ continuum-field theory. The unusual spectral properties associated with the zero-momentum forward-scattering character of the pseudoparticle interactions follow from the integrability of the Hubbard chain [7, 39, 40].

## 6.6 On the conductivity of the Hubbard chain

Solvable one-dimensional many-electron models such as the Hubbard chain are often used as an approximation for the study of the properties of quasi-one-dimensional

conductors [1, 2, 3, 4, 5]. Although the model has been diagonalized long ago [21, 41], the involved form of the Bethe-ansatz (BA) wave function has prevented the direct calculation of dynamic response functions, including the charge-charge and spin-spin response functions and their associate conductivity spectra.

Information on low-energy expressions for correlation functions can be obtained by combining BA with conformal-field theory [22, 23]. On the other hand, several approaches using perturbation theory [18], bosonization [42, 43, 44], the pseudoparticle formalism [8, 9], scaling methods [26], and spin-wave theory [45] have been used to investigate the low-energy transport properties of the model away from half filling and at the metal – insulator transition [41]. Some information on the transport properties at finite energies has also been obtained by numerical methods [27, 46, 47].

To study the optical conductivity of the Hubbard chain we start from its Lehmann representation, whose real part, $\mathcal{R}e\,\sigma(\omega)$, is given by [19, 24]

$$\begin{aligned}\mathcal{R}e\,\sigma(\omega) &= \frac{2\pi e^2}{\hbar}\left[D\delta(\hbar\omega)+\frac{1}{N_a}\sum_{m\neq 0}|\langle m|\hat{j}^{\rho}|0\rangle|^2\delta((E_m-E_0)^2-\hbar^2\omega^2)\right] \\ &\equiv \frac{2\pi e^2}{\hbar}\left[\,D\delta(\hbar\omega)+\sigma_{\rm reg}(\omega)\right]\,, \end{aligned} \tag{6.43}$$

with the charge stiffness $D$ given by

$$D=\frac{1}{N_a}\left[-\frac{1}{2}\langle 0|\hat{T}|0\rangle-\sum_{m\neq 0}\frac{|\langle m|\hat{j}^{\rho}|0\rangle|^2}{E_m-E_0}\right] \tag{6.44}$$

and $\hat{T}=-2t\sum_{k,\sigma}\cos(k)c^{\dagger}_{k,\sigma}c_{k,\sigma}$ being the model kinetic energy (all other quantities have been previously defined in the Chapter 2).

Following Kohn [32] and our previous discussion, the value of charge stiffness $D$ is a criterium for the metal-insulator transition. For such transition to occur, $D$ must change from non-zero to zero. According to Eq. (6.44), this is possible only if the two terms in this equation cancel indentically. For correlated systems with continuos spatial symmetry, the total current operator $\hat{j}^{\rho}=\sum_i\hat{p}_i/m=\hat{P}/m$ is a constant of motion ($m$ is the particle mass, $\hat{p}_i$ is the momentum of the particle $i$, and $\hat{P}$ is the total momentum). It follows that $[\hat{H},\hat{j}^{\rho}]=0$, which implies that $\hat{j}^{\rho}|m\rangle=\hat{P}_m/m|m\rangle$ and

$$\mathcal{R}e\,\sigma(\omega)=\frac{2\pi e^2}{\hbar}D\delta(\omega)\,,\qquad \sigma_{\rm reg}(\omega)=0\,,\qquad D=-\frac{1}{2N_a}\langle 0|\hat{T}|0\rangle\,. \tag{6.45}$$

Equation (6.45) then implies that for systems with continuos spatial symmetry a metal-insulator transition can not occur and the optical-conductivity is reduced to the $\omega = 0$ absorption peak. That is, the conductivity for a correlated system with continous spatial symmetry behaves like a independent-electron system.

The situation is different for lattice systems. In this case it may happen that $\hat{j}^{\rho}$ is no longer a constant of motion. Then $\langle 0|\hat{j}^{\rho}|m\rangle \neq 0$ for a set of Hamiltonian eigenstates $|m\rangle$ and the optical conductivity shows a non-zero regular spectrum ($\sigma_{\rm reg}(\omega) \neq 0$) and a metal-insulator transition may occur. Metal-insulator transitions can be induced, for instance, by the Peierls mechanism due to the dimerization of the lattice (the original band is splitted into two with the formation of a gap, due to the electron-phonon interaction), by Anderson localization, due to electron scattering with random distributed impurities, or by the Mott mechanism, associated with charge localization produced by electronic correlations. The latter mechanism occurs in the one-dimensional Hubbard model at half-filling.

In the pseudoparticle description of the Hubbard model, the metal-insulator transition is associated with the existance of a gap $\omega_0$ between the $c,0$ and the $c,\gamma$ bands. As we have remarked before, at half-filling and zero temperature the charge stiffness is zero and the real part of the optical conductivity, $Re\sigma(\omega)$, has a finite energy gap for all values of $U/t$. For this band filling the $c,0$-pseudoparticle band is full and charge excitations can only occur between the low-energy $\alpha,0$ band and the $c,\gamma$ heavy pseudoparticle bands. The form of the regular part of the optical conductivity is determined by this type of excitations.

As we have discussed in Section 6.2, to populate, for example, the lowest $c,\gamma$ energy-band (the $c,1$ band) with one $c,1$ heavy pseudoparticle one has to annihilate two $c,0$ and one $s,0$ pseudoparticles. The energy involved in this process is exactly $\epsilon^0_{c,1}(0)-\epsilon^0_{c,0}(2k_F)-\epsilon^0_{c,0}(-2k_F)-\epsilon^0_{s,0}(k_{F\downarrow}) = 2\mu(n=1)$, where $\mu(n=1)$ stands for the chemical potential in the limit of half-filling and $\epsilon^0_{\alpha,\gamma}(q)$ is the pseudoparticle energy dispersion. In addition, this excitation process is characterized by a topological excitation of the $s$ pseudoparticles of momentum $-k_{F\downarrow}$ [17], ensuring that the overall excitation has zero momentum, as required for the transitions induced by the current operator (Chapter 5). In general, the process of creating one $c,\gamma$ pseudoparticle has an minimum energy cost of $2\gamma\mu(1)$ and a maximum cost of $2\gamma\mu(1) + 8\gamma t$. Thus, in principle, these transitions should show up in $\sigma_{\rm reg}$ as a set of optical bands. As remarked in Section 6.2, it is possible to show that the creation of one $\alpha,\gamma$ pseudoparticle from the ground state involves, to leading order, a number $2\gamma$ of electrons. Since the currents are two-electron operators, it follows that the creation

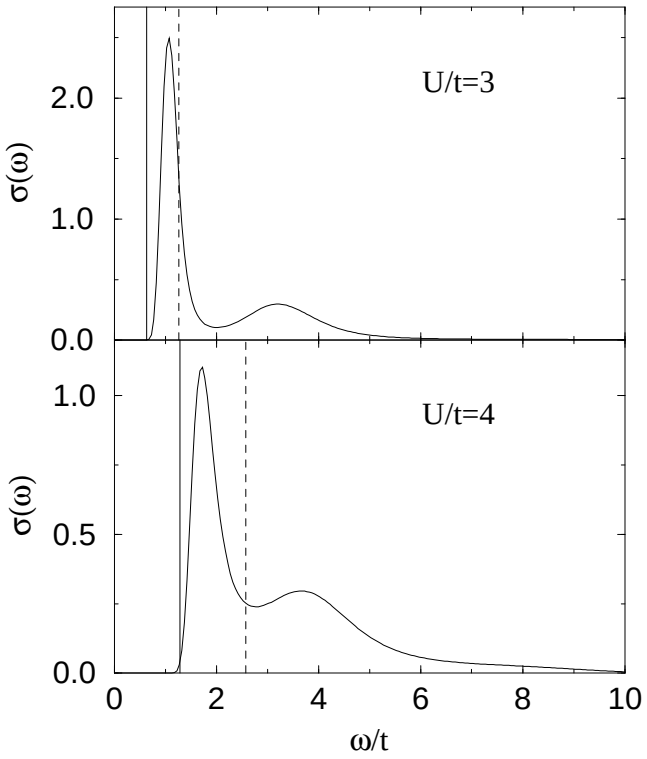



Figure 6.13: Optical conductivity results for 32-site Hubbard chains at half filling for values of $U/t = 3$ (top) and 4 (bottom), computed using maximum-entropy analytic continuation of quantum Monte Carlo data. The solid and dashed vertical lines indicate the theoretical predictions for the lower edges of the first two bands.

of one $\alpha, 1$ pseudoparticle from the ground state is the most important contribution to the transport of charge at finite energies. Moreover, for $U \gg 4t$ the creation of one $c, 1$ pseudoparticle is equivalent to the creation of a single doubly occupied site. Thus, for these values of $U$ only a single optical band should appear in $\sigma_{\rm reg}$. This is an exact result which can be confirmed by numerical studies in this regime [18, 27, 46].

In order to investigate the presence of more than one optical band for small and intermediate values of $U$, recent numerical studies have been performed [15], by use of a quantum Monte Carlo technique for systems with 32 sites. This corresponds to a considerably larger system than in previous exact diagonalization studies [27, 46]. The current-current correlation function has been computed in imaginary time

and continued to real frequency using the so called maximum-entropy method [48]. The resolution of this method is limited but, nevertheless, gives a semi-quantitative confirmation of a multi-band optical conductivity. In Fig. 6.13, the results are shown for $U/t = 3$ and 4 where two peaks are clearly resolved.

As indicated in the figure, the lower edges of the spectra agree with the predicted gaps (Chapter 3), and the second peak appears above the predicted lower edge of the second band, as computed from the pseudoparticle theory. This theory also allows the evaluation of the critical exponents associated with the conductivity edges [13, 14, 15]. Note that the weight of the first band is concentrated towards the lower end of the allowed band of width $8t$. The second peak seen in these results is probably dominated by the second optical band, but likely contains contributions also from the tail of the first band, as well as from higher bands that cannot be resolved due to the limitations of the method.

# Appendix A

# Normal-ordered solution of the BA equations with a flux $\phi$

In this appendix we derive the normal-ordered BA equations required for the evaluation of Eqs. (6.22) and (6.23). Writing $W^{\phi}(q)$ from Eq. (6.21) as

$$W^{\phi}(q) = \frac{dW(q)}{dq} L^{\phi}(q)\,, \tag{A.1}$$

where $L$ equals $L_{c,0}$, $L_{c,\gamma}$, or $L_{s,\gamma}$ when $W$ equals $K$, $R_{s,\gamma}$, or $R_{c,\gamma}$, respectively, we find that $W^{1,\phi}(q)$ obeys the following equality

$$W^{1,\phi}(q) = \frac{dW^{0}}{dq} L^{1,\phi}(q) + \frac{dW^{1}}{dq} L^{0,\phi}(q)\,. \tag{A.2}$$

Introducing the above equation in Eq. (6.19) and writing the distributions functions $N_{\alpha,\gamma}(q)$ as $N^{0}_{\alpha,\gamma}(q) + \delta N_{\alpha,\gamma}(q)$, we can expand $J \equiv \langle m|\, \hat{j}^{\zeta} |m\rangle$ in terms of the pseudomomentum deviations as

$$J = J^{0} + J^{1} + J^{2} \ldots\,, \tag{A.3}$$

where the first term, $J^{1}$, of the current normal-ordered expansion (A.3) can after some algebra be written as

$$\begin{aligned} J^{1} &= J^{1}_{0} - 2t \sum_{j=\pm 1} \frac{L^{0,\phi}_{c,0}(jq_{Fc}) L^{1}_{c,0}(jq_{Fc})}{2\pi\rho_{c,0}(Q)} \sin(Q) + \\ &+ \sum_{\gamma>0} \theta(N_{c,\gamma}) Re\, 4t \sum_{j=\pm 1} \frac{u^{2}[jr_{c,\gamma} - i\gamma]}{\sqrt{1 - u^{2}[jr_{c,\gamma} - i\gamma]^{2}}} \frac{L^{0,\phi}_{c,\gamma}(jq_{Fc,\gamma}) L^{1}_{c,\gamma}(jq_{Fc,\gamma})}{2\pi\rho_{c,\gamma}(r_{c,\gamma})} \end{aligned}$$

$$- \quad 2t \int_{-q_{Fc}}^{q_{Fc}} dq \frac{dK^{(0)}(q)}{dq} \sin(K^{(0)}(q)) \mathcal{L}_{c,0}^{1,\phi}(q) \,, \tag{A.4}$$

where the functions $2\pi\rho_{c,0}(k)$ and $2\pi\rho_{\alpha,\gamma}(r)$ were defined in Ref. [7] and

$$\begin{aligned} J_0^1 &= -2t \int_{-q_c}^{q_c} dq \delta N_c(q) \frac{dK^{(0)}(q)}{dq} \sin(K^{(0)}(q)) L_{c,0}^{0,\phi}(q) \\ &+ \sum_{\gamma>0} Re\, 4t \int_{-q_{c,\gamma}}^{q_{c,\gamma}} dq \delta N_{c,\gamma}(q) \frac{u^2[R_{c,\gamma}^{(0)}(q) - i\gamma]}{\sqrt{1 - u^2[R_{c,\gamma}^{(0)}(q) - i\gamma]^2}} \frac{dR_{c,\gamma}^{(0)}(q)}{dq} L_{c,\gamma}^{0,\phi}(q) \,. \end{aligned} \tag{A.5}$$

The function $\mathcal{L}^{1,\phi}(q)$ is defined as

$$\mathcal{L}^{1,\phi}(q) = L^{1,\phi}(q) - W^1(q) \frac{L^{0,\phi}(q)}{dq} \,. \tag{A.6}$$

In order to obtain the integral equations for $L^{0,\phi}(q)$ and $\mathcal{L}^{1,\phi}(q)$ (with $\mathcal{L} = \mathcal{L}_{c,0}, \mathcal{L}_{c,\gamma}$, and $\mathcal{L}_{s,\gamma}$), we start from the continuum limit of Eqs. (6.9), (6.10), and (6.11) which reads

$$\begin{aligned} K(q) &= q + \phi_\uparrow/N_a - \sum_{\gamma'} \frac{1}{2\pi} \int_{-q_{s,\gamma'}}^{q_{s,\gamma'}} dq' N_{s,\gamma'}(q') \, 2 \tan^{-1} \left( \frac{\sin(K(q))/u - R_{s,\gamma'}(q')}{(\gamma'+1)} \right) \\ &- \sum_{\gamma'>0} \frac{1}{2\pi} \int_{-q_{c,\gamma'}}^{q_{c,\gamma'}} dq' N_{c,\gamma'}(q') \, 2 \tan^{-1} \left( \frac{\sin(K(q))/u - R_{c,\gamma'}(q')}{\gamma'} \right) \,, \end{aligned} \tag{A.7}$$

$$\begin{aligned} 2Re\, \sin^{-1}[(R_{c,\gamma}(q) - i\gamma)u] &= q + \gamma(\phi_\uparrow + \phi_\downarrow)/N_a - \\ &- \frac{1}{2\pi} \int_{-q_c}^{q_c} dq' N_c(q') \, 2 \tan^{-1} \left( \frac{\sin(K(q'))/u - R_{c,\gamma}(q)}{\gamma} \right) \\ &+ \sum_{\gamma'>0} \frac{1}{2\pi} \int_{-q_{c,\gamma'}}^{q_{c,\gamma'}} dq' N_{c,\gamma'}(q') \Theta_{\gamma,\gamma'}(R_{c,\gamma}(q) - R_{c,\gamma'}(q') \,, \end{aligned} \tag{A.8}$$

and

$$\begin{aligned} q &= (\gamma+1)(\phi_\uparrow - \phi_\downarrow)/N_a + \frac{1}{2\pi} \int_{-q_c}^{q_c} dq' N_c(q') \, 2 \tan^{-1} \left( \frac{R_{s,\gamma}(q) - \sin(K(q'))/u}{(\gamma+1)} \right) \\ &- \sum_{\gamma'} \frac{1}{2\pi} \int_{-q_{s,\gamma}}^{q_{s,\gamma}} dq' N_{s,\gamma'}(q') \Theta_{\gamma+1,\gamma'+1}(R_{s,\gamma}(q) - R_{s,\gamma'}(q')) \,. \end{aligned} \tag{A.9}$$

It is convenient to write the function $\Theta_{\gamma,\gamma'}^{[1]}(x)$, defined by Eq. (A.9) of Chapter 4, as follows

$$\Theta^{[1]}_{\gamma,\gamma'}(x) = \sum_l \frac{2b_l^{\gamma,\gamma'}}{1+[x/l]^2}\,. \tag{A.10}$$

We emphasize that comparision term by term of Eq. (A.9) of Chapter 4 with expression (A.10) above fully defines the coefficients $b_l^{\gamma,\gamma'}$ and the corresponding set of integer numbers $l$.

Following equation (6.18), we have that $\phi_\uparrow = \phi_\downarrow$ for a charge-probe current and $\phi_\uparrow = -\phi_\downarrow$ for a spin probe. With the above equations written in terms of $\phi_\uparrow$ and $\phi_\downarrow$, Eq. (A.4) provides both the charge and spin currents. In what follows, we introduce in the functions $L^\phi(q)$ the index $\zeta = \rho, \sigma_z$ to label the equations for either the charge or the spin current, respectively. We start by expanding Eqs. (A.7), (A.8), and (A.9) up to first order in $\phi$. This procedure reveals that the functions $L^{\phi,\zeta}(q)$ obey the following integral equations

$$\begin{aligned} L^{\phi,\zeta}_{c,0}(q) &= \mathcal{C}^\zeta_{c,0} + \sum_{\gamma'} \frac{1}{(\gamma'+1)\pi}\int_{-q_{s,\gamma'}}^{q_{s,\gamma'}} dq'\frac{N_{s,\gamma'}(q')}{1+[\frac{\sin(K(q))/u - R_{s,\gamma'}(q')}{\gamma'+1}]^2}\frac{dR_{s,\gamma'}(q')}{dq'}L^{\phi,\zeta}_{s,\gamma'}(q') \\ &+ \sum_{\gamma'>0}\frac{1}{\pi\gamma'}\int_{-q_{c,\gamma'}}^{q_{c,\gamma'}} dq'\frac{N_{c,\gamma'}(q')}{1+[\frac{\sin(K(q))/u - R_{c,\gamma'}(q')}{\gamma'}]^2}\frac{dR_{c,\gamma'}(q')}{dq'}L^{\phi(q'),\zeta}_{c,\gamma'}(q')\,, \end{aligned} \tag{A.11}$$

$$\begin{aligned} L^{\phi,\zeta}_{c,\gamma}(q) &= \mathcal{C}^\zeta_{c,\gamma} + \frac{1}{\pi u\gamma}\int_{-q_c}^{q_c} dq'\frac{N_c(q')}{1+[\frac{\sin(K(q'))/u - R_{c,\gamma}(q)}{\gamma}]^2}\frac{dK(q')}{dq'}\cos(K(q'))L^{\phi,\zeta}_{c,0}(q') \\ &+ \sum_{\gamma'>0}\sum_l \frac{1}{\pi l}\int_{-q_{c,\gamma'}}^{q_{c,\gamma'}} dq'\frac{N_{c,\gamma'}(q')b_l^{\gamma,\gamma'}}{1+[\frac{R_{c,\gamma}(q) - R_{c,\gamma'}(q')}{l}]^2}\frac{dR_{c,\gamma'}(q')}{dq'}L^{\phi,\zeta}_{c,\gamma'}(q')\,, \end{aligned} \tag{A.12}$$

and

$$\begin{aligned} L^{\phi}_{s,\gamma}(q) &= \mathcal{C}^\zeta_{s,\gamma} + \\ &+ \frac{1}{u(\gamma+1)\pi}\int_{-q_c}^{q_c} dq'\frac{N_c(q')}{1+[\frac{\sin(K(q'))/u - R_{s,\gamma}(q)}{\gamma+1}]^2}\frac{dK(q')}{dq'}\cos(K(q'))L^{\phi,\zeta}_{c,0}(q') \\ &- \sum_{\gamma'}\sum_l \frac{1}{\pi l}\int_{-q_{s,\gamma'}}^{q_{s,\gamma'}} dq'\frac{N_{s,\gamma'}(q')b_l^{\gamma+1,\gamma'+1}}{1+[\frac{R_{s,\gamma}(q) - R_{s,\gamma'}(q')}{l}]^2}\frac{dR_{s,\gamma'}(q')}{dq'}L^{\phi,\zeta}_{s,\gamma'}(q')\,, \end{aligned} \tag{A.13}$$

where the coupling constants $\mathcal{C}^\zeta_{\alpha,\gamma}$ are defined by Eqs. (6.25) and (6.26). We again write the distributions functions $N_{\alpha,\gamma}(q)$ of Eqs. (A.11), (A.12), and (A.13) as $N^0_{\alpha,\gamma}(q) + \delta N_{\alpha,\gamma}(q)$. This allows us to obtain integral equations for $L^{0,\phi,\zeta}(q)$ and

$\mathcal{L}^{1,\phi}(q)$ (we remark that the functions $\mathcal{L}^{1,\phi}(q)$ are the same both for $\zeta = \rho, \sigma_z$). It is then straighforward to find the integral equations obeyed by $L^{0,\phi,\zeta}(q)$ and show that $L^{0,\phi,\zeta}(q)$ can be simply expressed in terms of linear combinations of phase shifts. The final result is

$$L^{0,\phi,\zeta}_{\alpha,\gamma}(q) = \mathcal{C}^{\zeta}_{\alpha,\gamma} + \sum_{\alpha',\gamma'} \sum_{j=\pm 1} j\theta(N_{\alpha',\gamma'}) \mathcal{C}^{\zeta}_{\alpha',\gamma'} \Phi_{\alpha,\gamma;\alpha',\gamma'}(q, jq_{F\alpha',\gamma'}) \,. \tag{A.14}$$

The integral equations obeyed by $\mathcal{L}^{1,\phi}(q)$ are related to the integral equations obeyed by $\tilde{\mathcal{L}}^{1,\phi}(r)$, where $r$ equals $\sin(K^{(0)}(q))/u$, $R^{(0)}_{c,\gamma}(q)$, and $R^{(0)}_{s,\gamma}(q)$ for $\mathcal{L} = \mathcal{L}_{c,0}$, $\mathcal{L}_{c,\gamma}$, and $\mathcal{L}_{s,\gamma}$, respectively. The functions $\tilde{\mathcal{L}}^{1,\phi}(r)$ obey the following integral equations

$$\tilde{\mathcal{L}}^{1,\phi}_{c,0}(r) = \tilde{\mathcal{L}}^{1,\phi,0}_{c,0}(r) + \frac{1}{\pi} \int_{-r_{s,0}}^{r_{s,0}} dr' \frac{\tilde{\mathcal{L}}^{1,\phi}_{s,0}(r')}{1 + (r - r')^2} \,, \tag{A.15}$$

$$\tilde{\mathcal{L}}^{1,\phi}_{c,\gamma}(r) = \tilde{\mathcal{L}}^{1,\phi,0}_{c,\gamma}(r) - \frac{1}{\pi\gamma u} \int_{-r_c}^{r_c} dr' \frac{\tilde{\mathcal{L}}^{1,\phi}_{c,0}(r')}{1 + (\frac{r-r'}{\gamma})^2} \,, \tag{A.16}$$

and

$$\begin{aligned} \tilde{\mathcal{L}}^{1,\phi}_{s,\gamma}(r) &= \tilde{\mathcal{L}}^{1,\phi,0}_{s,\gamma}(r) - \frac{1}{\pi(\gamma+1)u} \int_{-r_c}^{r_c} dr' \frac{\tilde{\mathcal{L}}^{1,\phi}_{c,0}(r')}{1 + (\frac{r-r'}{\gamma})^2} \\ &- \sum_l \frac{1}{\pi l} \int_{-r_{s,0}}^{r_{s,0}} dr' \frac{b_l^{\gamma+1,1} \tilde{\mathcal{L}}^{1,\phi}_{s,0}(r')}{1 + [\frac{r-r'}{l}]^2} \,, \end{aligned} \tag{A.17}$$

where the free terms $\tilde{\mathcal{L}}^{1,\phi,0}_{c,0}(r)$, $\tilde{\mathcal{L}}^{1,\phi,0}_{c,\gamma}(r)$, and $\tilde{\mathcal{L}}^{1,\phi,0}_{s,\gamma}(r)$ are, respectively, given by

$$\begin{aligned} \tilde{\mathcal{L}}^{1,\phi,0}_{c,0}(r) &= \sum_{\gamma'} \frac{1}{\pi\gamma'} \int_{-q_{c,\gamma'}}^{q_{c,\gamma'}} dq' \delta N_{c,\gamma'}(q') \frac{L^{0,\phi}_{c,\gamma'}(q')}{1 + [\frac{r - R^{(0)}_{c,\gamma'}(q')}{\gamma'}]^2} \frac{dR^{(0)}_{c,\gamma'}(q')}{dq'} \\ &+ \sum_{\gamma'} \frac{1}{\pi(\gamma'+1)} \int_{-q_{s,\gamma'}}^{q_{s,\gamma'}} dq' \delta N_{s,\gamma'}(q') \frac{L^{0,\phi}_{s,\gamma'}(q')}{(1 + [\frac{r - R^{(0)}_{s,\gamma'}(q')}{\gamma'+1}]^2)} \frac{dR^{(0)}_{s,\gamma'}(q')}{dq'} \\ &+ \sum_{\gamma'} \theta(N_{c,\gamma'}) \frac{1}{\gamma'\pi} \sum_{j=\pm 1} \frac{jL^1_{c,\gamma'}(jq_{Fc,\gamma'})}{2\pi\rho_{c,\gamma'}(r_{c,\gamma'})} \frac{L^{0,\phi}_{c,\gamma'}(jq_{Fc,\gamma'})}{(1 + [\frac{r - jr_{c,\gamma'}}{\gamma'}]^2)} \\ &+ \sum_{\gamma'} \theta(N_{s,\gamma'}) \frac{1}{(\gamma'+1)\pi} \sum_{j=\pm 1} \frac{jL^1_{s,\gamma'}(jq_{Fs,\gamma'})}{2\pi\rho_{s,\gamma'}(r_{s,\gamma'})} \frac{L^{0,\phi}_{s,\gamma'}(jq_{Fs,\gamma'})}{(1 + [\frac{r - jr_{s,\gamma'}}{\gamma'+1}]^2)} \,, \end{aligned} \tag{A.18}$$

$$\begin{aligned}
\tilde{\mathcal{L}}^{1,\phi,0}_{c,\gamma}(r) &= -\frac{1}{\pi u\gamma}\int_{-q_c}^{q_c} dq'\delta N_c(q')\frac{L^{0,\phi}_{c,0}(q')}{1+[\frac{\sin(K^{(0)}(q'))/u-r}{\gamma}]^2}\cos(K^{(0)}(q'))\frac{dK^{(0)}(q')}{dq'} \\
&- \sum_{\gamma'}\sum_{l}\frac{1}{\pi l}\int_{-q_{c,\gamma'}}^{q_{c,\gamma'}} dq'\delta N_{c,\gamma'}(q')\frac{b_l^{\gamma,\gamma'}L^{0,\phi}_{c,\gamma'}(q')}{1+[\frac{r-R^{(0)}_{c,\gamma'}(q')}{l}]^2}\frac{dR^{(0)}_{c,\gamma'}(q')}{dq'} \\
&- \frac{1}{\gamma u\pi}\sum_{j=\pm 1}\frac{jL^1_{c,0}(jq_{Fc})}{2\pi\rho_{c,0}(Q)}\frac{L^{0,\phi}_{c,0}(jq_{Fc})}{(1+[\frac{r-jr_{c,0}}{\gamma}]^2)}\cos(Q) \\
&- \sum_{\gamma'}\theta(N_{c,\gamma'})\sum_{l}\frac{1}{\pi l}\sum_{j=\pm 1}\frac{jb_l^{\gamma,\gamma'}L^1_{c,\gamma'}(jq_{Fc,\gamma'})}{2\pi\rho_{c,\gamma'}(r_{c,\gamma'})}\frac{L^{0,\phi}_{c,\gamma'}(jq_{Fc,\gamma'})}{(1+[\frac{r-jr_{c,\gamma'}}{l}]^2)}\,, \qquad \text{(A.19)}
\end{aligned}$$

and

$$\begin{aligned}
\tilde{\mathcal{L}}^{1,\phi,0}_{s,\gamma}(r) &= \frac{1}{\pi u(\gamma+1)}\int_{-q_c}^{q_c} dq'\delta N_c(q')\frac{L^{0,\phi}_{c,0}(q')}{1+[\frac{\sin(K^{(0)}(q'))/u-r}{\gamma+1}]^2}\cos(K^{(0)}(q'))\frac{dK^{(0)}(q')}{dq'} \\
&- \sum_{\gamma'}\sum_{l}\frac{1}{\pi l}\int_{-q_{s,\gamma'}}^{q_{s,\gamma'}} dq'\delta N_{s,\gamma'}(q')\frac{b_l^{\gamma+1,\gamma'+1}L^{0,\phi}_{s,\gamma'}(q')}{1+[\frac{r-R^{(0)}_{s,\gamma'}(q')}{l}]^2}\frac{dR^{(0)}_{s,\gamma'}(q')}{dq'} \\
&+ \frac{1}{(\gamma+1)u\pi}\sum_{j=\pm 1}\frac{jL^1_{c,0}(jq_{Fc})}{2\pi\rho_{c,0}(Q)}\frac{L^{0,\phi}_{c,0}(jq_{Fc})}{(1+[\frac{r-jr_{c,0}}{\gamma+1}]^2)}\cos(Q) \\
&- \sum_{\gamma'}\theta(N_{s,\gamma'})\sum_{l}\frac{1}{\pi l}\sum_{j=\pm 1}\frac{jb_l^{\gamma+1,\gamma'+1}L^1_{s,\gamma'}(jq_{Fs,\gamma'})}{2\pi\rho_{s,\gamma'}(r_{s,\gamma'})}\frac{L^{0,\phi}_{s,\gamma'}(jq_{Fs,\gamma'})}{(1+[\frac{r-jr_{s,\gamma'}}{l}]^2)}\,. \qquad \text{(A.20)}
\end{aligned}$$

Introducing the functions $\mathcal{L}^{1,\phi}(q)$ obtained from Eqs. (A.15), (A.16), and (A.17) in Eq. (A.4) and keeping terms only up to second order in the density of heavy pseudoparticles, we obtain Eq. (6.19) with $j^{\zeta}_{\alpha,\gamma}(q)$ given by

$$j^{\zeta}_{\alpha,\gamma}(q) = v_{\alpha,\gamma}(q)L^{0,\phi,\zeta}_{\alpha,\gamma}(q) + \sum_{\alpha',\gamma'}\sum_{j=\pm 1} j\theta(N_{\alpha',\gamma'})v_{\alpha',\gamma'}L^{0,\phi,\zeta}_{\alpha',\gamma'}(jq_{F\alpha',\gamma'})\Phi_{\alpha',\gamma';\alpha,\gamma}(jq_{F\alpha',\gamma'},q)\,. \qquad \text{(A.21)}$$

Inserting Eq. (A.14) in Eq. (A.21) we obtain Eq. (6.23).

# Appendix B

# Static masses for the heavy pseudoparticles

The $\alpha, \gamma$ pseudoparticle static mass, $m^*_{\alpha,\gamma}$, is defined in Ref. [7] as

$$\frac{1}{m^*_{\alpha,\gamma}} = \left.\frac{2t\, d\eta_{\alpha,\gamma}(r)/dr}{(2\pi\rho_{\alpha,\gamma}(r))^2}\right|_{r=r^0} - \left.\frac{2t\eta_{\alpha,\gamma}(r)(2\pi\, d\rho_{\alpha,\gamma}(r)/dr)}{(2\pi\rho_{\alpha,\gamma}(r))^3}\right|_{r=r^0} , \tag{B.1}$$

where the functions $2t\eta_{\alpha,\gamma}(r)$ and $2\pi\rho_{\alpha,\gamma}(r)$ are defined in Ref. [7] and $r^0$ stands for $W^0_{\alpha,\gamma}(q_{F\alpha,\gamma})$ which represents $Q$, $r_{c,\gamma}$, and $r_{s,\gamma}$.

After some straightforward algebra, the general expressions (B.1) lead to the following simple expressions for $1/m^*_{\alpha,\gamma}$

$$\frac{1}{m^*_{c,\gamma}} = \frac{-4tu^2/(1+u^2\gamma^2)^{3/2} + \Lambda^\eta_{c,\gamma}}{(2u/\sqrt{1+u^2\gamma^2} - \Lambda^\rho_{c,\gamma})^2} , \qquad \gamma > 0 , \tag{B.2}$$

and

$$\frac{1}{m^*_{s,\gamma}} = \frac{\Lambda^\eta_{c,\gamma+1} - \Lambda^\eta_{s,\gamma} - \Lambda^\eta_{s,\gamma+2}}{(\Lambda^\rho_{c,\gamma+1} - \Lambda^\rho_{s,\gamma} - \Lambda^\rho_{s,\gamma+2})^2} , \qquad \gamma > 0 . \tag{B.3}$$

In Eqs. (B.2) and (B.3) the functions $\Lambda^\eta_{\alpha,x}$ and $\Lambda^\rho_{\alpha,x}$ read

$$\Lambda^\eta_{\alpha,x} = 2\int_{-q_{F\alpha,0}}^{q_{F\alpha,0}} \frac{dq}{\pi x^3} \frac{v_{\alpha,0}(q) R^{(0)}_{\alpha,0}(q)}{[1 + (R^{(0)}_{\alpha,0}(q)/x)^2]^2} , \tag{B.4}$$

and

$$\Lambda^\rho_{\alpha,x} = \int_{-q_{F\alpha,0}}^{q_{F\alpha,0}} \frac{dq}{\pi x} \frac{1}{1 + [R^0_{\alpha,0}(q)/x]^2} , \tag{B.5}$$

with

$$R_{c,0}^{(0)}(q) = \frac{\sin(K^{(0)}(q))}{u}\,. \tag{B.6}$$

In the limit of fully polarized ferromagnetism, these expressions lead to the following closed-form expressions for the static masses

$$\frac{1}{m_{c,\gamma}^{*}} = \frac{t\pi}{8[\eta_{1,\gamma}]^2}\left(-\frac{\pi + 2[\eta_{1,\gamma}]}{\sqrt{1+[u\gamma]^2}} - \frac{u\gamma\sin(2n\pi)}{[u\gamma]^2+\sin^2(n\pi)}\right) \tag{B.7}$$

and

$$\frac{1}{m_{s,\gamma}^{*}} = \frac{t\pi}{[\eta_{2,\gamma+1}]}\left(\frac{1}{\sqrt{1+[u(\gamma+1)]^2}} - \frac{u(\gamma+1)}{2[\eta_{2,\gamma+1}]}\frac{\sin(2n\pi)}{[u(\gamma+1)]^2+\sin^2(n\pi)}\right)\,, \tag{B.8}$$

where

$$\eta_{1,x} = \tan^{-1}[\cot(n\pi)\frac{xu}{\sqrt{1+u^2x^2}}]\,, \tag{B.9}$$

and $\eta_{2,x} = \pi/2 - \eta_{1,x}$. We remark that the static masses of the $c,\gamma$ pseudoparticles are, in general, negative. The static masses of the $\alpha, 0$ pseudoparticles have been studied in Ref. [49].

# Appendix C

# Charge and spin stiffnesses at zero temperature

In this Appendix we show that the direct use of Eq. (6.35) leads to the stiffness expressions (135) - (137) of Ref. [8, 9].

The calculation of the charge and spin stiffnesses (6.35) requires the expansion of Eq. (6.12) and of Eqs. (A.7), (A.8), and (A.9) up to second order in $\phi$. As in the case of the charge and spin current, both he charge and spin stiffnesses can be computed from Eq. (6.35), and we obtain one or the other depending on the coupling constants we choose in Eqs. (A.7), (A.8), and (A.9). Expanding the ground-state energy up to second order in $\phi$, we obtain

$$\left.\frac{d^2(E_0/N_a)}{d(\phi/N_a)^2}\right|_{\phi=0} = \frac{1}{2\pi}\int_{-q_{Fc}}^{q_{Fc}} dq \left[2tK^{0,\phi\phi}(q)\sin(K^{(0)}(q)) + 2t[K^{0,\phi}(q)]^2\cos(K^{(0)}(q))\right] , \tag{C.1}$$

where the function $K^{0,\phi\phi}(q)$ is the second derivative of the rapidity function defined by Eq. (A.7) in order to $\phi/N_a$ at $\phi = 0$. The functions $K^{0,\phi}(q)$ and $K^{0,\phi\phi}(q)$ can be written as

$$K^{0,\phi}(q) = \frac{dK^{(0)}(q)}{dq} L_{c,0}^{0,\phi}(q) , \tag{C.2}$$

and

$$K^{0,\phi\phi}(q) = \frac{d}{dq}\left(\frac{dK^{(0)}(q)}{dq}[L_{c,0}^{0,\phi}(q)]^2\right) + 2\frac{dK^{(0)}(q)}{dq} L_{c,0,*}^{0,\phi\phi} , \tag{C.3}$$

respectively. The use of Eqs. (C.2) and (C.3) in Eq. (C.1) leads then to

$$\left.\frac{d^2(E_0/N_a)}{d(\phi/N_a)^2}\right|_{\phi=0} = \frac{1}{2\pi}\int_{-q_{Fc}}^{q_{Fc}} dq 2t\sin(K^{(0)}(q))2\frac{dK^{(0)}(q)}{dq}L_{c,0,*}^{0,\phi\phi}(q) + \frac{1}{2\pi}\sum_{j=\pm 1}\frac{2t\sin(Q)[L_{c,0}^{0,\phi}(jq_{Fc})]^2}{2\pi\rho_{c,0}(Q)}\,, \quad \text{(C.4)}$$

where the function $L_{c,0}^{0,\phi}(jq_{Fc})$ is defined in Appendix A. The function $L_{c,0,*}^{0,\phi\phi}(q)$ obeys the following integral equation

$$L_{c,0,*}^{0,\phi\phi}(q) = \frac{1}{2\pi}\sum_{j=\pm 1}\frac{j[L_{s,0}^{0,\phi}(jq_{Fs,0})]^2}{2\pi\rho_{s,0}(r_{s,0})(1+[\sin(K^{(0)}(q))/u - jr_{s,0}]^2)} + \frac{1}{\pi}\int_{-q_{Fs,0}}^{q_{Fs,0}} dq'\frac{dR_{s,0}^{(0)}(q')}{dq'}\frac{L_{s,0,*}^{0,\phi\phi}(q')}{1+[\sin(K^{(0)}(q))/u - R_{s,0}^{0}(q')]^2}\,, \quad \text{(C.5)}$$

which was obtained by performing the type of expansions developed in Appendix A. Moreover, $L_{s,0,*}^{0,\phi\phi}(q)$ is given by

$$\begin{aligned} L_{s,0,*}^{0,\phi\phi}(q) &= \frac{1}{2u\pi}\sum_{j=\pm 1}\frac{j[\cos(Q)L_{c,0}^{0,\phi}(jq_{Fc})]^2}{2\pi\rho_{c,0}(Q)(1+[R_{s,0}^{(0)}(q) - jr_{c,0}]^2)} \\ &- \frac{1}{4\pi}\sum_{j=\pm 1}\frac{j[L_{s,0}^{0,\phi}(jq_{Fs,0})]^2}{2\pi\rho_{s,0}(r_{s,0})(1+[(R_{s,0}^{(0)}(q) - jr_{s,0})/2]^2)} \\ &- \frac{1}{2\pi}\int_{-q_{Fs,0}}^{q_{Fs,0}} dq'\frac{dR_{s,0}^{(0)}(q')}{dq'}\frac{L_{s,0,*}^{0,\phi\phi}(q')}{1+[(R_{s,0}^{(0)}(q) - R_{s,0}^{(0)}(q'))/2]^2} \\ &+ \frac{1}{\pi u}\int_{-q_{Fc}}^{q_{Fc}} dq'\frac{dK^{(0)}(q')}{dq'}\frac{\cos(K^{(0)}(q'))L_{c,0,*}^{0,\phi\phi}(q')}{1+(\sin(K^{(0)}(q'))/u - R_{s,0}^{(0)}(q))^2}\,. \end{aligned} \quad \text{(C.6)}$$

Introducing Eqs. (C.5) and (C.6) in Eq. (C.4) we obtain, after some algebra, the following expression for the (charge and spin) stiffness $D^{\zeta}$

$$4\pi D^{\zeta} = \sum_{j=\pm 1} v_{c,0}[L_{c,0}^{0,\phi,\zeta}(jq_{Fc,0})]^2 + \sum_{j=\pm 1} v_{s,0}[L_{s,0}^{0,\phi,\zeta}(jq_{Fs,0})]^2\,, \quad \text{(C.7)}$$

where the functions $L^{0,\phi,\zeta}(jq_{F\alpha,0})$ are defined by Eq. (A.14). After some simple algebra, expression (C.7) can be shown to be the same as expressions (135) - (137) of Ref. [8, 9].

# Appendix D

# The zero magnetic-field solution

For the case of zero magnetic field it is possible to cast the equations for the energy bands, phase shifts, and rapidities in a simpler form. After some algebra, the $\epsilon^0_{s,\gamma}(q)$ band (with $\gamma = 0, 1, 2, \ldots, \infty$) and the $\epsilon^0_{c,\gamma}(q)$ band with ($\gamma = 1, 2, \ldots, \infty$) can at zero magnetic field be rewritten as

$$\epsilon^0_{s,\gamma}(q) = -\delta_{\gamma,0}\left[2t\int_0^\infty d\omega \frac{\cos(\omega R^{(0)}_{s,0}(q))}{\omega\cosh(\omega)}\Upsilon_1(\omega)\right], \tag{D.1}$$

and

$$\begin{aligned}\epsilon^0_{c,\gamma}(q) &= Re\, 4t\sqrt{1-u^2(R^{(0)}_{c,\gamma}(q)+i\gamma)^2} - \\ &- 4t\int_0^\infty d\omega \frac{e^{-\gamma\omega}}{\omega}\cos(\omega R^{(0)}_{c,\gamma}(q))\Upsilon_1(\omega)\,,\end{aligned} \tag{D.2}$$

where $\Upsilon_1(\omega)$ obeys the integral equation

$$\Upsilon_1(\omega) = \Upsilon^0_1(\omega) + \int_{-\infty}^{\infty} d\omega'\Upsilon_1(\omega')\Gamma(\omega',\omega)\,. \tag{D.3}$$

Here the free term and the kernel read

$$\Upsilon^0_1(\omega) = \frac{1}{2\pi}\int_{-Q}^{Q} dk\sin(k)\sin(\omega\sin(k)/u)\,, \tag{D.4}$$

and

$$\Gamma(\omega',\omega) = \frac{\sin((\omega-\omega')r_{c,0})}{\pi(\omega-\omega')(1+e^{2|\omega'|})}\,, \tag{D.5}$$

respectively. The kernel (D.5) was already obtained in Ref. [50] (see Eq. (A5) of that reference). Equation (D.1), together with the fact that in the limit of zero

magnetic field the width of the $s,\gamma>0$ momentum pseudo-Brillouin zone vanishes [see Eq. (6.36)], shows that the $s,\gamma$ bands collapse for $\gamma>0$ and all values of $U$ and $n$ to the point zero.

In this limit it is also possible to cast the integral equations for the phase shifts, whose expressions are given in Ref. [7], in the following alternative form

$$\bar{\Phi}_{c,0;c,0}(r,r') = -B(r-r') + \int_{-r_{c,0}}^{r_{c,0}} dr'' \bar{\Phi}_{c,0;c,0}(r'',r') A(r-r'')\,, \tag{D.6}$$

$$\bar{\Phi}_{c,0;c,\gamma'}(r,r') = -\frac{1}{\pi}\tan^{-1}(\frac{r-r'}{\gamma'}) + \int_{-r_{c,0}}^{r_{c,0}} dr'' \bar{\Phi}_{c,0;c,\gamma'}(r'',r') A(r-r'')\,, \tag{D.7}$$

$$\begin{aligned}\bar{\Phi}_{c,0;s,\gamma'}(r,r') &= -\delta_{0,\gamma'}\frac{1}{2\pi}\tan^{-1}[\sinh(\pi/2(r-r'))] + \\ &+ \int_{-r_{c,0}}^{r_{c,0}} \frac{dr''}{\gamma'+1}\bar{\Phi}_{c,0;s,\gamma'}(r'',r') A(r-r'')\,,\end{aligned} \tag{D.8}$$

$$\bar{\Phi}_{c,\gamma;c,0}(r,r') = \frac{1}{\pi}\tan^{-1}(\frac{r-r'}{\gamma}) - \int_{-r_{c,0}}^{r_{c,0}} \frac{dr''}{\pi\gamma}\frac{\bar{\Phi}_{c,0;c,0}(r'',r')}{1+(\frac{r-r''}{\gamma})^2}\,, \tag{D.9}$$

$$\bar{\Phi}_{c,\gamma;c,\gamma'}(r,r') = \frac{1}{2\pi}\Theta_{\gamma,\gamma'}(r-r') - \int_{-r_{c,0}}^{r_{c,0}} \frac{dr''}{\pi\gamma}\frac{\bar{\Phi}_{c,0;c,\gamma'}(r'',r')}{1+(\frac{r-r''}{\gamma})^2}\,, \tag{D.10}$$

$$\bar{\Phi}_{c,\gamma;s,\gamma'}(r,r') = -\int_{-r_{c,0}}^{r_{c,0}} \frac{dr''}{\pi\gamma}\frac{\bar{\Phi}_{c,0;s,\gamma'}(r'',r')}{1+(\frac{r-r''}{\gamma})^2}\,, \tag{D.11}$$

$$\bar{\Phi}_{s,\gamma;c,0}(r,r') = 0\,, \tag{D.12}$$

$$\bar{\Phi}_{s,\gamma;c,\gamma'}(r,r') = \delta_{0,\gamma}\frac{1}{4}\int_{-r_{c,0}}^{r_{c,0}} dx'' \frac{\bar{\Phi}_{c,0;c,\gamma'}(r'',r')}{\cosh(\pi/2(r''-r))}\,, \tag{D.13}$$

$$\begin{aligned}\bar{\Phi}_{s,0;s,\gamma'}(r,r') &= \frac{1}{\pi}\int_0^\infty d\omega \frac{\sin(\omega[r-r'])}{\omega(1+e^{2\omega})}[e^{-\gamma'\omega} + (1-\delta_{0,\gamma'})e^{-(\gamma'-2)\omega}] \\ &+ \frac{1}{4}\int_{-r_{c,0}}^{r_{c,0}} \frac{dr''}{\gamma'+1}\frac{\bar{\Phi}_{c,0;s,\gamma'}(r'',r')}{\cosh(\pi/2(r-r''))}\,,\end{aligned} \tag{D.14}$$

and

$$\bar{\Phi}_{s,\gamma>0;s,\gamma'}(r,r') = \frac{1}{2\pi}\Theta_{\gamma+1,\gamma'+1}(r-r') -$$
$$- \quad \frac{1}{\pi}\int_0^\infty d\omega \frac{\sin[\omega(r-r')]}{\omega(1+e^{2\omega})} e^{-(\gamma'+\gamma)\omega}[2-\delta_{0,\gamma'}+e^{-2\omega}+(1-\delta_{0,\gamma'})e^{2\omega}]\,. \quad \text{(D.15)}$$

The functions $A(r)$ and $B(r)$ are defined as

$$A(r) = \frac{1}{\pi}\int_0^\infty d\omega \frac{\cos(r\omega)}{1+e^{2|\omega|}}\,, \quad \text{(D.16)}$$

and

$$B(r) = \frac{1}{\pi}\int_0^\infty d\omega \frac{\sin(r\omega)}{\omega(1+e^{2|\omega|)}}\,, \quad \text{(D.17)}$$

respectively.

At $n = 1$ we have that $\Upsilon_1(x) = \Upsilon_1^0(x) = J_1(x/u)$, where $J_1(x/u)$ is the Bessel function of order one, and the bands (D.1) and (D.2) are obtained in closed form.

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# Chapter 7

# Conclusions

In this Thesis we have focused our attention on the one-dimensional Hubbard model. As it became clear from Chapters 1 and 2, the Hubbard Hamiltonian, as introduced by Hubbard, Gutzwiller, and Kanamori [1, 2, 3], is the simplest model for the description of interacting electrons in a lattice.

Introduced firstly to study itinerant ferromagnetism in transition metals, the Hubbard model revealed later to have an antiferromagnetic ground state [4]. With the discovery of a new class of superconducting materials, by Berdnoz and Müller in 1986 [6] and the proposal, by Anderson [5], that the 2D Hubbard model would retain the essential physics of these new materials, the model gained renewed interest. It soon became clear that, for the values of the physical parameters imposed by the experimental results, the usual theoretical tools would not suffice to deal with this model (and its "relatives") [7] and that, accordingly, the search for non-perturbative methods should be pursued. The claim by Anderson that the 2D Hubbard model should present many similarities with its one-dimensional counterpart [5], for which an exact solution is available, together with better crystals of quasi one-dimensional materials, and more refined experimental methods (e.g. angle resolved photoemission measurements) [8], renewed the interest in the one-dimensional Hubbard model.

At present, the theoretical goal associated with the study of the Hubbard model is to investigate the role of electron-electron interactions in relation with the thermodynamic and transport properties of a non-perturbative electron liquid. Based on the exact Bethe-ansatz solution of the Hubbard chain and on its symmetries, we presented an algebraic representation for all the eigenstates of the model (Chapter 3). Our representation is much simpler than the starting Bethe-ansatz wave function. The latter is a complicated sum of permutations written in terms of

the original electronic operators, while the former representation is a simple Slater determinant of pseudoholes and heavy pseudoparticles (Chapter 3). These latter operators are the quantum operators that diagonalize the Hubbard Hamiltoninan. In this representation it is then simpler to select and characterize the relevant eigenstates which contribute to a given physical property of the model. For example, the low-temperature thermodynamics for electronic fillings less than one and finite magnetization is controlled by the eigenstates with no heavy-pseudoparticles occupancy; on the other hand, the optical conductivity is controlled, at half filling, by eigenstates with one $c, 1$ heavy pseudoparticle and two $c, 0$ pseudoholes. This kind of characterization is by no means possible for the usual Bethe-ansatz wave function, and it is essencial for a simple calculation of correlation functions using conformal-field theory methods [9, 10, 11, 12].

The pseudoparticle perturbation theory (PPT) described in Chapter 4, combined with the results of Chapter 3 and with new results on conformal theory methods [11, 12], allow the calculation of correlation functions at low $(\omega - \omega_0)$ frequency values (note that $\omega_0$ can be very large). This possibility goes much beyond both bosonization studies [13], and the spinon and holon conformal-field theory of Framh and Korepin [9, 10]. The possibility opened up by our pseudoparticle theory, namely that of giving finite energy results for the spectral functions of the model, allows the comparison of finite energy spectral functions in real materials with the results obtained for the Hubbard model. This is a topic that deserves further research.

The use of the algebraic representation introduced in Chapter 3 permits the computation of the energy eigenvalues for all the eigenstates of the model. This can be accomplished, at least in principle, by means of the PPT developed in Chapter 4. This PPT is an expansion of the Hamiltoninan in the density of excited pseudoparticles, relatively to a suitable reference state. The most convenient choice for the reference state is, for most of the physical properties, the ground state or the generalized ground-state, both introduced in Chapter 3.

The normal-ordered PPT Hamiltonian describes the physics associated with the Hilbert subspace spanned by the reference state and all Hamiltonian eigenstates differing from it by the occupancies of a small density of pseudoparticles. Combined with a generalized conformal-field theory, the PPT provides the leading-order expressions of correlation functions for low-energies $(\omega - \omega_0)$. These expressions refer either to the low-energy functions ($\omega_0 = 0$) [9, 10, 14] or to energy values closed to the energy gaps, $\omega_0$, of Hamiltonian eigenstates with heavy-pseudoparticle occupancy [11, 12].

Very important for the description of excitations that change the number of electrons $N_\uparrow$ and/or $N_\downarrow$ (change of canonical ensemble) and/or the number of pseudoparticles (change of sub-canonical ensemble) is the study of the collective pseudo momentum shifts of value $\pm\pi/N_a$. These momentum shifts are generated by the topological momentum shift operators introduced in Chapter 5. These are important in two ways: (i) they contribute to the momentum of state transitions connecting different canonical ensembles and sub-canonical ensembles [15, 16]; (ii) in transitions between ground states, the final pseudoparticle momenta are such that the final ground state has the lowest possible energy [17]. The importance of these types of excitations had not been recognized before in the literature in its full relevance.

The problem of charge and spin transport in the one-dimensional many-body problem, in general, and in one-dimensional integrable models, in particular, is a difficult and subtle issue [18, 19, 20, 21, 22]. By using the Bethe-ansatz equations with twisted boundary conditions, we have obtained a general formula for the mean value of the charge and spin current operators (Chapter 6). However, the functional character of this expression does not seem amenable to practical calculations. Combining this general functional with the PPT, and performing equivalent calculations to those presented in Chapter 4, we were able to compute the mean value of the charge and spin currents for a given subset of eigenstates of the model. The obtained normal-ordered functional provides the current for states that differ from the reference state by a small density of excited pseudoparticles. Our current functional provided the values for the transport mass of the charge and spin carriers. These masses provide important information on the role of electronic correlations in the transport properties. Our functional representation can also provide information on the transport of charge and spin at finite temperatures. Althougt the PPT does not cover the full range of temperatures $T$ from 0 to $\infty$, it provides some information in some regimes. For example, away from half filling, the regime where PPT can be used is $T \ll v_{Fc,0}q_{Fc,0}$, while at half filling it is $T \ll \Delta$, where $\Delta$ is the smallest of the energy gaps $\omega_0$ derived in Chapter 4. Studies on finite-temperature transport by use of the PPT is a subject of current research.

The study of the Bethe-ansatz equations, together with the PPT, gave the coupling constants of the pseudoparticles to the external charge and spin probes. These coupling constants provide selection rules for the ground state transitions. Conformal-field theory provides asymptotic expressions for correlation functions, including their $x, t$ (space and time) and $k, \omega$ (momentum and frequency) depen-

dences. However, it does not provide the multiplicative constants determined by the weights of the ground-state transitions, which control these expressions and dependences. Often, due to symmetry and selection rules, these weights and corresponding constants vanish. Therefore, the above couplings provide relevant information on such rules, which goes beyond conformal-field theory.

Both the coupling constants and the mean value of the charge and spin current operators can also be derived from a semi-classical transport description of the quantum liquid. Comparing this approach to the Bethe-ansatz exact solution (PPT theory), one confirms that the kinetic approach gives exact results for small $(\omega-\omega_0)$, while for a Fermi liquid the same kinetic approach gives exact results for small $\omega$ only. This difference can be traced back to the existence of only forward scattering among the pseudoparticles at all energy scales, and it is peculiar of integrable one-dimensional models.

The formalism presented here is applicable to other one-dimensional integrable systems [23]. Examples of these are the super-symmetric $t-J$ and the lattice spinless fermion models. Both these models present interesting transport properties, since the charge current operator does not commute with the Hamiltonian. Besides the charge stiffness, there is a finite-energy absorption that can be studied by combinig the methods presented in Chapters 3, 4, 5, and 6 with the thechniques of conformal-field theory [9, 10, 11, 12]. Also the study of finite-temperature transport can be fulfilled by developing the apropriate PPT for these models. Following the results presented here, calculations for the lattice spinless fermion model are currently being developed [24].

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