Theoretical study of gapless low-dimensional systems: graphene and the Luttinger model

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2014
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Chapter 1

Introduction

Exploring electronic properties of low-dimensional systems is one of the most exciting fields of solid state physics in the last few decades. Due to experimental realizations, materials with less than three spatial dimensions became the object of intense investigation. Quasi two-dimensional systems are available in quantum wells of semiconductor heterostructures and have tremendous number of applications in electronic circuits, optical devices, etc. These tools are already parts of our everyday life. Quantum wells have also enabled to study interesting correlated many body phenomena, such as fractional quantum Hall effect observed in the presence of high magnetic field. One-dimensional systems also attracted lots of interest partially due to their realizations in carbon nanotubes, in huge organic molecules or at the edges of topological insulators but mostly because of their theoretical importance. Namely, theoretical techniques, such as Bethe Ansatz or bosonization, provide exact solutions to the interacting one-dimensional system which is not possible in two- or three dimensional systems to date.

One of the most remarkable low dimensional system is the two-dimensional graphene\[1\] which is also the subject of the first part of this dissertation. This material is a one-atomic thick layer of carbon atoms arranged in a honeycomb lattice, which was first fabricated by mechanical exfoliation from bulk graphite. Extracting graphene flakes from graphite with for example a scotch tape results in a stack of carbon debris which consist of not only monolayer but also bilayer, trilayer and other multilayer graphene. Since the optical transmission of graphene on SiO\textsubscript{2} substrate highly depends on the number of layers, the monolayer flakes can simply be isolated by using optical microscope.
Immediately after its discovery in 2004, monolayer graphene triggered intensive research due to its high potential for industrial applications. The mechanical strength [2], the high mobility of charge carriers[3], and the high optical transmission rate[4] make graphene suitable for invisible electric circuits, efficient solar cells or for high-frequency transistors but it could also be used as hydrogen storage, p-n junctions with negative refractive index[5], just to mention several items from the long list of potential applications of graphene.

Graphene has been attracting lots of interest from theoretical point of view as well. While electronic properties of standard metals are described as free electron gases with parabolic energy spectrum, electrons in graphene behave as massless Dirac fermions with linear isotropic dispersion relation [6, 7, 8]. Since the Fermi velocity is three-hundred times smaller than the speed of light, relativistic phenomena, such as the Klein paradox, became experimentally observable. Due to the gapless nature of band structure of massless fermions, undoped (half filled) graphene behaves as zero gap semiconductor or sometimes called a semimetal, placing it somewhere between good metals and insulators. Applying appropriate gate voltage leads to electron or hole pockets and metallic behavior. The linear dispersion results in a linearly vanishing density of states near half filling which essentially influences the transport and optical properties.

Another peculiarity of electrons in graphene is that they possess a so-called pseudospin degree of freedom beside the real spin. This additional degree of freedom stems from the lattice structure, namely, the unit cell of the honeycomb lattice contains two atoms. For the low energy electron states, the direction of pseudospin is equal to the direction of its momentum, while for hole states they point just in the opposite direction. Hence, quasi-particles of electron and hole states in graphene may be referred to as chiral particles and are analogous to relativistic massless particles and anti-particles, respectively. This chirality is closely related to the non-trivial topology of electronic states which is manifested, for example, in the half-integer quantum Hall effect [9] observable even at room temperature, showing the robustness of the topologically protected states.

Although graphene shows many exciting phenomena due to the massless, chiral nature of the electrons, researchers make efforts to open a gap in the spectrum in order to use graphene as a substitute material of silicon in electric circuits. There are various suggested methods to make progress, for example, by cutting graphene nanoribbons, applying appropriate strain,
or gate voltages but none of them is experimentally well controllable. Another possible way of opening a bandgap is to somehow control the strength of Coulomb interaction between electrons. The effect of electron-electron interactions on the electronic structure is, therefore, one of the most exciting field of graphene physics[10]. Due to the strong tight-binding character of the electrons of carbon atoms and the weak intrinsic screening, one would expect strong electron correlations in graphene. However, for a long time no experimental evidence of the relevance of electron-electron interaction in graphene had been found. In 2011, the electron structure of suspended monolayer was found to be strongly influenced by interaction effects [11] but no energy gap has been found yet.

To summarize all that has been mentioned so far, graphene exhibits interesting physical phenomena and is also a promising material in future industrial applications. In the present thesis, we study several aspects of the electronic structure of graphene, including the interaction between substitutional impurities and electrons, effects of Coulomb interaction and dynamical properties in terms of optical conductivity. In the course of our investigations, we shed light on what fundamental properties of graphene are responsible for unconventional observations, such as universal value of the optical conductivity or unconventional critical behaviour of the Mott transition, and the results enable one to make predictions on the behaviour of other particular systems.

Almost at the same time of the discovery of graphene, low-dimensional systems became available in cold atomic systems [12] opening a new route to understanding the nature of fundamental quantum processes by controlling the parameters of the system artificially. To establish ultracold systems, atoms are confined in a magnetic or optical trap and the temperature is decreased by laser cooling typically down to several microkelvins. Although these systems could be used in principle in quantum information processes, more importantly, they allow one to accurately realize simple, well-studied models, such as the Bose-Hubbard model or the Luttinger model [12, 13]. The parameters of the model can be tuned artificially in the experiment, leading to the observation of correlated phenomena, for example, superfluid-insulator transition of the Bose-Hubbard model.

The controllability of model parameters also provide the opportunity to study the time evolution of closed interacting quantum systems due to the weak coupling between the atoms and the environment. While equilibrium properties of interacting systems can be understood
very well by mean-field theory or renormalization group theory, non-equilibrium dynamics of quantum systems is much less clear. One of the most interesting question is how a quantum system prepared in a specific initial state thermalizes. The possibility to simulate non-equilibrium processes in ultracold atomic systems motivates a lot of theorists to answer this kind of questions. In experiments, special initial states can be achieved by performing a quantum quench driving the system away from equilibrium. Therefore, theoretical works usually focus on the time evolution of interacting systems following a quantum quench and relaxation of different physical quantities and correlation functions.

For the sake of simplicity, the time evolution is usually studied in systems with one spatial dimension. In this thesis, we investigate the dynamics of the Luttinger model after a quantum quench midst of which the interaction strength is switched on following a time dependent protocol. Since the final Hamiltonian describes an integrable system, there is a macroscopic number of constants of motion and the system does not achieve the thermal equilibrium in the long time limit. Full description of this peculiar steady state is given by the so-called diagonal ensemble which we determine in this dissertation. We also make predictions on some directly measurable physical quantities, such as the statistics of energy and work done on the system during the quench.

More detailed introduction of these topics will be found at the beginning of the upcoming chapters. The dissertation is organized as follows. In Chapter 2, electronic properties of graphene are reviewed within tight-binding approximation. These results have been known for a long time but are worth revisiting. New results on graphene are presented in Chapters 3, 4 and 5. In Chapter 3, we study impurity scattering of electrons on a well localized impurity and by analyzing the short wavelength pattern of the Friedel oscillation we make predictions on experiments probing the electron density around the impurity. In Chapter 4, we focus on the critical behaviour of the Mott transition in graphene and general gapless systems. The results are obtained in a very general framework, allowing us to explain or predict critical exponents in a wide class of systems. In Chapter 5, we study the dynamical properties of graphene and show that its universal behaviour is not related to its peculiar linear dispersion relation but is a consequence of the two-dimensionality and its chiral nature. The results are extended to general chiral systems in which the optical conductivity shows universal behaviour in the low frequency regime.
In Chapter 6, we study the dynamical properties of the Luttinger model after a quantum quench. New results of this chapter are the finite temperature effects in the density matrix of the steady state and the Loschmidt echo. We also make predictions on the statistics of total energy and work done measured on systems at finite temperature. In Chapter 7, the results of the dissertation are summarized focusing on the new results and the thesis statements are also listed.
In this chapter we review the basics of electronic structure of graphene which has been known for a long time [14]. We also introduce notations which are used consistently throughout the dissertation.

Graphene is a two-dimensional material consisting of carbon atoms arranged in a honeycomb lattice (see Fig. 2.1.a). The unit cell of the lattice contains two carbon atoms which are usually denoted by $A$ and $B$. Note that both the $A$ and the $B$ atoms build up a triangular lattice, shifted by $c$ with respect to each other, which will henceforth be referred to as sublattice $A$ and $B$.

Figure 2.1: a) Honeycomb lattice and its elementary lattice vectors. b) Brillouin zone of the honeycomb lattice and elementary reciprocal vectors. The two inequivalent corners of the Brillouin zone are $K$ and $-K$. 
The unit vectors of the lattice are given as

\[
\mathbf{a}_1 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \quad \text{and} \quad \mathbf{a}_2 = \frac{a}{2} \begin{pmatrix} -1 \\ \sqrt{3} \end{pmatrix}
\]  

(2.1)

with \(a\) being the lattice constant, i.e., the distance of two neighbouring \(A\) atoms or \(B\) atoms.

We set the coordinate system in such a way that its origin coincide with an \(A\) atom and, hence, the position of \(A\) atoms are given by the lattice vectors, \(\mathbf{r}_A = \mathbf{R}\), while the \(B\)-atomic positions are given as \(\mathbf{r}_B = \mathbf{R} + \mathbf{c}\) where \(\mathbf{c} = (\mathbf{a}_1 + \mathbf{a}_2)/3\) is the vector pointing from the \(A\) atom to the \(B\) atom in the same unit cell.

The point group of the two-dimensional honeycomb lattice is the \(C_{6v}\) symmetry group consisting of two-, three- and six-fold rotations and reflections against two inequivalent axes. We note that if graphene is considered as a three-dimensional object due to the finite width of the monolayer, the proper point group is \(D_{6h}\) [15].

The reciprocal lattice is again a triangular lattice spanned by the elementary reciprocal vectors

\[
\mathbf{b}_1 = \frac{2\pi}{\sqrt{3}a} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix} \quad \text{and} \quad \mathbf{b}_2 = \frac{2\pi}{\sqrt{3}a} \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix}.
\]  

(2.2)

The Brillouin zone is a perfect hexagon which has two inequivalent corners

\[
\mathbf{K} = \frac{\mathbf{b}_1 - \mathbf{b}_2}{3} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{K}' = -\mathbf{K}.
\]  

(2.3)

Wavenumbers are equivalent if their difference is given by a reciprocal lattice vector. In this sense other corners of the Brillouin zone are equivalent with either \(\mathbf{K}\) or \(\mathbf{K}'\) as shown in Fig. 2.1.b.

Now we review the bandstructure calculation within tight-binding approximation. In the atomic limit, each carbon atom has four electrons on the outer shells (2s, 2p). When putting atoms together in a graphene crystal, three of the four electrons participate in bonds between carbon atoms and do not contribute to the low energy behaviour of graphene. The forth electron, which occupies the \(p_z\) orbital in the atomic limit with the \(z\)-axis perpendicular to the graphene sheet, is not localized and contributes to transport phenomena.

In the following calculation, we take into account nearest neighbour hopping only. Next nearest neighbour coupling does not influence the low energy behaviour of quasi-particles significantly and, hence, can be neglected. Within tight-binding approximation, the Hamiltonian
of the non-interacting \( p_z \) electrons can be written as

\[
\hat{H} = t \sum_{R \sigma} \left[ a_{R \sigma}^{\dagger} b_{R \sigma} + a_{R \sigma}^{\dagger} b_{R-\mathbf{a}_1 \sigma} + a_{R \sigma}^{\dagger} b_{R-\mathbf{a}_2 \sigma} + \text{h.c.} \right] \tag{2.4}
\]

where \( t < 0 \) is the hopping integral and \( a_{R \sigma} \) and \( b_{R \sigma} \) are the annihilation operators of electrons on sublattice \( A \) and \( B \), respectively, in the unit cell given by \( R \) and with spin orientation \( \sigma \). After Fourier transformation, the Hamiltonian is block-diagonal in momentum representation,

\[
\hat{H} = \sum_{k \sigma} \begin{pmatrix} a_{k \sigma}^{\dagger} & b_{k \sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & t f^*(k) \\ t f(k) & 0 \end{pmatrix} \begin{pmatrix} a_{k \sigma} \\ b_{k \sigma} \end{pmatrix}, \tag{2.5}
\]

where

\[
f(k) = 1 + e^{i k a_1} + e^{i k a_2} \tag{2.6}
\]

and \( a_{k \sigma} \) and \( b_{k \sigma} \) are the annihilation operators with momentum \( k \). After diagonalization the electron spectrum reads as

\[
\varepsilon_{\pm}(k) = \pm \varepsilon(k) \quad \varepsilon(k) = |t| |f(k)| \tag{2.7}
\]

defining the two bands of pure graphene which are plotted in Fig. 2.2. An interesting feature of graphene is that the valance and conductance bands touch each other at the corners of the Brilluoin zone. In the case of neutral (undoped or half filled) graphene the Fermi level is exactly at this touching point usually called the Dirac point.

![Figure 2.2: Dispersion relation of the valance and conductance bands of graphene within tight binding approximation. In the calculation only nearest neighbour hopping was considered.](image)
The eigenvectors of the momentum dependent Hamilton matrix appearing in (2.5) is obtained as
\[ \frac{1}{\sqrt{2}} \left( \mp e^{-i\delta(k)} \right) \]
(2.8)
where \( \delta(k) \) is the argument of the complex-valued function \( f(k) = |f(k)|e^{i\delta(k)} \). The two components of the vector correspond to the two sublattices. Note that the absolute value of the two components are equal which implies that the probability of occupying an A site equals the probability that the electron sits on a B site. This property of the eigenvector is a consequence of the inversion symmetry of the honeycomb lattice.

The two component structure allows one to introduce the concept of the so called pseudospin. The pseudospin operator is defined as \( \vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \) where \( \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z \) are the Pauli matrices,
\[
\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]
(2.9)
In real space representation the eigenstates are rewritten as
\[
\Psi_{\pm,k}(r) = \frac{1}{\sqrt{2N}} \sum_R e^{ikR} \left[ \mp e^{-i\delta(k)} \varphi(r-R) + \varphi(r-R-c) \right],
\]
(2.10)
with \( \varphi(r) \) denoting the well-localized wavefunction of the \( p_z \) orbital. In the formula \( N \) is the number of unit cells in the graphene sample.

As already mentioned, in neutral graphene (at half filling) the Fermi energy is at the Dirac point where the valance and conduction band touch each other. By applying an appropriate gate voltage, the Fermi level can be shifted to positive or negative direction but remains always near the Dirac point in experimental situations since the order of the bandwidth is \( \sim 10 \) eV. It follows that only electron states in the vicinity of Dirac point play an important role in transport phenomena. In theoretical works, its manifestation is the linear approximation of the dispersion relation. The approximation remains valid even at finite temperature because the energy scale of the temperature (at room temperature \( \sim 10 \) meV) is also much less than the bandwidth.

In the vicinity of the Dirac point, i.e. near the corners of the Brillouin zone, the function \( f(k) \) vanishes linearly with the momentum measured from \( \mathbf{K} \) or \( \mathbf{K}' \). To leading order in
\[ \delta \mathbf{k} = \mathbf{k} - \mathbf{K} \text{ or } \delta \mathbf{k} = \mathbf{k} - \mathbf{K}', \text{ it is obtained as} \]

\[
\begin{equation}
    f(k) \approx -\frac{\sqrt{3}a}{2}(s\delta k_x + i\delta k_y) \tag{2.11}
\end{equation}
\]

where \( s = 1 \) if \( \delta \mathbf{k} \) is measured from \( \mathbf{K} \) and \( s = -1 \) if from \( \mathbf{K}' \). The index \( s \) is usually called valley index distinguishing the electron states of the two valleys. From now on, we suppress the notation \( \delta \mathbf{k} \) and use \( \mathbf{k} \) instead for the sake of brevity. The valley index identifies the valley which the wavenumber corresponds to. In the linear approximation, the Hamilton matrix reads as

\[
    H_s(k) = \hbar v_F (sk_x \sigma_x + k_y \sigma_y) \tag{2.12}
\]

where \( \sigma_x \) and \( \sigma_y \) are Pauli matrices.

Under time reversal transformation one valley is transformed to the other one, \( s \rightarrow -s \) and \( \mathbf{k} \rightarrow -\mathbf{k} \), and the wavefunctions are complex conjugated. It follows that the Hamiltonian is time reversal invariant, \( \tilde{H}_s(k) \rightarrow \tilde{H}_s^*(-\mathbf{k}) = \tilde{H}_s(\mathbf{k}) \). The pseudospin operator is transformed as \( \tilde{\mathbf{\sigma}} = (\tilde{\sigma}_x, \tilde{\sigma}_y, \tilde{\sigma}_z) \rightarrow (\tilde{\sigma}_x, -\tilde{\sigma}_y, \tilde{\sigma}_z) \) because of the complex conjugation. Interestingly, this behaviour is different from that of the real spin.

In the linear approximation, the energy spectrum vanishes linearly as

\[
    \varepsilon_\pm(k) = \pm \hbar v_F k \tag{2.13}
\]

in both valleys. Here, the Fermi velocity is defined as \( \hbar v_F = \sqrt{3}|t|a/2 \) and is three-hundred times smaller than the speed of light. Due to this property and that the Hamiltonian (2.12) is analogous to the Dirac Hamiltonian of relativistic massless fermions, graphene enables us to investigate relativistic effects experimentally, see for example Ref. [16].

Close to the Dirac point,

\[
    e^{i\delta(k)} \approx -se^{-is\gamma} \tag{2.14}
\]

where \( \gamma \) is the polar angle of the wavenumber \( \mathbf{k} \), measured from the \( k_x \) axis. The eigenvectors in the two-component vector representation are

\[
    |\pm, s, k\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm se^{-is\gamma} \\ 1 \end{pmatrix}. \tag{2.15}
\]
We note that the eigenfunctions are sufficient to be considered as $e^{ikr}|\pm, sk\rangle$ in many cases when the short wavelength behaviour does not influence physical properties or is not in the scope of investigation. In the case of Friedel oscillation, however, short wavelength pattern turned out to be decisive in the long range behaviour of the envelope of the oscillation.

An interesting feature of the eigenvectors given in Eq. (2.15), is that the expectation value of the pseudospin operator

$$\langle \pm, s, \mathbf{k}|\vec{\sigma}|\pm, s, \mathbf{k}\rangle = \pm s \begin{pmatrix} \cos \gamma \\ \sin \gamma \\ 0 \end{pmatrix}$$

(2.16)

is proportional to the unit vector $\mathbf{k}/k$. This property is similar to the helicity of neutrinos, therefore the electrons in graphene are called chiral particles. We will show later that a whole family of graphene materials exhibit chiral nature. Chirality is also related to non-trivial topological invariants. For example, electrons can be characterized by the so called winding number which counts how many times the pseudospin of the particle winds around while the state is adiabatically propagated along a closed loop around $\mathbf{K}$. In monolayer graphene, the winding number is 1. This non-trivial topology explains unconventional phenomena, such as half integer quantum Hall effect [17], or angle dependence of intensity in angle resolved photo emission spectroscopy measurements [18].

In the vicinity of the Dirac point, the density of states normalized to a unit cell is obtained as

$$\rho_0(\varepsilon) = \frac{A_c}{\pi \hbar^2 v_F^2} |\varepsilon|$$

(2.17)

for one spin direction where we have already taken into account the valley degeneracy. In Eq. (2.17), $A_c = \sqrt{3}a^2/2$ is the area of the unit cell.

Note that in real systems the dispersion is not perfectly linear and for more precise description higher order terms should be taken into account. Many phenomena, however, can be explained without going beyond the linear approximation.

Finally, we briefly introduce the electronic structure of multilayer graphene consisting of $M$ layers of graphene, for comparison see for example Ref. [19]. The elementary lattice vectors are the same as in monolayers but the unit cell of the multilayer graphene contains $2M$ carbon atoms. There are many different ways how the layers can be oriented with respect
to each other and the stacking of layers strongly affects the electronic structure as well [20].

In this thesis, we will study the so-called chirally stacked multilayer graphene or sometimes called $ABC$-stacked multilayer graphene. In this case, along a straight line perpendicular to the sheets, $A$, $B$, $C$, $A$, $B$, … sites of subsequent layers follow each other as illustrated in Fig. 2.3. Here, a $C$ site stands for the center of a hexagon of the honeycomb lattice. Near half filling, the low energy behaviour is given by the effective Hamiltonian

$$
\hat{H}_{\text{multiLG},s}^{\text{eff}} = c_M \begin{pmatrix}
0 & (sk_x - ik_y)^M \\
(sk_x + ik_y)^M & 0
\end{pmatrix}
$$

(2.18)

where $s = \pm 1$ is the valley index and $c_M$ is a momentum independent constant. If $M > 1$, this effective Hamiltonian is derived from the $2M \times 2M$ tight-binding Hamiltonian in the limit when the interlayer coupling is much smaller than the intralayer hopping.

The quasiparticles described by (2.18) are referred to as chiral particles due to their non-trivial topological properties, for instance, their winding number is $M$.

Figure 2.3: Chirally stacked multilayer graphene. Source: Phys. Rev. B 88, 205428 (2013)
Chapter 3

Short wavelength pattern of Friedel oscillation in monolayer graphene

Friedel oscillation is an obvious fingerprint of the interaction between impurities and itinerant electrons in solids. Jacques Friedel showed that in the presence of a single impurity, the change of the electron density exhibits oscillations with the wavenumber $2k_F$ where $k_F$ is the Fermi wavenumber [21]. Sufficiently far from the impurity, the envelope of the oscillation shows power law decay with an exponent equal to the number of spatial dimensions of the system. This power law decay gives rise to the Rudemann-Kittel-Kasuya-Yosida interaction which is an electron mediated long range coupling between impurities. The Friedel oscillation also accounts for the screening properties, since the electron density change due to a single well localized impurity is closely related to the polarizability. How charged impurities are screened by the surrounding electrons, is a crucial issue to explain transport phenomena, such as doping dependence of the conductivity. Thus, Friedel oscillation is an important quantity to examine the electronic structure of the system. Moreover, it can be observed directly, for example in scanning tunneling microscopy measurements.

In graphene, earlier theoretical works suggested long wavelength oscillations with an envelope decaying as $r^{-3}[22, 23]$, as opposed to the $r^{-2}$ decay in conventional two-dimensional gases. The difference was argued to be a consequence of the absence of back scattering off the impurity due to the chiral nature of quasi-particles in graphene. To be more precise, let us consider electron states near the Dirac point within linear approximation, i.e. the eigenfunctions $e^{ikr}|\pm, s, k\rangle/\sqrt{A}$ where $|\pm, s, k\rangle$ is defined in Eq. (2.15), $+$ ($-$) corresponds...
to the conductance (valance) band, $A$ is the area of the graphene sample and $s$ is the valley index. The transition probability of scattering from $k$ to $k'$ in a given valley due to the single impurity described by Dirac delta potential reads as

$$\left| \int d^2r e^{-i\mathbf{kr} + i\mathbf{k'}r} \frac{A}{A} \delta(\mathbf{r}) \langle l, s, k|l, s, k' \rangle \right|^2 = \frac{1}{A^2} \cos^2 \left( \frac{\gamma - \gamma'}{2} \right)$$

(3.1)

with $\gamma$ and $\gamma'$ being the polar angle of $k$ and $k'$. Here, only elastic scattering processes are considered, i.e. intraband transitions are allowed only, and $l$ is the band index. In the case of $k' = -k$ the transition probability is zero, thus, backscattering of chiral particles is suppressed due to quantum interference.

This description, however, does not take into account intervalley processes, which are inevitable in the case of well localized impurities. Moreover, it assumes an impurity equally present on the two sublattices which is not physically expected in the case of a substitutional impurity. Therefore, the unusual $r^{-3}$ power-law decay cannot be explained simply by the suppressed backscattering but needs further investigations. In Ref. [24], intervalley processes are considered leading to $r^{-2}$ oscillation. In this chapter, we investigate the short-wavelength pattern of Friedel oscillation in graphene around a well localized single impurity. Our goal is to explore under what conditions the envelope decays as $r^{-2}$ or $r^{-3}$.

In the first section, we briefly review Friedel oscillations in conventional electron gases showing that the exponent of the power-law decay coincides with the number of spatial dimensions. In the second and third sections, electron Green’s functions are analyzed in pristine graphene and in the presence of a well localized impurity. In the fourth and fifth sections, we examine the change in the local density of states and in particle density, respectively.

### 3.1 Friedel oscillation around a short range scatterer in conventional fermion gases

In this section Friedel oscillations in conventional Fermi gases are presented for one, two and three spatial dimensions. The spectrum and the eigenstates of free electrons are given by

$$\varepsilon(k) = \frac{\hbar^2k^2}{2m} \quad \Psi_k(r) = \frac{1}{\sqrt{\Omega}} e^{ikr}$$

(3.2)
for arbitrary dimension where Ω is the volume (or area or length) of the sample. In the pure system (without any impurities), the Green’s function of the electrons is defined as

\[
G^0(z, \mathbf{r}, \mathbf{r}') = \sum_k \frac{\Psi_k(\mathbf{r})\Psi^*_k(\mathbf{r}')}{z - \varepsilon(k)} = \frac{1}{\Omega} \sum_k \frac{e^{ik(\mathbf{r}-\mathbf{r}')}}{z - \varepsilon(k)}
\]  

(3.3)

with \( z \) being the complex energy variable. By using Eq. (3.2), the retarded Green’s functions can be evaluated as

\[
G^0(\varepsilon + i\delta, \mathbf{r}, \mathbf{r}') = \frac{m}{2i\hbar^2} \begin{cases} 
\frac{2e^{ik|\mathbf{r}-\mathbf{r}'|}}{k} & 1D \\
H_0^{(1)}(k|\mathbf{r}-\mathbf{r}'|) & 2D \\
\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{\pi|\mathbf{r}-\mathbf{r}'|} & 3D
\end{cases}
\]

(3.4)

where \( k = \sqrt{2m\varepsilon}/\hbar \) and \( H_0^{(1)}(x) \) is the Hankel function of the first kind. Note that due to the continuous translational invariance of the system, the Green’s function depends on the difference of space variables only. In Eq. (3.4), \( \delta \to 0^+ \) limit was taken in order to obtain the retarded Green’s function. The local density of states is homogeneous in the unperturbed system,

\[
\rho_0(\varepsilon) = -\frac{1}{\pi} \text{Im} G^0(\varepsilon + i\delta, \mathbf{r}, \mathbf{r}) = \frac{m}{2\pi\hbar^2} \begin{cases} 
\frac{2}{k} & 1D \\
1 & 2D \\
\frac{k}{\pi} & 3D
\end{cases}
\]

(3.5)

which is also a consequence of the continuous translational invariance of the gas.

In the presence of impurities, the Green’s function of the electrons modifies due to scattering. In the case of a single well-localized impurity, we determine the Green's function within Born approximation. Up to first order within perturbation theory, the Green’s function is obtained as

\[
G(z, \mathbf{r}, \mathbf{r}') = G^0(z, \mathbf{r}, \mathbf{r}') + G^0(z, \mathbf{r}, 0)uG^0(z, 0, \mathbf{r}')
\]

(3.6)

where \( u \) measures the strength of the impurity potential, \( U(\mathbf{r}) = u\delta(\mathbf{r}) \). The local density of states reads as

\[
\rho(\varepsilon, \mathbf{r}) = -\frac{1}{\pi} \text{Im} [G(\varepsilon + i\delta, \mathbf{r}, \mathbf{r})] = \rho_0(\varepsilon) + \Delta\rho(\varepsilon, \mathbf{r})
\]

(3.7)
where $\rho_0(\varepsilon)$ corresponds to the pure system and the first order correction is obtained as

$$\Delta \rho(\varepsilon, r) = \begin{cases} \frac{u_m^2}{4\pi\hbar^4} \sin(2kr) & \text{1D} \\ 2J_0(kr)Y_0(kr) & \text{2D} \\ -\frac{1}{4\pi\hbar^4} \sin(2kr) & \text{3D} \end{cases}$$

(3.8)

where $J_0(x)$ and $Y_0(x)$ are Bessel functions of the first and second kind.

At zero temperature, the leading correction to the density is evaluated by integrating $\Delta \rho(\varepsilon, r)$ up to the Fermi level with respect to $\varepsilon$. Sufficiently far from the impurity ($r \gg (2k_F)^{-1}$), the integration leads to the compact formula

$$\Delta n(r) = \frac{m k_F^d}{\hbar^2(2\pi)^d} \cos \left( 2k_F r - \frac{\pi}{2}(d + 1) \right)$$

(3.9)

which is the Friedel oscillation. The wavelength of the spherical oscillation $\pi/k_F$ is comparable to the mean distance between neighbouring particles. The envelope is decaying as $r^{-d}$ in a $d$-dimensional system.

### 3.2 Green’s functions in graphene

Now we investigate the case of graphene and first analyze the Green’s function of the pure system. Since the impurity we will consider is non-magnetic, the electron spin does not play any role in the forthcoming discussion, therefore spin indices are suppressed, and all the results refer to one spin orientation.

The real space representation of the Green’s function of complex energy variable $G(z, r, r')$ is of central importance for our subject. For pristine graphene, not perturbed by impurities, the free Green’s function is defined as

$$G^0(z, r, r') = \sum_{k,l=\pm} \frac{\Psi_{l,k}(r)\Psi_{l,k}^*(r')}{z - \varepsilon_l(k)}$$

(3.10)

where $\varepsilon_\pm(k)$ are the conductance and valance bands and $\Psi_{l,k}(r)$ are the corresponding wavefunctions, all of them defined in Chapter 2. Substituting Eq. (2.10), we obtain

$$G^0(z, r, r') = \sum_{RR'} \varphi(r - R)G^0(z, R - R')\varphi^+(r' - R')$$

(3.11)

where $\varphi(r) = [\varphi(r), \varphi(r - c)]$ is a row vector formed by the orbitals of the A and B sites in the unit cell and the summations run over all lattice vectors. The Green’s matrix is given by
\[ G^0(z, R) = \frac{1}{N} \sum_k \frac{e^{ikR}}{\varepsilon(k)^2} \begin{pmatrix} z & tf^*(k) \\ tf(k) & z \end{pmatrix} \]  

(3.12)

where \( f(k) \) is the complex valued function defined in Eq. (2.6). The free Green’s function in Eq. (3.11) is invariant under translations by a lattice vector only, \( G^0(z, r, r') = G^0(z, r + R, r' + R) \). Elements of the point group of graphene are also symmetries of the Green’s function, \( G^0(z, \hat{O}r, \hat{O}r') = G^0(z, r, r') \) with \( \hat{O} \) denoting a point group transformation, e.g., a threefold rotation.

It is instructive to consider the local density of states of the pure system given by

\[ \rho_0(\varepsilon, r) = \rho_0(\varepsilon) \sum_R \left(|\varphi(r - R)|^2 + |\varphi(r - R - c)|^2\right) \]  

(3.13)

where \( \rho_0(\varepsilon) \) is the density of states. Note that the local density of states is not homogeneous, as opposed to conventional electron gases, but it has a spatial dependence determined by the \( p_z \) orbitals.

Due to the well-localized nature of the atomic wavefunctions, there is only one non-negligible term in Eq. (3.11) which is determined by the proximity of \( r \) and \( r' \) to a lattice point given by either \( r_A (= R) \) on sublattice \( A \), or by \( r_B (= R + c) \) on the B sublattice. For example, if \( r \) is in the vicinity of the \( A \)-atomic position \( R_1 \) and \( r' \) is near the \( B \)-atomic position \( R_2 + c \), the only non-negligible term is

\[ G^0(z, r, r') = \varphi(r - R_1)G^0_{AB}(z, R_1 - R_2)\varphi(r - R_2 - c) \]  

(3.14)

where \( G^0_{AB}(z, R_1 - R_2) \) is the \( AB \) element of the Green’s matrix. We note that this approximation does not break the symmetries of the Green’s function.

The diagonal elements of the Green’s matrix in Eq. (3.12) are even functions of \( R \), e.g., \( G^0_{AA}(z, -R) = G^0_{AA}(z, R) \), while the off-diagonal elements transform into each other upon reflection, \( G^0_{AB}(z, -R) = G^0_{BA}(z, R) \).

### 3.3 Impurity scattering

Let us now consider a substitutional impurity characterized by a short range scattering potential energy \( U(r) = u\delta(r) \) located at the origin, which is an \( A \) atomic position. We note
that in real graphene samples, impurities have non-zero extent ensuring that the matrix element of the scattering potential between \( p_z \) states does not vanish. In the presence of the potential scatterer, the point group of the system is reduced. The translational invariance and sixfold rotational symmetry is broken and only threefold rotation and reflections against axes including the origin leave the system unchanged. However, by considering only the \( A \) sublattice, the sixfold symmetry is still present.

Up to first order within Born approximation, the Green’s function of the electrons reads as

\[
G(z, r, r') = G^0(z, r, r') + G^0(z, r, 0)uG^0(z, 0, r')
\]

which is the same as in the case of conventional electron gases in Eq. (3.6). We note that the Born approximation is valid if the site energy difference of the impurity and a carbon atom is smaller than the hopping.

First order correction to the local density of states in Born approximation is determined by

\[
\Delta \rho(\varepsilon, r) = -\frac{1}{\pi} \text{Im} \Delta G(\varepsilon + i\delta, r, r)
\]

where

\[
\Delta G(z, r, r) = G^0(z, r, 0)uG^0(z, 0, r)
\]

Depending on whether \( r \) is in the vicinity of an \( A \) or a \( B \) site, the first order correction to the Green’s function can be expressed as

\[
\Delta G(z, r, r) = u_0|\varphi(r - r_A)|^2G^0_{AA}(z, r_A)G^0_{AA}(z, -r_A) \quad \text{or} \quad (3.18)
\]

\[
\Delta G(z, r, r) = u_0|\varphi(r - r_B)|^2G^0_{BA}(z, r_B - c)G^0_{AB}(z, -r_B + c) \quad (3.19)
\]

where \( u_0 = u|\varphi(0)|^2 \). The spatial pattern of (3.18) and (3.19) is dominated by the density profile of the atomic orbital centered on the given lattice site, while the multiplicative factor on that site depends on the corresponding Green’s matrix elements. Note that both \( r_A \) and \( r_B - c \) are lattice vectors, therefore, they are valid variables of the Green’s matrix elements.

\[
G^0_{AA}(z, r_A) = \frac{1}{N} \sum_k \frac{e^{ikr_A}}{z^2 - \varepsilon(k)^2}
\]

\[
G^0_{BA}(z, r_B - c) = \frac{1}{N} \sum_k \frac{e^{ikr_B}g(k)}{z^2 - \varepsilon(k)^2}
\]

\[
G^0_{AB}(z, -r_B + c) = G^0_{BA}(z, r_B - c)
\]
where
\[ g(k) = f(k)e^{-ikc} = e^{-ikc} + e^{ik(a_1-c)} + e^{ik(a_2-c)} \]

with the vectors \( c, c - a_1 \) and \( c - a_2 \) pointing to the nearest B atoms from an A atom (see Fig. 2.1). The positions of the three nearest neighbours show threefold rotational symmetry and, therefore, \( g(\hat{C}_3 k) = g(k) \) with \( \hat{C}_3 \) denoting the operator of the threefold rotation. It follows that the Green’s matrix element is also symmetric,

\[ G_{BA}^0(z, \hat{C}_3 r_B - c) = 1 \sum_k t e^{i(\hat{C}_3 r_B g(k))} \frac{e^{-ikc}}{z^2 - \varepsilon(k)^2} = 1 \sum_k t e^{i(\hat{C}_3 r_B g(k))} \frac{e^{-ikc}}{z^2 - \varepsilon(k)^2}. \]

The last equation holds true because both the Brillouin zone and the dispersion relation \( \varepsilon(k) \) are symmetric. The sixfold rotational symmetry of the diagonal Green’s matrix elements can similarly be proven, \( G_{AA}^0(z, \hat{C}_6 r_A) = G_{AA}^0(z, r_A) \).

Up to this point, we have taken into account the whole spectrum plotted in Fig. 2.2 but the sum over \( k \) in Eqs. (3.20) and (3.21) cannot be calculated analytically. In order to evaluate the relevant Green’s matrix elements from Eq. (3.12), we observe that the most important contributions come from around the points \( K \) and \( K' = -K \). Within linear approximation, the dispersion is obtained as \( \varepsilon(k) = \hbar v_F k \) and \( g(k) = -\sqrt{3}a (s\delta k_x + i\delta k_y) \) because of \( Kc = 0 \). The summation over the wavevectors in Eqs. (3.20) and (3.21) is now restricted to the circles around the two corners of the Brillouin zone whose radius is the cutoff \( k_c \), such that \( k_F \ll k_c \ll a^{-1} \). Remember, that in graphene the Fermi wavenumber is much smaller than the inverse lattice constant. The linear approximation of the Green’s function is valid for energies in the vicinity of the Dirac point. This is also a proper approximation of the Friedel oscillations for distances from the impurity much larger, and for characteristic spatial variations much longer than \( 1/k_c \).

The Green’s matrix elements consist of two terms stemming from the two valleys. These are led by fast oscillations of the type \( e^{ikR} \) and \( e^{-ikR} \) and modulated by functions of slow
Green's functions can be obtained as analytic continuation of the retarded Grenn's functions.

where \( G_{AB}(z, r_B - c) = G^0_{BA}(z, r_B - c) \) (3.26)

where \( H^0_1(z) \) is the Hankel function of the first kind, \( H^0_1(z) = -dH^1_0(z)/dz \) and \( \vartheta \) is the polar angle of \( r_B \). We note that the exponential prefactors in the Green’s matrix elements describing short wavelength oscillations are exact, as opposed to the spatial dependence described by the Hankel functions which are obtained within linear approximation. Eqs. (3.24) and (3.25) are valid for \( |z| \ll \hbar v_F k_c \) and for \( \text{Im} z > 0 \) only, which is enough for the prescribed analytic continuation of the retarded Greun’s functions.

In order to obtain the retarded Green’s functions, we have to take the \( \lim_{\delta \to 0^+} G^0(\varepsilon + i\delta) \) limit with \( \varepsilon \) being the real energy variable. Regarding the analytic properties of the Hankel functions, namely, that they have a branch cut along the negative real axis, the retarded Green’s functions can be obtained as

\[
G^0_{AA}(\varepsilon + i\delta, r_A) = \left( e^{iK_{rA}} + e^{-iK_{rA}} \right) \left( \frac{-iA_c \varepsilon}{(2\hbar v_F)^2} \right) \left( J_0 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) + i \text{sgn}(\varepsilon) Y_0 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) \right),
\]

(3.27)

\[
G^0_{BA}(\varepsilon + i\delta, r_B - c) = \left( e^{iK_{rB} + \vartheta} - e^{i(-K_{rB} - \vartheta)} \right) \left( \frac{A_c \varepsilon}{(2\hbar v_F)^2} \right) \left( J_1 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) + i \text{sgn}(\varepsilon) Y_1 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) \right)
\]

(3.28)

where \( J(x) \) and \( Y(x) \) are the Bessel functions of the first and second kind, respectively. The first order correction to the Green’s functions of continuous space variables is obtained as

\[
\Delta G(\varepsilon + i\delta, r, r) = -u_0 |\varphi(r - r_A)|^2 \cos^2(K r_A) \left[ \frac{A_c \varepsilon}{2\hbar v_F} \left( J_0 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) + i \text{sgn}(\varepsilon) Y_0 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) \right) \right]^2
\]

(3.29)

if \( r \) is in the vicinity of an \( A \) atom positioned at \( r_A \). If \( r \) is near a \( B \) atom at \( r_B \), the Green’s function is evaluated as

\[
\Delta G(\varepsilon + i\delta, r, r) = -u_0 |\varphi(r - r_B)|^2 \sin^2(K r_B + \vartheta) \left[ \frac{A_c \varepsilon}{2\hbar v_F} \left( J_1 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) + i \text{sgn}(\varepsilon) Y_1 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) \right) \right]^2.
\]

(3.30)

We note again that both results are valid only for energies \( |\varepsilon| \ll \hbar v_F k_c \).
3.4 Change of the local density of states

The change of the local density of states in graphene due to the impurity can be obtained as

$$\Delta \rho(\varepsilon, \mathbf{r}) = -\frac{1}{\pi} \text{Im} \Delta G(\varepsilon + i\delta, \mathbf{r}, \mathbf{r})$$  (3.31)

where we have to substitute Eqs. (3.29) and (3.30). The short wavelength spatial pattern is described by the atomic wavefunctions and \(\cos^2(Kr_A)\) and \(\sin^2(Kr_B + \vartheta)\). If the impurity is unable to produce intervalley scattering, for example because it is extended and has no large wavenumber Fourier components, then the factors \(\cos^2(Kr_A)\) and \(\sin^2(Kr_B + \vartheta)\) should be replaced by \(1/2\).

After substituting the Green’s functions, the change in the local density of states is evaluated as

$$\Delta \rho(\varepsilon, \mathbf{r}) = \pi u_0 \rho_0^2(\varepsilon) sgn(\varepsilon) J_0 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right) \frac{Y_0 \left( \frac{|\varepsilon| r_A}{\hbar v_F} \right)}{2}$$  (3.32)

if \(\mathbf{r}\) is in the vicinity of an A site, and

$$\Delta \rho(\varepsilon, \mathbf{r}) = \pi u_0 \rho_0^2(\varepsilon) sgn(\varepsilon) J_1 \left( \frac{|\varepsilon| r_B}{\hbar v_F} \right) \frac{Y_1 \left( \frac{|\varepsilon| r_B}{\hbar v_F} \right)}{2}$$  (3.33)

if \(\mathbf{r}\) is in the vicinity of a B site. Here, \(\rho_0(\varepsilon)\) is the density of states in pure graphene as defined in Eq. (2.17) for one spin direction and the factors describing the short wavelength spatial behavior are incorporated into the functions

$$c_A(\mathbf{r}) = |\varphi(\mathbf{r} - r_A)|^2 \cos^2(Kr_A)$$  (3.34)

$$c_B(\mathbf{r}) = |\varphi(\mathbf{r} - r_B)|^2 \sin^2(Kr_B + \vartheta).$$  (3.35)

These are shown in Fig. 3.1 where the three-dimensional plots of the density of atomic orbitals are viewed from above the graphene plane and their weights are given by the trigonometric factors. The impurity is at the center on both subfigures.

It can be proven that these factors are invariant under the symmetry operations of the system. Here, we show the threefold rotational symmetry of the factor \(c_B(\mathbf{r})\) only but all other symmetries can be demonstrated in a very similar way. Note that if \(\mathbf{r}\) is in the vicinity of the B-atomic position \(r_B\), then \(\hat{C}_3\mathbf{r}\) is near \(\hat{C}_3 r_B\). Since the atomic wavefunction is rotational invariant, under threefold rotation \(|\varphi(\hat{C}_3\mathbf{r} - \hat{C}_3 r_B)|^2 = |\varphi(\mathbf{r} - r_B)|^2\) and, hence,

$$c_B(\hat{C}_3\mathbf{r}) = |\varphi(\mathbf{r} - r_B)|^2 \sin^2 \left( \frac{2\pi}{3} \right) = |\varphi(\mathbf{r} - r_B)|^2 \sin^2 \left( \frac{1}{3} \right) \left( \hat{C}_3^{-1} K \right) r_B + \vartheta + \frac{2\pi}{3}. \right)$$  (3.36)
Upon threefold rotation, $\hat{C}_3^{-1}K = K - b_1$ which leads to

$$c_B(\hat{C}_3 r) = |\varphi(r - r_B)|^2 \sin^2 \left( (K - b_1)(R_B + c) + \vartheta + \frac{2\pi}{3} \right) =$$

$$= |\varphi(r - r_B)|^2 \sin^2 \left( K r_B - b_1 c + \frac{2\pi}{3} + \vartheta \right) = c_B(r)$$

(3.37)

where we have introduced the lattice vector $R_B = r_B - c$ and used $b_1 c = 2\pi/3$. Symmetries, such as sixfold and threefold rotational invariance on the A and B sublattice, respectively, can be readily seen in Fig. 3.1.

Remember that for intravalley scattering only, the weights of the density of atomic orbitals would be the same on each lattice sites on both figures and the short wavelength pattern is given by $c_{A/B}(r) = |\varphi(r - r_{A/B})|^2/2$.

The isotropic spatial dependence in the local density of states is given by the Bessel functions in Eqs. (3.32) and (3.33). The characteristic wavenumber of these oscillations, $k = |\varepsilon|/\hbar v_F$, is much smaller than the cutoff $k_c$ and $a^{-1}$. Consequently, the isotropic spatial dependence describes very long wavelength behaviour. Therefore, instead of $r_A$ and $r_B$, one may use the continuous variable $r$ measuring the distance from the impurity. For distances...
large enough to satisfy $kr \gg 1$ we use the leading asymptotic expressions

\begin{align}
J_0(kr)Y_0(kr) &= -\frac{1}{\pi kr} \cos(2kr) \quad (3.38) \\
J_1(kr)Y_1(kr) &= \frac{1}{\pi kr} \cos(2kr). \quad (3.39)
\end{align}

Due to this sign change on the two sublattices, it is useful to define a composite short wavelength pattern

\[
c(r) = \begin{cases} 
-c_A(r) & \text{if } r \text{ is near an } A \text{ site} \\
-c_B(r) & \text{if } r \text{ is near a } B \text{ site.} 
\end{cases} \quad (3.40)
\]

Then the change of the local density of states due to an impurity at the origin is given by the following compact formula:

\[
\Delta \rho(\varepsilon, r) = u_0 c(r) \rho_0^2(\varepsilon) \frac{\hbar v_F}{2\varepsilon r} \cos\left(\frac{2\varepsilon r}{\hbar v_F}\right), \quad (3.41)
\]

indicating a long wavelength oscillation with an $r^{-1}$ decay and a short wavelength spatial pattern given by $c(r)$, and shown in Fig. 3.2. Although a very rich structure can be seen on the plot, the overall threefold rotational symmetry is apparent, and appears to have been observed experimentally\[25\] where the change in local density of states could be seen on atomic scale due to the good resolution of the tip.

However, if the resolution of the STM tip is worse, it will measure a spatial average of the pattern given by $c(r)$. In the simple case of an extended impurity not producing intervalley scattering, $c(r)$ has atomic densities with equal weight on each site of one sublattice and the same weight with opposite sign on each site of the other sublattice. A resolution worse than an elementary cell of graphene will lead to cancellation of the leading $r^{-1}$ decay in Eq. (3.41), leaving us with the next to leading $r^{-2}$ decay of local density of states.

On the other hand, for a short range impurity potential, when intervalley scattering contributes as well, the short wavelength spatial pattern is shown in Fig. 3.2, where no cancellation within one unit cell occurs. However, averaging $c(r)$ over three neighboring unit cells leads to cancellation of the weights of the atomic densities. Contributions of atoms in the unit cells given by lattice vectors $R$, $R + a_1$ and $R + a_1 - a_2$ sum up to

\[
-\cos^2(KR) - \cos^2(K(R + a_1)) - \cos^2(K(R + a_2)) + \\
\sin^2(K(R + c) + \vartheta) + \sin^2(K(R + a_1 + c) + \vartheta) + \sin^2(K(R + a_2 + c) + \vartheta) = 0 \quad (3.42)
\]
Figure 3.2: Short wavelength spatial dependence of the local density of states due to an impurity at the center. $c_A(\mathbf{r}) + c_B(\mathbf{r}) = |c(\mathbf{r})|$ is shown, and the color code indicates the opposite sign on the two sublattices.

far enough from the impurity where $\vartheta$ is the same in the three unit cells. It can be shown in a similar way that the weights of the atomic densities cancel on the six sites of any hexagon of the honeycomb lattice. Therefore an STM with resolution worse than three elementary cells will not be able to measure the leading $r^{-1}$ decay either.

We still have to investigate whether the next-to-leading order, $r^{-2}$, vanishes for similar reasons. The next-to-leading corrections in the asymptotic expressions of the Bessel functions have different prefactors and not only different signs,

$$J_0(kr)Y_0(kr) = -\frac{1}{\pi kr} \cos(2kr) - \frac{1}{4\pi(kr)^2} \sin(2kr)$$  \hspace{1cm} (3.43) \\
$$J_1(kr)Y_1(kr) = \frac{1}{\pi kr} \cos(2kr) + \frac{3}{4\pi(kr)^2} \sin(2kr).$$  \hspace{1cm} (3.44)

Therefore, the $r^{-2}$ contributions are present in the local density of states even if the leading order is cancelled.

### 3.5 Friedel oscillation

The change in the particle density at zero temperature due to the impurity is obtained by integrating the local density of states up to the Fermi energy. Since $\Delta \rho(\varepsilon, \mathbf{r})$ is an odd function
of energy, $\Delta n(r)$ is even in $\varepsilon_F$, therefore we integrate up to $-|\varepsilon_F|$. Hence,

$$\Delta n(r) = \int_{-|\varepsilon_F|}^{-\hbar v_F k_c} d\varepsilon \Delta \rho(\varepsilon, r) = -u_0 \frac{A_c^2}{2\pi \hbar v_F} \frac{c_A(r)}{r_A} \int_{-k_c r_A}^{-k_F r_A} x^2 J_0(x)Y_0(|x|)dx$$

(3.45)

if $r$ is near an A site and

$$\Delta n(r) = -\frac{u_0 A_c^2}{2\pi \hbar v_F} \frac{c_B(r)}{r_B} \int_{-k_c r_B}^{-k_F r_B} x^2 J_1(|x|)Y_1(|x|)dx$$

(3.46)

if $r$ is in the vicinity of a B site where $k_F = |\varepsilon_F|/\hbar v_F$ is the Fermi wavenumber.

At half filling, when the chemical potential is at the Dirac point and $k_F = 0$, the above integrals have only unphysical spatial dependence through $k_c r$ where $k_c$ is the cutoff. Therefore, the change of the particle density does not show oscillation but a $r^{-3}$ decay only [26]. The question arises whether something physical is missed due to the linear approximation. First, we substitute Eqs. (3.20) and (3.21), which contains the complete tight-binding dispersion $\varepsilon(k) = |t||f(k)|$, into Eqs. (3.18) and (3.19), respectively, leading to

$$\Delta n(r) = \frac{u_0}{2N^2} \begin{cases} 
-|\varphi(r - r_A)|^2 \sum_{kk'} e^{i(k-k')r_A} \left( |\varepsilon(k)| + |\varepsilon(k')| \right) & \text{near an A atom} \\
|\varphi(r - r_B)|^2 \sum_{kk'} e^{i(k-k')(r_B - c) - i\delta(k) + i\delta(k')} \left( |\varepsilon(k)| + |\varepsilon(k')| \right) & \text{near a B atom}
\end{cases}$$

(3.47)

where the summations run over the whole Brillouin zone. This expression shows that at large distances the major contribution comes from small values of $k - k'$ and, because of the denominator, from the vicinity of nodal points, confirming the validity of the linear approximation.

Second, exact diagonalization of the Hamiltonian on a honeycomb lattice of $21 \times 21$ unit cells also shows that the $r^{-3}$ decay is present [27]. In Fig. 3.3, the change in the number of electron multiplied by $r^3$ is plotted. The modified values show non-decaying behaviour at large distances and, hence, confirm the $r^{-3}$ power-law. The short wavelength pattern is also confirmed by our numerical calculations, see Fig. 3.3.

In doped graphene, we investigate distances $k_F r \gg 1$ which allows one to use the asymptotic expressions of the Bessel functions and integrate Eqs. (3.32) and (3.33) up to $-|\varepsilon_F|$ leading to the change of the particle density

$$\Delta n(r) = -\frac{u_0 A_c}{4\pi} \frac{c_A(r)\rho_0(\varepsilon_F)}{r_A^2} \frac{\sin(2k_F r_A)}{r_A},$$

(3.48)
Figure 3.3: Numerical results at half filling (exact diagonalization of the tight-binding Hamiltonian): absolute value of the change of the density multiplied by $r^3$. On both sublattices the modified weights show constant envelope, which confirms the analytical $r^{-3}$ dependence. a) Sublattice A. The sign of the change is negative and the sixfold rotational symmetry is plain. b) Sublattice B. The sign is positive and the threefold symmetry is present.

If $\mathbf{r}$ is near an $A$ site and

$$
\Delta n(\mathbf{r}) = \frac{u_0 A_c}{4\pi} c_B(\mathbf{r}) \rho_0(\varepsilon_F) \frac{\sin(2k_F r_B)}{r_B^2},
$$

(3.49)

If $\mathbf{r}$ is in the vicinity of a $B$ atom. The oscillations due to the cutoff at the lower limit of integration are disregarded as unphysical. The oscillating part of Eqs. (3.48) and (3.49) describes long wavelength behaviour. Therefore, the distances $r_A$ or $r_B$ can be replaced by $r$, since $\mathbf{r}$ is in the same unit cell as $\mathbf{r}_A$ or $\mathbf{r}_B$, respectively. Hence, the change of density is rewritten by means of the composite short wavelength pattern $c(\mathbf{r})$,

$$
\Delta n(\mathbf{r}) = \frac{u_0 A_c}{4\pi} c(\mathbf{r}) \rho_0(\varepsilon_F) \frac{\sin(2k_F r)}{r^2}.
$$

(3.50)

This result shows the Friedel oscillation with wavenumber $2k_F$ and with amplitude decaying on both sublattices as $r^{-2}$. Similarly to the case of the local density of states, limited experimental resolution leads to cancellation of the leading power laws, and only the $r^{-3}$ decay will be observed. For resolution of about a unit cell this happens for an extended impurity not producing internodal scattering. This explains earlier theoretical results where the intervalley scattering was not taken into account while averaging over the unit cell was included. If the
resolution is worse than about three unit cells or a hexagon of the honeycomb lattice, leading order cancels even for a pointlike impurity.

We note again that, while the long range and long wavelength behaviour is described within linear approximation of the energy spectrum, the short wavelength pattern is exact.

### 3.6 Conclusion

In this chapter Friedel oscillation around a well localized, non-magnetic impurity has been investigated. Assuming a weak scattering potential, we performed the calculation within Born approximation. As opposed to earlier theoretical works, we have focused on the short wavelength pattern of the change in the local density of states and particle density for which intervalley scattering and the atomic wavefunctions are necessarily taken into account. As a consequence of this approach, the short wavelength spatial pattern described by \( c(r) \) in Eqs. (3.41) and (3.50), can be considered exact and also reflects the symmetry properties of the system. Using a linearized electronic spectrum affects only the rest of the spatial dependence. For energies close to the Dirac point and for distances far from the impurity, linear approximation is an excellent approximation as we have seen by comparing numerical and analytical results.

The Friedel oscillation decays as \( r^{-2} \) with a wavenumber \( 2k_F \) on both sublattices but with alternating sign. Detailed analysis of the short wavelength pattern leads to the conclusion that experimental resolution worse than a hexagon of the lattice leads to cancellation of the leading power law decay yielding the next-to-leading behaviour. An extended impurity potential can also be considered by restricting the calculation to intravalley scattering. This affects the short wavelength behaviour only, making the atomic densities equal on the two sublattices but with opposite sign. This means that in the case of an extended impurity experimental resolution worse than one unit cell can already lead to cancellation. If the experimental resolution falls between one and three unit cells, distinction can be made between localized and extended defects, since the observed power law decay of the Friedel oscillation should be observed as \( r^{-2} \) for the former and \( r^{-3} \) for the latter. The results are published in Ref. [28].

We have also studied the case of undoped graphene when the change of density shows non-oscillating behaviour with an envelope decaying as \( r^{-3} \) far from the impurity. This result
is closely related to the fact that the susceptibility is a linear function of the wavenumber,

\[ \chi(q) = -\frac{e^2 q}{4\hbar v_F} \tag{3.51} \]

if both spin directions are taken into account. This highly unusual behaviour of the susceptibility is a consequence of the linear spectrum and the vanishing Fermi surface in undoped graphene. Within random phase approximation, the electric potential of a point charge is obtained as \( \Phi(q) = Q/(2\varepsilon_0 q - \chi(q)) \) where \( \varepsilon_0 \) is the vacuum permittivity. Due to the unusual behaviour of the susceptibility of half filled graphene, this leads to a long range potential \( \Phi(q) = Q'/(2\varepsilon q) \) with renormalized electric charge \( Q' = Q/(1 + \frac{e^2}{8\varepsilon_0\hbar v_F}) \). This weak intrinsic screening suggests that the Coulomb interaction between electron should play an important role in the case of undoped graphene.
Chapter 4

Mean-field quantum phase transitions in graphene and in general gapless systems

Interaction effects between electrons in graphene has been studied by researchers for a long time [10]. At the end of the previous chapter we have shown that in undoped graphene screening of intrinsic electrons is very weak, therefore interaction effects should play an important role in the electronic properties. In 1960, Pauling proposed [29], that due to strong coupling graphene should be a Mott insulator. On the other hand, Wallace predicted that graphene is a semimetal, i.e. a gapless system with zero density of states at the Fermi level [14]. More than 40 years later, after the production of real graphene, semimetal behaviour was confirmed and electron interaction seemed to have no effects on the electronic properties. However, the coupling constant, measuring the strength of the interaction between electrons, is inversely proportional to the dielectric constant which highly depends on the environment. Since first graphene samples were produced on silicon substrate, one may ask the question whether the environment could be chosen in such a way that correlation effects occur in the electronic structure. In Refs. [30, 31, 32], Drut and Lähde showed by Monte Carlo simulations that in vacuum the coupling between electrons is strong enough to form a Mott insulator while on a silicon substrate it is not. According to their result, suspended graphene would possess a gap which would be very useful in potential applications of graphene in electrical
circuits. These simulations make predictions on the critical value of the coupling constant but do not account for the gap produced inside the insulating phase. In Ref. [33], Sorella and Tosatti apply lattice simulation on the Hubbard model of honeycomb lattice and found Mott transition at $U_c/|t| = 4.5 \pm 0.5$. They also demonstrate that the gap vanishes linearly in the vicinity of the critical point within mean-field theory which differs from the behaviour usually found in finite temperature phase transitions where the gap vanishes as $\Delta \sim |T_c - T|^{1/2}$.

Here we study the Mott transition accompanied by an antiferromagnetic ordering in undoped graphene at zero temperature. The control parameter of the transition is the interaction strength and the goal of the present chapter is to explore the quantum critical behaviour near the critical point. On the basis of Ref. [33] we expect unconventional critical exponents which, as we will see, differ from those in the usual Landau theory.

Landau proposed that in the vicinity of a critical point of a second order phase transition the free energy can be written as

$$ F(m) = F_0 + a(T)m^2 + cm^4 - hm $$

(4.1)

where $m$ is the order parameter, $a(T)$ is proportional to the deviation of the temperature from its critical value, $T - T_c$ and $c > 0$ does not depend on the temperature significantly. In Eq. (4.1), $h$ is the external field conjugated to the order parameter. By minimizing the free energy function, one can obtain the usual mean field exponents, listed below.

<table>
<thead>
<tr>
<th>exponent</th>
<th>definition</th>
<th>mean-field value</th>
</tr>
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<tr>
<td>$\alpha$</td>
<td>$E_{\min} \sim (T_c - T)^{2-\alpha}$</td>
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</tr>
<tr>
<td>$\delta$</td>
<td>$</td>
<td>m</td>
</tr>
</tbody>
</table>

Table 4.1

In order to understand the unconventional behavior in graphene, we will extend our investigations to systems with power law density of states near the Fermi energy, $\rho(\varepsilon) \sim |\varepsilon|^r$. We propose another free energy function for quantum phase transitions and show how the critical exponents are determined by the DOS exponents. Beside monolayer graphene, there exist other materials exhibiting power law DOS. For example, in chirally stacked multilayer
graphene, the DOS exponent is given as \( r = 2/M - 1 \) with \( M \) denoting the number of layers or in VO\(_2\)/TiO\(_2\) nano-heterostructures[34] the DOS varies as \( \sim |\varepsilon|^{1/2} \). Disorder can also modify the DOS exponent to almost arbitrary power-law [35] as \( \sim |\varepsilon|^r \) with \( 0 < r < 1 \). We note that generalization of the density of states to arbitrary power law function has been investigated in quantum impurity models [36, 37] but bulk correlations have been studied systematically in Ref. [38] first.

This chapter is organized as follows. In the first section we establish the mean-field theory of the Hubbard model in monolayer graphene. In the second chapter the critical behaviour of the Mott transition is discussed in details. In the third section we extend the mean-field calculation to general gapless systems and demonstrate how the critical exponents and the critical coupling depend on the DOS exponent.

### 4.1 Mean-field theory of the Hubbard model in graphene

In Chapter 2, we have introduced the tight-binding Hamiltonian of the non-interacting electrons in monolayer graphene as

\[
\hat{H}_0 = \sum_{k\sigma} \begin{pmatrix} a_{k\sigma}^+ & b_{k\sigma}^+ \end{pmatrix} \begin{pmatrix} 0 & tf^*(k) \\ tf(k) & 0 \end{pmatrix} \begin{pmatrix} a_{k\sigma} \\ b_{k\sigma} \end{pmatrix}
\]  

(4.2)

where \( a_{k\sigma} \) and \( b_{k\sigma} \) are the annihilation operators of Bloch states corresponding to the sub-lattice \( A \) and \( B \), respectively, \( t \) is the nearest neighbour hopping integral and \( f(k) = 1 + e^{ika_1} + e^{ika_2} \). As we have discussed in Chapter 2, the spectrum can be approximated as a linear, isotropic dispersion in the vicinity of the Dirac point, \( \varepsilon(k) = \hbar v_F k \). We note that the wavenumber \( K \) does not play any role in this chapter, as opposed to the case of Friedel oscillation. Therefore, the valley degeneracy is taken into account only as a factor of 2 in the density of states which is a linear function of the energy near the Dirac point,

\[
\rho_0(\varepsilon) = \frac{2A_c}{\pi \hbar^2 v_F^2} |\varepsilon|.
\]  

(4.3)

This linearity is a consequence of the linear spectrum and the two-dimensionality of the system because in a \( d \)-dimensional system with dispersion like \( \varepsilon \sim k^z \), the DOS exponent is given as \( r = d/z - 1 \). In Eq. (4.3), spin degeneracy is also taken into account and \( A_c \) is the area of the unit cell.
Interaction between electrons has been neglected so far. One of the easiest way to take it into account is introducing an on-site interaction, leading to the Hubbard model of graphene described by

\[ \hat{H} = \hat{H}_0 + U \sum_{\mathbf{R}} \left( \hat{a}_{\mathbf{R} \uparrow}^+ \hat{a}_{\mathbf{R} \uparrow} \hat{a}_{\mathbf{R} \downarrow}^+ \hat{a}_{\mathbf{R} \downarrow} + b_{\mathbf{R} \uparrow}^+ b_{\mathbf{R} \downarrow}^+ \right) \]  

(4.4)

where \( U \) is the energy cost of double occupancy. Using the Fourier transform of the creation and annihilation operators, one may introduce the following quantities:

\[
\begin{align*}
\hat{n}(\mathbf{q}) &= \frac{1}{4N} \sum_{\mathbf{k}} \left( a_{\mathbf{k}+\mathbf{q} \uparrow}^+ a_{\mathbf{k} \uparrow} + b_{\mathbf{k}+\mathbf{q} \uparrow}^+ b_{\mathbf{k} \uparrow} + a_{\mathbf{k}+\mathbf{q} \downarrow}^+ a_{\mathbf{k} \downarrow} + b_{\mathbf{k}+\mathbf{q} \downarrow}^+ b_{\mathbf{k} \downarrow} \right) \\
\hat{m}(\mathbf{q}) &= \frac{1}{4N} \sum_{\mathbf{k}} \left( a_{\mathbf{k}+\mathbf{q} \uparrow}^+ a_{\mathbf{k} \uparrow} - b_{\mathbf{k}+\mathbf{q} \uparrow}^+ b_{\mathbf{k} \uparrow} - a_{\mathbf{k}+\mathbf{q} \downarrow}^+ a_{\mathbf{k} \downarrow} + b_{\mathbf{k}+\mathbf{q} \downarrow}^+ b_{\mathbf{k} \downarrow} \right) \\
\hat{p}(\mathbf{q}) &= \frac{1}{4N} \sum_{\mathbf{k}} \left( a_{\mathbf{k}+\mathbf{q} \uparrow}^+ a_{\mathbf{k} \downarrow} - b_{\mathbf{k}+\mathbf{q} \uparrow}^+ b_{\mathbf{k} \downarrow} + a_{\mathbf{k}+\mathbf{q} \downarrow}^+ a_{\mathbf{k} \uparrow} - b_{\mathbf{k}+\mathbf{q} \downarrow}^+ b_{\mathbf{k} \uparrow} \right) \\
\hat{s}(\mathbf{q}) &= \frac{1}{4N} \sum_{\mathbf{k}} \left( a_{\mathbf{k}+\mathbf{q} \uparrow}^+ a_{\mathbf{k} \uparrow} - b_{\mathbf{k}+\mathbf{q} \uparrow}^+ b_{\mathbf{k} \uparrow} - a_{\mathbf{k}+\mathbf{q} \downarrow}^+ a_{\mathbf{k} \downarrow} + b_{\mathbf{k}+\mathbf{q} \downarrow}^+ b_{\mathbf{k} \downarrow} \right) 
\end{align*}
\]

(4.5)  

(4.6)  

(4.7)  

(4.8)

which are all Fourier components of well defined physical observables, namely, \( \hat{n}(\mathbf{q}) \) is the electron density, \( \hat{m}(\mathbf{q}) \) is the magnetization, \( \hat{p}(\mathbf{q}) \) is the polarization measuring the charge ordering and \( \hat{s}(\mathbf{q}) \) is the staggered magnetization. In the formulas, \( N \) is the number of unit cells and, hence, the number carbon atoms is given as \( 2N \). In terms of the physical quantities defined above, the Hamiltonian can be rewritten as

\[ \hat{H} = \hat{H}_0 + 2UN \sum_{\mathbf{q} \in \text{BZ}} \left( \hat{n}(\mathbf{q})\hat{n}(-\mathbf{q}) - \hat{m}(\mathbf{q})\hat{m}(-\mathbf{q}) + \hat{p}(\mathbf{q})\hat{p}(-\mathbf{q}) - \hat{s}(\mathbf{q})\hat{s}(-\mathbf{q}) \right). \]

(4.9)

Since the Hubbard model cannot be solved exactly, we determine the ground state within mean-field approximation. By neglecting correlations, the Hamiltonian is obtained as

\[
\begin{align*}
\hat{H} &= \hat{H}_0 + 2UN \sum_{\mathbf{q} \in \text{BZ}} \left[ -|\langle \hat{n}(\mathbf{q}) \rangle|^2 + |\langle \hat{m}(\mathbf{q}) \rangle|^2 - |\langle \hat{p}(\mathbf{q}) \rangle|^2 + |\langle \hat{s}(\mathbf{q}) \rangle|^2 + 2\hat{n}(-\mathbf{q})\langle \hat{n}(\mathbf{q}) \rangle - 2\hat{m}(-\mathbf{q})\langle \hat{m}(\mathbf{q}) \rangle + 2\hat{p}(-\mathbf{q})\langle \hat{p}(\mathbf{q}) \rangle - 2\hat{s}(-\mathbf{q})\langle \hat{s}(\mathbf{q}) \rangle \right]
\end{align*}
\]

(4.10)

In this chapter we are interested in the ground state properties of the interacting electron system at half filling. In principle, Eq. (4.10) could describe any order in which the number of electrons is preserved. However, the honeycomb lattice is bipartite, in which strong on-site repulsion favors antiferromagnetic order at half filling. We assume that the only non-vanishing
expectation value is

\[ \langle \hat{s}(q) \rangle = s \delta_{q,0} \quad (4.11) \]

describing the staggered magnetization illustrated in Fig. 4.1 and because of half filling \( \langle n(q) \rangle = \delta_{q,0}/2 \).

![Figure 4.1: Staggered magnetization in monolayer graphene.](image)

All other expectation values are assumed to be zero, i.e., \( \langle \hat{m}(q) \rangle = 0 \) and \( \langle \hat{p}(q) \rangle = 0 \). Substituting into Eq. (4.10) leads to the mean-field Hamiltonian

\[
\hat{H}_{MF} = \frac{UN}{2} + 2UNs^2 + \sum_{k\sigma} \begin{pmatrix} a_{k\sigma}^+ & b_{k\sigma}^+ \end{pmatrix} \begin{pmatrix} -Us\sigma & tf^*(k) \\ tf(k) & Us\sigma \end{pmatrix} \begin{pmatrix} a_{k\sigma} \\ b_{k\sigma} \end{pmatrix} \quad (4.12)
\]

where \( \sigma = 1 \) for up spins and \( \sigma = -1 \) for down spins. By diagonalizing the mean-field Hamiltonian, we get a gapped quasiparticle spectrum,

\[
\xi_{\pm}(k) = \pm \xi(k) \quad \xi(k) = \sqrt{\Delta^2 + \varepsilon(k)^2}, \quad (4.13)
\]

where the gap is proportional to the staggered magnetization, \( \Delta = U|s| \). The energy spectrum is plotted in Fig. 4.2. Note that for different spin directions the eigenvalues are the same but the eigenvectors are different.

At half filling, the total energy, i.e., the zero temperature free energy, is obtained as

\[
E(s) = \frac{UN}{2} + 2UNs^2 - \sum_{k\sigma} \sqrt{\Delta^2 + \varepsilon(k)^2} = \frac{UN}{2} + 2UNs^2 - \int_{-W}^0 d\varepsilon \rho_0(\varepsilon) \sqrt{\Delta^2 + \varepsilon^2} \quad (4.14)
\]
where $W$ is the bandwidth. In Eq. (4.14), the term proportional to $s^2$ can be identified as the general energy cost of the staggered magnetization which competes with the kinetic energy gain described by the last term. This competition governs the phase transition and determines the equilibrium value of $s$.

Due to gap-opening, the energy spectrum is modified mostly in the vicinity of the Dirac point, where the linearized spectrum is valid and the density of states normalized to a unit cell is given by \( \rho_0(\varepsilon) = \frac{2 A \, |\varepsilon|}{\pi \hbar^2 v_F^2} \). In linear approximation, a cutoff $W$ is introduced preserving the total number of electrons,

\[
2N = \int_{-W}^{0} d\varepsilon \, N\rho_0(\varepsilon) \quad \Rightarrow \quad W = \sqrt{\frac{3\pi}{2}}|t|, \tag{4.15}
\]

leading to

\[
\frac{E(s)}{N} = \frac{U}{2} + 2Us^2 - \frac{4}{3W^2} \left[ ((Us)^2 + W^2)^{\frac{3}{2}} - (Us)^3 \right]. \tag{4.16}
\]

By minimizing the energy one can find the equilibrium value of the staggered magnetization at different interaction strengths. If $U < W$, the energy is minimal at $s_0 = 0$ and at

\[
|s_0| = \frac{1}{2} \left( 1 - \frac{W^2}{U^2} \right) \tag{4.17}
\]

if $U > W$. Thus, for weak interaction strength undoped graphene is a paramagnetic semimetal and by tuning $U$ we find a second order quantum phase transition at the critical point $U_c = W$. For stronger interaction, the system behaves as a regular Mott insulator with antiferromagnetic order. The presented results agree qualitatively with the renormalization group analysis.
in the presence of long-range Coulomb interaction [39, 40], namely that around the Dirac point, weak interactions cannot trigger phase transitions but there is a finite critical coupling.

As claimed in Ref. [10], this explains the absence of electron correlations in graphene samples exfoliated on silicon dioxide where the electron interaction is weakened by screening of the electrons of the substrate. The coupling in these samples is too weak to form a correlated phase. The question whether a correlated phase emerges in graphene in vacuum where electron-electron interaction is expected to be large, was answered later in Ref. [11] by measuring the dispersion of suspended graphene which is reshaped by the interaction but no gap has been formed (not larger than 0.1 meV). The strength of the interaction compared to the kinetic energy, however, can be larger than that in vacuum when appropriate strain is applied [41].

### 4.2 Critical behaviour of Mott transition in graphene

In the previous section, the critical value of the interaction has been obtained as $U_c = W \approx 2.33|t|$ within mean-field theory and linear approximation. One could, however, go beyond the linear approximation and take into account the full tight-binding spectrum (2.7), leading to the critical coupling $U_c = 2.23|t|$ [33]. The smaller value of the critical interaction strength can be explained by the fact that in the semimetallic phase eigenenergies are farther from the Fermi level in the linearized model than in the full spectrum. It follows that the gap-opening produces larger kinetic energy gain and smaller interaction is sufficient to establish the Mott phase in the case of full tight-binding spectrum.

In mean-field theory, however, the stability of the ordered phase is overestimated and the real critical value, if such a phase transition exists at all, should be larger because of the quantum fluctuations. Monte Carlo simulations [33, 31, 32] confirm the existence of the semimetal-insulator transition and the critical interaction strength was found $U_c / |t| = 4.5 \pm 0.5$ [33]. Numerical studies, however, do not account for the critical exponents of the Mott transition except the $\beta$ exponent, defined as $|s| \sim (U - U_c)^\beta$ close to $U_c$, which was found 1 in Ref. [33]. Here we calculate all the exponents and explore what fundamental properties of graphene are responsible for this unconventional behaviour.

The critical behaviour can be obtained from the expansion of the total energy (4.16) for
small values of $s$,
\[
\frac{E(s)}{N} = \frac{E(0)}{N} - a(U)s^2 + c|s|^3,
\]
with
\[
E(0) = \frac{UN}{2} \left(1 - \frac{8W}{3U}\right), \quad a(U) = 2U \left(\frac{U}{W} - 1\right), \quad c = \frac{4U^3}{3W^2}.
\]

Here the second order term is followed by a third order term instead of $s^4$ usually found in standard Landau theory, see (4.1). The unconventional third order term is induced by the linear behaviour of the density of states at the Fermi level. In all other aspects, Eq. (4.18) works like standard Landau theory. The coefficient of the second order term, $a(U)$, changes sign at the critical point while the coefficient of the third order counterterm is positive on both sides of the transition. It follows that the minimalization of the ground state energy provides paramagnetic state below the critical interaction strength and ordered phase above.

The equilibrium value of the order parameter is already calculated in Eq. (4.17). Just above the critical point, if $U - U_c \ll U_c$, it is rewritten as
\[
|s_0| = \frac{U - U_c}{U_c}
\]
being linear in the deviation of the control parameter from its critical value which results in $\beta = 1$, as opposed to the standard mean-field value $1/2$.

The specific heat exponent is defined through $E_{\text{min}} - E(0) \sim (U - U_c)^{2-\alpha}$ for $U > U_c$ where $E_{\text{min}}$ is the minimal ground state energy. Of course, $E_{\text{min}} = E(0)$ in the semimetallic phase, but in the magnetic phase
\[
\frac{E_{\text{min}}}{N} = \frac{E(0)}{N} - 2\frac{(U - U_c)^3}{3W^2}
\]
near the critical point, leading to $\alpha = -1$. In conventional Landau theory, the specific heat exponent was obtained as $\alpha = 0$.

The conjugate field of the staggered magnetization is the alternating external magnetic field which has different sign on the two sublattices but with the same amplitude $h$. In the presence of an external field, the full Hamiltonian is given as
\[
\hat{H}_{MF,h} = \hat{H}_{MF} - N\hat{h}\hat{s}(0) = \hat{H}_0 + \frac{UN}{2} + 2UNs^2 - 4UN \left(s + \frac{h}{4U}\right) \hat{s}(0)
\]
where $\hat{s}(0)$ is the staggered magnetization operator. This formula suggests that in the total energy $s$ should be replaced by $s + h/(4U)$ everywhere except in the term stemming from the
general energy cost of the magnetic order. Remember that in conventional Landau theory the conjugate field can easily be taken into account by adding $-h s$ to the ground state energy. In our model, however, close to the critical point

$$\frac{E_h(s)}{N} = \frac{E(0)}{N} + 2 U s^2 - \frac{2 U^2}{W} \left(s + \frac{h}{4U}\right)^2 + c \left|s + \frac{h}{4U}\right|^3$$

(4.23)

is the correct form. The critical exponent of the conjugate field is defined as $s \sim h^{1/\delta}$ when the interaction takes its critical value, $U = U_c$. Exactly at the critical point, the energy is minimal at

$$|s(h)| = \sqrt{\frac{h}{4W}}$$

(4.24)

to leading order in the external field. Therefore, the critical exponent of the conjugate field is obtained as $\delta = 2$, as opposed to that of a normal Landau theory, $\delta = 3$.

The susceptibility is calculated by determining the staggered magnetization in the presence of a weak external field and the corresponding exponent is defined as $\chi = (\partial s/\partial h)|_{h=0} \sim |U - U_c|^{-\gamma}$. Below the critical point, $s = 0$ in the absence of magnetic field. Hence, $s$ is small for a weak external field and the third order term is negligible. The minimalization then leads to

$$s(h) = -\frac{h}{4(U - U_c)} \quad U < U_c.$$  

(4.25)

Above the critical point the minimum value of the ground state energy (4.22) was found at $s = 2a(U)/3c$. In the presence of a weak external field, the deviation from this value is

$$s(h) - s(h = 0) = \frac{h}{4(U - U_c)} \quad U > U_c$$

(4.26)

leading to

$$\chi = \frac{1}{4|U - U_c|},$$

(4.27)

which provides the susceptibility exponent $\gamma = 1$.

We note that the susceptibility is the inverse of the second derivative of the ground state energy with respect to $s$ and evaluated at the minimum. Additionally, the same result can be obtained from microscopic theory within random phase approximation. The bare susceptibility is derived within linear response theory as

$$\chi_0 = \frac{1}{N} \sum_{\mathbf{R}} \int_0^\infty dt \frac{i}{\hbar} \langle [\hat{s}(\mathbf{R}, t), \hat{s}(0, 0)] \rangle = \frac{1}{8N} \sum_k \left(1 - \frac{\Delta^2}{\xi(k)^2}\right) \frac{1}{\xi(k)}$$

(4.28)
where \( \hat{s}(\mathbf{R}, t) \) is the time dependent staggered magnetization in the unit cell characterized by the lattice vector \( \mathbf{R} \), which is the Fourier transform of (4.8). In Eq. (4.28), \( \xi(k) \) is mean-field dispersion relation which is gapped above the critical point and coincides with \( \varepsilon(k) \) below. Using the linear approximation of the spectrum, the bare susceptibility is obtained as

\[
\chi_0 = \begin{cases} 
\frac{1}{W} & \text{if } U < U_c \\
\frac{1}{2U} \frac{W^2}{U^2 + W^2} & \text{if } U > U_c 
\end{cases}
\]  

(4.29)

which leads to

\[
\chi_{\text{RPA}} = \frac{\chi_0}{1 - 4U\chi_0} = \begin{cases} 
\frac{1}{W} \frac{1}{W - U} & \text{if } U < U_c \\
\frac{1}{2U} \frac{W^2}{U^2 + W^2} & \text{if } U > U_c 
\end{cases}
\]  

(4.30)

within random phase approximation. Near the critical point, the RPA susceptibility yields

\[
\chi_{\text{RPA}} \approx \frac{1}{4 |U - U_c|}
\]  

(4.31)

on both sides of the transition in accordance with Eq. (4.27).

The correlation length \( (\xi) \) and the relaxation time \( (\tau) \) are the typical length and time scales of the correlation function defined as

\[
C(\mathbf{R}, \mathbf{R}', t, t') = \langle \hat{s}(\mathbf{R}, t) \hat{s}(\mathbf{R}', t') \rangle - \langle \hat{s}(\mathbf{R}, t) \rangle \langle \hat{s}(\mathbf{R}', t') \rangle.
\]  

(4.32)

In the ordered phase, the Fourier transform of the correlation function is obtained as

\[
\tilde{C}(q, \omega) = \frac{i \hbar A_c \Delta}{\pi^2 \hbar^2 v_F} \int_0^{\frac{W}{2}} dx S(x, \xi_q, \tau \omega)
\]  

(4.33)

with

\[
S(x, Q, \Omega) = x \int_0^{2\pi} d\varphi \frac{1 + \frac{x^2 + xQ \cos \varphi - 1}{\sqrt{1 + x^2} \sqrt{1 + x^2 + 2xQ \cos \varphi + Q^2}}}{\Omega - \sqrt{1 + x^2} - \sqrt{1 + x^2 + 2xQ \cos \varphi + Q^2}}
\]  

(4.34)

and

\[
\xi = \frac{\hbar v_F}{\Delta}, \quad \tau = \frac{\hbar}{\Delta}.
\]  

(4.35)

The corresponding critical exponents are defined as \( \xi \sim (U - U_c)^{-\nu} \) and \( \tau \sim (U - U_c)^{-\nu z} \) and can be readily seen as \( \nu = 1 \) and \( z = 1 \).
The calculated critical exponents fulfill scaling relations, such as \[42\]

\[\alpha + 2\beta + \gamma = 2\]

\[\alpha + \beta(1 + \delta) = 2.\]  \hspace{1cm} (4.36)

The renormalization group eigenvalues corresponding to the universality class described by the above critical exponents are \(y_t = 1\) and \(y_h = 2\). The effective dimension, which differs from the number of spatial dimensions in the case of quantum phase transitions, is obtained as \(d_{\text{eff}} = d + z = 3\). By using scaling relations, the exponent of the correlation function is calculated as \(\eta = 1\). The exponents are summarized in Table 4.2.

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<th>exponent</th>
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<td>(0)</td>
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<td>(\beta)</td>
<td>(</td>
<td>s</td>
<td>\sim (U - U_c)^{\beta})</td>
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<tr>
<td>(\gamma)</td>
<td>(\chi \sim (U - U_c)^{-\gamma})</td>
<td>(1)</td>
<td>(1)</td>
</tr>
<tr>
<td>(\delta)</td>
<td>(</td>
<td>s</td>
<td>\sim h^{1/\delta}, U = U_c)</td>
</tr>
<tr>
<td>(\nu)</td>
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<td>(1)</td>
<td>(_)</td>
</tr>
<tr>
<td>(z)</td>
<td>(\tau \sim (U - U_c)^{-\nu z})</td>
<td>(1)</td>
<td>(_)</td>
</tr>
<tr>
<td>(\eta)</td>
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<td>(_)</td>
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</tbody>
</table>

Table 4.2: Critical exponents of quantum phase transitions in graphene at \(T = 0\) within mean-field theory. The exponents are compared to the ones of the standard Landau theory (in which correlation length, relaxation time and correlation function exponents depend on further properties of the system).

The critical exponents of the quantum phase transition differ from those of finite temperature thermal mean-field exponents. In Landau language, the difference is the consequence of the counterterm of the free energy functional proportional to \(s^3\), as opposed to the conventional theory with \(s^4\). This unconventional counterterm originates from the linear energy dependence of the density of states. In order to understand this relation in more details and see if other properties of the system influence the critical behaviour, we extend our investigation to general gapless systems with arbitrary power-law density of states in the next section.
4.3 Generalization to gapless systems

In undoped graphene, the density of states vanishes linearly at the Fermi level and the system is regarded as a semimetal. In this section, we generalize this behaviour to arbitrary power law energy dependence of the density of states and we are concerned with general gapless systems described by

\[ \rho(\varepsilon) = \kappa |\varepsilon|^r \]  

(4.37)

where the energies are measured from the Fermi level. Note that \( r > -1 \) must hold so that the total number of electrons \( N \) does not diverge. We introduce a cut-off energy \( W \) in such a way that

\[ N = \int_{-W}^{0} d\varepsilon \rho(\varepsilon) = \frac{\kappa}{r + 1} W^{r+1}. \]  

(4.38)

As mentioned in the introduction of this chapter, there are numerous real systems with such power-law DOS. In undoped graphene \( r = 1 \) and in general a \( d \)-dimensional non-interacting electron system with power-law momentum dependence results in

\[ \varepsilon(k) \sim \pm k^z \Rightarrow \rho(\varepsilon) \sim |\varepsilon|^\frac{d-1}{2}. \]  

(4.39)

By switching on the electron-electron interaction, an ordered phase can develop. We assume that within mean-field approximation an energy gap opens in the quasi-particle dispersion relation

\[ \xi_{\pm}(k) = \pm \sqrt{\varepsilon(k)^2 + \Delta^2}. \]  

(4.40)

The control parameter of the quantum phase transition is the interaction strength \( U \) and the order parameter is denoted by \( s \) describing arbitrary ordering with spin or charge or pairing character and it is proportional to the energy gap \( \Delta = Us \). We set \( s \) being positive but it is not a restriction if we assume that the system is symmetric under \( s \rightarrow -s \). Phase transitions with gap-opening described above include for example the BCS theory, spin density wave theories, certain magnetic transitions, e.g. the one described in the previous section, etc. In standard theories, the density of states is usually approximated as a constant function of the energy, which is recovered if \( r = 0 \) in this scheme and will be discussed in more details later.
Using the density of states, the zero temperature total energy of the half-filled system is obtained as

$$\frac{E(s)}{N} = U s^2 - \frac{1}{N} \int_{-W}^{0} d\varepsilon \sqrt{\varepsilon^2 + \Delta^2} \rho(\varepsilon) = U s^2 - U s \, _2F_1\left(\frac{-1}{2}, \frac{r + 1}{2}, \frac{r + 3}{2}; -\frac{W^2}{(Us)^2}\right).$$

(4.41)

where $_2F_1$ is the Gauss hypergeometric function. Here we assumed that the general energy cost of the ordered phase can be written as $Us^2$ which is also very general in mean-field theories. Similarly to the case of undoped monolayer graphene, Eq. (4.41) consists of two competing terms, namely, the general energy cost and the kinetic energy gain. In order to describe the critical behaviour, if phase transition occurs at all, the total energy is expanded with respect to $Us/W$ as

$$\frac{E(s)}{N} = \frac{E(0)}{N} - a(U) s^2 + c s^{r+2} + b s^4.$$

(4.42)

The coefficients and the ground state energy of the unordered phase are given by

$$a(U) = U^2 \left(\frac{r + 1}{2rW} - \frac{1}{U}\right), \quad c = U^{r+2} \frac{r + 1}{W^{r+1}} \Gamma\left(\frac{2 + r}{2}\right) \Gamma\left(\frac{1 + r}{2}\right),$$

$$b = U^4 \frac{r + 1}{8W^3(r - 2)} \quad E(0) = -NW \frac{r + 1}{r + 2}.$$

(4.43)

(4.44)

where $\Gamma(x)$ is the gamma function. Higher order terms in the expansion are higher even powers of $Us/W$ (6, 8, ...), not influencing the critical behaviour. The term proportional to $s^4$ is also negligible if $r < 2$. For $r \geq 2$, the leading terms are $a(U)s^2$ and $bs^4$ which recover the
conventional Landau theory and the critical exponents. In this regime, the critical coupling, which is calculated by solving $a(U_c) = 0$, is obtained as

$$U_c = \frac{2rW}{r+1}. \quad (4.45)$$

When $-1 < r < 2$, the expression of the energy (4.42) differs from the usual Landau expansion because of the term $s^{r+2}$, producing unconventional critical exponents. First we investigate the region of $0 < r < 2$, which includes the case of graphene $r = 1$. Then we study the interesting region of $-1 < r < 0$ where the density of states diverges at the Fermi level. Finally, we discuss the special point of $r = 0$. In all cases we determine the critical interaction strength and the critical exponents $\alpha$, $\beta$, $\gamma$ and $\delta$ in the same way as in the case of undoped monolayer graphene. The correlation length and relaxation time exponents cannot be determined directly within our model, defined by (4.37), but may be obtained by using scaling arguments.

### 4.3.1 Pseudogap regime

For $0 < r < 2$, the density of state vanishes at the Fermi level but no finite energy gap is present in the semimetallic phase. Therefore, this regime is often called the pseudogap regime. The relevant terms in the ground state energy are

$$\frac{E(s)}{N} = \frac{E(0)}{N} - a(U)s^2 + cs^{r+2} \quad (4.46)$$

where the coefficients are defined by Eq. (4.43). The critical interaction strength is calculated from $a(U_c) = 0$ which yields

$$U_c = \frac{2rW}{r+1}, \quad (4.47)$$

therefore there is always a finite critical interaction, and no conventional weak-coupling solution exists. By increasing the interaction, $a(U)$ changes sign at the critical point and the ordered phase becomes more favourable energetically. In Fig. 4.4, the energy as a function of the order parameter is illustrated.

In the ordered phase, $U > U_c$, the total energy is minimal at

$$s_0 = \left( \frac{2a(U)}{(r+2)c} \right)^{\frac{1}{r}} \sim (U - U_c)^{\frac{1}{r}}, \quad (4.48)$$
Figure 4.4: The total energy of the system as a function of the order parameter for different interaction strengths. Below the critical point the minimum of the energy function is at $s = 0$, while above the $U_c$ the minimum is at a finite value of $s$. The density of states exponent was chosen as $r = 1.5$ but the shape of the energy function is typical in the whole $0 < r < 2$ region and is also reminiscent of that of the conventional Landau theory.

giving $\beta = 1/r$. In the ordered phase the ground state total energy reads as

$$
\frac{E_{\text{min}} - E(0)}{N} = - \frac{r}{r + 2} \left( \frac{2}{(r + 2)c} \right)^{\frac{2}{r+1}} a(U)^{\frac{2}{r+1}} \sim (U - U_c)^{\frac{2}{r+1}},
$$

yielding $\alpha = 1 - \frac{2}{r}$. Upon introducing an appropriate external field $h$ which is conjugate to the order parameter, it appears in the Hamiltonian in the additional term $-h \dot{s}$, similarly to the case of monolayer graphene. The total energy is written as

$$
\frac{E_h(s) - E(0)}{N} = Us^2 - \frac{U^2}{U_c} \left( s + \frac{h}{U} \right)^2 + c \left( s + \frac{h}{U} \right)^{r+2}.
$$

We note that, just like in the case of graphene, a numeric prefactor may appear in front of $h/U$ but it does not influence the scaling properties.

Exactly at the critical point, $U = U_c$, the total energy is extremal at

$$
\alpha = \left( \frac{h}{2(r + 2)c} \right)^{\frac{1}{r+1}} \sim h^{\frac{1}{r+1}},
$$

to leading order in $h$. The critical exponent of the conjugate field is, thus, $\delta = r + 1$.

If the external field is weak,

$$
s(h) = \begin{cases} 
\frac{h}{U_c - U} & \text{if } U < U_c, \\
\frac{h}{(U - U_c)r} + s(h = 0) & \text{if } U > U_c,
\end{cases}
$$

where $s(h = 0)$ is the equilibrium value of the order parameter in the absence of external field given by (4.48). The susceptibility, then, scales as

$$
\chi \sim \frac{1}{|U - U_c|} \quad \Rightarrow \quad \gamma = 1.
$$
The exponents calculated above fulfill scaling relations. The renormalization group eigenvalues cannot be derived from the energy function (4.46). However, if we assume that the power law density of states originates from a power law dispersion $\varepsilon(k) \sim k^z$ with $z = d/(r+1)$ in a $d$-dimensional system, then by using scaling and hyperscaling relations the eigenvalues may be obtained as

$$y_h = d, \quad y_t = d \frac{r}{r+1}.$$  \hspace{1cm} (4.54)

The two eigenvalues correspond to the relevant variables $h$ and $U$. The exponent of the correlation length is given as $\nu = 1/y_t = (r + 1)/(rd)$ and the relaxation time scales as $\tau \sim h/\Delta \sim (U - U_c)^{-1/r}$. The effective dimension describing the quantum phase transition is $d_{\text{eff}} = d + z = d(r + 2)/(r + 1)$ and the exponent of the correlation function is given by $\eta = d_{\text{eff}} + 2 - 2y_h = 2 - d/(r + 1)$.

To summarize, in the $0 < r < 2$ region significant $r$-dependence has been found in the critical exponents of the quantum phase transition. This calculation shows that in the case of monolayer graphene, $r = 1$, the unconventional critical behaviour is related solely to the linear energy dependence of the density of states and is not directly associated with the two-dimensionality of graphene or the linear dispersion or any other peculiarities of graphene.

In the whole region, the critical coupling is finite, i.e., there is no weak coupling solution.

The regime $0 < r < 2$ was investigated in the Kondo problem using renormalization group. In Ref. [36], a quantum phase transition was identified at finite coupling and the Kondo temperature was found to be a power-law function of the coupling with the exponent $1/r$ close to the critical point, in agreement with the above results.

### 4.3.2 Diverging density of states

In the regime of $-1 < r < 0$, the density of states diverges at the Fermi level. Such behaviour can be found, for instance, in chirally stacked multilayer graphene with more than two layers or near a van Hove singularity. Within mean-field theory, the relevant terms of the ground state energy are given by

$$\frac{E(s)}{N} = \frac{E(0)}{N} + cs^{r+2} - a(U)s^2$$  \hspace{1cm} (4.55)

where the leading correction due to ordering is proportional to $s^{r+2}$. Its coefficient $c$ is negative for arbitrary interaction strength due to the Gamma functions in Eq. (4.43). The
counterterm is now the $s^2$ term with the coefficient $a(U)$ which is negative independently from the strength of the interaction. Because of $c < 0$, the function $E(s)$ decreases for small values of $s$ until the counterterm, which is positive, turns the function increasing. Hence, the minimum is always at a finite value of $s_0$ as long as $U > 0$. Thus, in the region $-1 < r < 0$ weak coupling solution is found, i.e. the system is ordered for any finite interaction.

As the interaction strength goes to zero, the coefficients vanish as $a(U) \approx -U$ and $c \sim -Ur^2$ and the equilibrium value of the order parameter $s_0$ becomes infinitesimally small as illustrated in Fig. 4.5. Hence, the critical coupling is $U_c = 0$ and the deviation from the critical value is $U$ itself. Therefore, $U$-dependence of both $a(U)$ and $c(U)$ plays an important role in the forthcoming discussion.

![Figure 4.5](image)

Figure 4.5: The total energy of the system as a function of the order parameter for different interaction strengths, $U_1 > U_2 > U_3 > 0$. As the coupling decreases, the equilibrium value of the order parameter is reduced. In particular, in the $U \to 0$ limit, $s_0 \to 0$. The density of states exponent was chosen as $r = -0.9$ for the plot.

Near the critical point the total energy reaches its minimum at

$$s_0 = \left(\frac{2|a(U)|}{|c(U)|(r+2)}\right)^{\frac{1}{r}} \sim U^{-1 - \frac{1}{r}} \quad \Rightarrow \quad \beta = -1 - \frac{1}{r}.$$  \hspace{1cm} (4.56)

The minimum energy scales as

$$\frac{E_{\min}}{N} = -\frac{r}{r+2}a(U) \left(\frac{2|a(U)|}{|c(U)|(r+2)}\right)^{\frac{2}{r}} \sim U^{-1 - \frac{2}{r}} \quad \Rightarrow \quad \alpha = 3 + \frac{2}{r}.$$  \hspace{1cm} (4.57)

The linear response to an external field is obtained as the inverse second derivative of the ground state energy with respect to $s$ and evaluated at $s_0$.

$$\chi = \left(\frac{1}{N} \frac{\partial^2 E(s)}{\partial s^2}\right)^{-1} \bigg|_{s=s_0} = \frac{1}{2a(U)r} \sim U^{-1} \quad \Rightarrow \quad \gamma = 1.$$  \hspace{1cm} (4.58)

In the presence of an external field, a $-\hbar \hat{s}$ operator appears in the Hamilton operator. The ground state energy is rewritten as

$$\frac{E(s)}{N} = \frac{E(0)}{N} + c(U) \left(s + \frac{h}{U}\right)^{r+2} + Us^2 - U^2r^2 + \frac{1}{2rW}\left(s + \frac{h}{U}\right)^2.$$  \hspace{1cm} (4.59)
In order to determine the $\delta$ exponent, we have to calculate its minimum to leading order in $h$ and in the $U \to 0$ limit. The latter limit can be taken only after dividing the equation $\partial E(s)/\partial s = 0$ by $U$, leading to

$$s(h) = \frac{(r+1)(r+2)}{8\sqrt{\pi}} \Gamma\left(-\frac{2+r}{2}\right) \Gamma\left(\frac{1+r}{2}\right) \left(\frac{h}{W}\right)^{r+1} \Rightarrow \delta = \frac{1}{r+1}.$$  \tag{4.60}

This behaviour can be understood by the following dimensional analysis as well. Exactly in the critical point $U = U_c = 0$, the only relevant energy scale is determined by the external field $h$. Therefore, the only way to derive a dimensionless quantity is $s_0 \sim \kappa h^{r+1}$ which also leads to $\delta = 1/(r+1)$.

The critical exponents calculated above fulfill appropriate scaling relations. Assuming again that the dynamical critical exponent is $d/(r+1)$, the renormalization group eigenvalues are obtained as

$$y_h = d \frac{1}{r+1}, \quad y_t = d \frac{|r|}{r+1}$$ \tag{4.61}

in a $d$-dimensional system. The critical exponent of the correlation length is obtained as $\nu = 1/y_t = (r+1)/(d|\lambda|)$. The effective dimension is again $d_{\text{eff}} = d(r+2)/(r+1)$ and the exponent of the correlation function is given by $\eta = 2 + dr/(r+1)$.

### 4.3.3 Constant density of states

Finally, we study the case of constant density of states at the Fermi level, $r = 0$, which is well known but it is instructive to revisit the calculation in our framework. In the special case of $r = 0$, Eq. (4.41) can be rewritten as

$$\frac{E(s)}{N} = U s^2 - \frac{U^2 s^2}{2W} \text{arcsinh} \left(\frac{W}{Us}\right) - \frac{1}{2} \sqrt{(Us)^2 + W^2}$$ \tag{4.62}

which is expanded for small values of $Us/W$ as

$$\frac{E(s)}{N} = \frac{E(0)}{N} + U s^2 - \frac{U^2}{2W} s^2 \ln \left(\frac{2W}{Us}\right).$$ \tag{4.63}

The total energy acquires logarithmic corrections in the counterterm which is proportional to $s^2 \ln s$ and may be regarded as a power-law function with the exponent $2 + 0$. Similarly to the $-1 < r < 0$ regime, the critical coupling is found $U_c = 0$ and the deviation of the control parameter is $U$ itself.
The energy is minimal at

\[ s_0 = \frac{W}{U \sqrt{e^{-2W}}} \]  

(4.64)

which is in accordance with the well known weak-coupling solution of the gap equation \( \Delta \sim We^{-2W/U} \). This exponential behaviour may be regarded as a power law function of the control parameter with infinite exponent and, hence, the critical exponent of the order parameter is \( \beta = \infty \).

The minimal energy reads as

\[ \frac{E_{\text{min}} - E(0)}{N} = -\frac{We^{-4W}}{U} \]  

(4.65)

which may be interpreted as a power law function of \( U \) with the exponent \( \alpha = -\infty \).

Interestingly, the \( \gamma \) exponent is obtained as

\[ \chi = \left( \frac{1}{N} \frac{\partial^2 E(s)}{\partial s^2} \right)^{-1} \bigg|_{s=s_0} = \frac{W}{U^2} \Rightarrow \gamma = 2 \]  

(4.66)

which differ from that in all other regions where \( \gamma = 1 \). This is, however, expected after both \( \alpha \) and \( \beta \) have singular behaviour at \( r = 0 \), see Fig. 4.6.

The \( \delta \) exponent can be obtained from the energy function

\[ \frac{E(s)}{N} = \frac{E(0)}{N} + Us^2 - \frac{U^2}{2W} \left( s + \frac{h}{U} \right)^2 \ln \left( \frac{2W}{U \left( s + \frac{h}{U} \right)} \right) \]  

(4.67)

in similar way as we have done in the previous subsection. The energy is minimal at

\[ s(h) = \frac{h}{2W} \ln \frac{W}{h} \]  

(4.68)

to leading order in the external field and exactly at the critical point. This may be regarded as a power law function with \( \delta = 1 + 0 \).

4.4 Conclusion

In this chapter we studied the critical behaviour of the Mott transition in undoped monolayer graphene. In the previous chapter we have shown that the screening is very weak and, therefore, strong interaction effects are expected at half filling. Another motivation was that opening a bulk gap in graphene in a controllable way would be extremely useful in industrial applications.
The Mott transition accompanied by antiferromagnetic ordering has already been predicted by numerical and analytical calculations [31, 33], but no comprehensive study of the critical behaviour has been done before. In this chapter, all the mean-field critical exponents of the semimetal-insulator transition have been determined which differ from that of the conventional Landau theory. In order to understand what fundamental properties of graphene cause this difference, the mean-field calculation has been extended to general gapless systems. The results imply that the linear energy dependence of the density of states in graphene is sufficient to explain the unusual critical behaviour of the Mott transition and no other properties of graphene influence this behaviour.

General gapless systems are electron systems with density of states obeying power-law energy dependence at the Fermi level, \( \rho(\varepsilon) \sim |\varepsilon|^r \). This energy dependence can be found for example in chirally stacked multilayer graphene where \( r = 2/M - 1 \) with \( M \) denoting the number of layers. In general gapless systems, only the critical coupling of the Kondo problem and, in a few cases, the coupling dependence of the Kondo temperature have been investigated using renormalization group techniques [36, 43]. Bulk correlated phases, however, have not been studied within mean-field theory before. For \( r > 2 \), the conventional Landau theory is recovered, while in the \( -1 < r < 2 \) regime the critical exponents depend remarkably on the density of states exponent. These dependences are summarized in Table 4.3 and plotted in Fig. 4.6. The presented results extend the mean-field universality class covering a much broader region of values of critical exponents than that of the conventional Landau theory.

<table>
<thead>
<tr>
<th>exponents</th>
<th>( \alpha )</th>
<th>( \beta )</th>
<th>( \gamma )</th>
<th>( \delta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r \geq 2 )</td>
<td>0</td>
<td>( \frac{1}{2} )</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>( 0 &lt; r &lt; 2 )</td>
<td>1 - ( \frac{2}{r} )</td>
<td>( \frac{1}{r} )</td>
<td>1</td>
<td>( r + 1 )</td>
</tr>
<tr>
<td>( r = 0 )</td>
<td>( -\infty )</td>
<td>( \infty )</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>( -1 &lt; r &lt; 0 )</td>
<td>3 + ( \frac{2}{r} )</td>
<td>( -1 - \frac{1}{r} )</td>
<td>1</td>
<td>( \frac{1}{r + 1} )</td>
</tr>
</tbody>
</table>

Table 4.3: Summary of the mean-field quantum critical exponents for general gapless phases. The exponents for \( -1 < r < 0 \) can be obtained from the \( 0 < r < 2 \) exponents by the \( r \rightarrow -r/(r + 1) \) replacement.
Figure 4.6: The critical exponents and the critical interaction strength as a function of the density of states exponent, $r$ are plotted. For $r > 2$, the conventional mean-field exponents are recovered.

Extension of the low-energy model of monolayer graphene enabled us to understand which features of the system determine the critical behaviour of the Mott transition. In the next chapter, we will follow the same strategy to investigate optical properties of monolayer and chirally stacked multilayer graphene.
Chapter 5

Low-frequency optical conductivity in graphene and other scale-invariant systems

One of the most fascinating properties of monolayer graphene is that the optical conductivity is universal and independent of the frequency [44, 45, 46, 47, 48],

\[ \sigma_{\text{monoLG}}(\omega) = \frac{e^2}{4\hbar} \]  

being proportional to the conductance quantum, \( 2e^2/h \approx 7.75 \cdot 10^{-5} \Omega^{-1} \). This feature was argued to be a consequence of the linear spectrum and the structure of the Dirac cones [44] but here we will show that linearity does not play any role in this phenomenon.

Similar universal behaviour has been found in chirally stacked multilayer graphene, namely the optical conductivity is independent of the frequency, \( \sigma_{\text{multiLG}}(\omega) = Me^2/(4\hbar) \) with \( M \) being the number of layers. Electronic and optical properties of multilayer graphene have also been investigated experimentally and theoretically [49, 50, 51]. As we have discussed in Chapter 2, the low energy behaviour of quasiparticles show chiral nature and can be characterized by the pseudospin winding number which is equal to the number of layers. Chiral nature of quasiparticles has been proven to play an important role in various phenomena, such as quantum Hall effect [52], THz radiation measurements [53] and angle-resolved photoemission spectroscopy measurements [18].

In this chapter, we generalize the low-energy model of graphene in order to understand
the underlying physics behind the universal frequency dependence of Eq. 5.1 and explore the relation between chirality and universal nature.

First, we review the Kubo formula of the optical conductivity of generic solids and show how the resulting formulas can be written if tight-binding approximation is applied. Then, we restrict our investigation to two band systems where the electronic states are described by two-component vectors and, therefore, possess a pseudospin degree of freedom. Finally, we present a wide class of two band systems which exhibit universal frequency dependence.

5.1 Optical conductivity in generic solids

Physical quantities measured in optical experiments can usually be expressed by means of the optical conductivity. Using the Kubo formula the optical conductivity is written as

\[
\sigma_{\alpha\beta}(r, r', \omega) = -\frac{e^2 n(r)}{i\omega m} \delta(r - r') \delta_{\alpha\beta} + \frac{1}{i\omega} \lim_{\delta \to 0^+} \int_0^\infty dt \frac{i}{\hbar} \langle [j_\alpha(r, t), j_\beta(r', 0)] \rangle_0
\]  

(5.2)

where \( n(r) \) is the density of electrons, \( j_\alpha(r, t) \) is the current density operator and the expectation value shall be evaluated in the equilibrium state. The first term in (5.2) is the diamagnetic term which, as we will see, does not contribute to the real part of the optical conductivity at finite frequencies.

In generic solids of arbitrary dimension and with arbitrary lattice structure, the one-particle eigenstates are the Bloch states which obey the Schrödinger equation

\[
H(r) \Psi_{lk}(r) = E_l(k) \Psi_{lk}(r)
\]  

(5.3)

where \( H(r) = -\hbar^2 \Delta/(2m) + U(r) \) is the Hamilton operator with a lattice periodic potential. Because of Bloch's theorem, the eigenfunctions can be written as

\[
\Psi_{lk}(r) = \frac{1}{\sqrt{\Omega}} e^{i kr} u_{lk}(r)
\]  

(5.4)

where \( \Omega \) is the volume of the sample and \( u_{lk}(r) \) is a periodic function of space variables, possessing the same translational symmetries as the potential \( U(r) \). If the Coulomb interaction between electrons is neglected, then the one-particle eigenstates are filled following the Fermi distribution function \( f(E) = (e^{\beta E} + 1)^{-1} \).

In this chapter we investigate optical transitions, i.e. when electrons absorb or emit photons. During these inelastic scattering processes the momentum of photons are negligible,
therefore electron momentum is preserved. Optical transitions are described by the homogeneous \((\mathbf{q} = 0)\) dynamical conductivity,

\[
\sigma_{\alpha\beta}(\omega) = \sigma_{\alpha\beta}^{\text{dia}}(\omega) + \frac{1}{\Omega} \int d^d r \int d^d r' \frac{1}{i\omega} \lim_{\delta \to 0^+} \int_0^\infty dt \, e^{i\omega t - \delta t} \frac{i}{\hbar} \langle [j_\alpha(r, t), j_\beta(r', 0)] \rangle_0 = 
\]

\[
= \sigma_{\alpha\beta}^{\text{dia}}(\omega) - \frac{2e^2}{i\omega \Omega} \sum_{ll'kk'} V_{\alpha,ll'kk'} V_{\beta,ll'kk'} \frac{f(E_l(k)) - f(E_{l'}(k'))}{\hbar \omega + i\delta + E_l(k) - E_{l'}(k')} 
\]

\[(5.5)\]

where \(\mathbf{k}\) and \(\mathbf{k}'\) run over the whole Brillouin zone. The prefactor 2 comes from spin degeneracy.

The matrix elements \(V_{ll'kk'} = \langle \Psi_{l'k'} | \mathbf{v} | \Psi_{lk} \rangle\) of the velocity operator may be rewritten as

\[
V_{ll'kk'} = \delta_{kk'} \left[ i \omega_{ll'}(k) A_{ll'}(k) + v_l(k) \delta_{ll'} \right] 
\]

\[(5.6)\]

with \(\hbar \omega_{ll'}(k) = E_l(k) - E_{l'}(k)\). In the formula, \(\hbar v_l(k) = \partial E_l / \partial k\) is the quasiparticle velocity in the \(l\)th band and

\[
A_{ll'}(k) = \frac{i}{\Omega} \int d^d r u_{l'k}^*(r) \nabla_k u_{lk}(r) 
\]

\[(5.7)\]

is the self-adjoint Berry connection matrix.

Note that the first term in (5.6) describes transitions between two different bands and equals to zero if \(l = l'\). The second term is non-zero only if \(l = l'\) and is the quasiparticle velocity. However, in (5.5) only terms corresponding to two different bands survive for non-zero frequencies because of the Fermi functions. Therefore,

\[
\sigma_{\alpha\beta}(\omega) = \sigma_{\alpha\beta}^{\text{dia}}(\omega) - \frac{2e^2}{i\hbar \omega \Omega} \sum_{ll'kk'} \omega_{ll'}(k)^2 A_{\alpha,ll'}(k) A_{\beta,ll'k} \frac{f(E_l(k)) - f(E_{l'}(k))}{\omega + i\delta + \omega_{ll'}(k)}. 
\]

\[(5.8)\]

In the followings, we focus on the real part of the optical conductivity. The imaginary part may be calculated using Kramers-Kronig relations. The diamagnetic conductivity is purely imaginary so it does not appear in the real part at non-zero frequencies. The \(\delta \to 0^+\) limit of the second term in (5.8) can be divided into a principal value part and a Dirac-delta part because

\[
\lim_{\delta \to 0^+} \frac{1}{x + i\delta} = \text{P} \frac{1}{x} - i\pi \delta(x). 
\]

\[(5.9)\]

Since the Hamiltonian does not depend on the spin, the system is time reversal invariant leading to \(E_l(k) = E_l(-k)\) and \(A_{ll'}(k) = A_{l'l}(-k)\). Using these relations one can easily see that the real part of Eq. (5.8) equals the Dirac-delta part.
We note that this statement is true even if the Hamiltonian is different for up and down spins. Due to the time reversal properties of a spin-dependent Hamiltonian, \( E_s^\lambda(k) = E_i^{−s}(−k) \) and \( A_s^{ll'}(k) = A_i^{−s}(−k) \) hold where \( s \) denotes the different spin directions. In this case, one has to sum up with respect to \( s \) in (5.8) instead of just simply having the prefactor 2. The time reversal properties of the dispersion relation and Berry curvature ensure again that the real part coincides with the Dirac delta part of the optical conductivity. Spin-dependent Hamiltonian occurs, for example, in the presence of an external magnetic field. In this chapter, however, we do not consider magnetic effects, and continue with spin-independent Hamiltonian.

The real part of the optical conductivity is obtained as

\[
\text{Re} \sigma_{\alpha\beta}(\omega) = \frac{2e^2}{\hbar} \frac{\pi \omega}{\Omega} \sum_{ll'k} A_{\alpha, ll'}(k) A_{\beta, ll'}(k) \left[ f(E_l(k)) - f(E_i^{−s}(−k)) \right] \delta(\omega - \omega_{ll'}(k)).
\]  

(5.10)

Due to the difference of the Fermi functions in Eq. (5.10), intraband processes do not contribute for non-zero frequencies. We note that in the presence of disorder, intraband contributions are negligible only for frequencies larger than the scattering rate. The optical conductivity is now expressed in terms of the Berry connection matrix. It is well known that the Berry connection is essential in determining the dc Hall conductivity[54]. However, Eq. (5.10) shows that this topological quantity plays an important role in dynamical quantities as well.

Using Eq. (5.10) one can calculate the optical conductivity of solids generally. To do so, first the energy spectrum and the Berry connection matrix have to be computed in band structure calculations. Since the bandstructure and the eigenstates cannot be determined exactly, one has to apply some kind of approximation. In tight binding approximation the Hilbert space is restricted to several atomic orbits per unit cell and the eigenfunctions are given as \( e^{i\mathbf{k} \cdot \mathbf{r}} |\mathbf{k}, l\rangle / \sqrt{\Omega} \) where we have introduced \( |\mathbf{k}, l\rangle \) as finite-dimensional vectors representing the eigenstates on this subspace. See for example, Eq. (2.8) in the case of monolayer graphene where the two components correspond to the \( p_z \) orbitals of an \( A \) and a \( B \) atom. In order to calculate the Berry connection matrix elements, one may use \( A_{ll'}(k) = i \langle k, l | \nabla_k | k, l' \rangle \) instead of (5.7). This expression, however, depends on the choice of the basis in the tight binding subspace. Before continuing the evaluation of the optical conductivity, we show in the next section that in most cases \( i \langle k, l | \nabla_k | k, l' \rangle \) deviates from (5.7) negligibly in the so-called "natural" tight binding basis.
5.2 Berry connection in tight-binding approximation

The Berry connection matrix, defined originally in Eq. (5.7) in terms of the periodic functions $u_{lk}(r)$ can usually be rewritten as $A_{ll'}(k) = i\langle k, l|\nabla_k|k, l'\rangle$ within tight-binding approximation, if the vectors $|k, l\rangle$ are given in the "natural" TB basis.

Within tight binding approximation, we restrict the Hilbert space to $L$ atomic orbitals $\varphi_b(r)$ ($b = 1, \ldots, L$) per unit cell. Then the corresponding Bloch functions are

$$\varphi_{bk}(r) = \frac{1}{\sqrt{N}} \sum_{b} e^{\frac{i}{\sqrt{N}} R} \varphi_b(r - R)$$  (5.11)

where $R$ runs over all lattice vectors. We call this set of functions "natural" TB basis because this basis is directly derived from the atomic orbitals. Note that TB basis is not necessarily orthonormal but can be Löwdin-orthonormalized[55]. We now assume that

$$\int dr \varphi_{bk}(r)^* \varphi_{bk'}(r) = \delta_{kk'} \delta_{bb'}.$$  (5.12)

The Hamiltonian $H(r) = -\hbar^2 \Delta/(2m) + U(r)$ acts on the "natural" TB basis elements (5.11) as

$$H(r)\varphi_{bk}(r) = \sum_{b'} H_{b'b}(k) \varphi_{bk'}(r) + (H - PHP)\varphi_{bk}(r)$$  (5.13)

where $H_{b'b}(k) = \int dr \varphi_{bk'}(r)^* H(r) \varphi_{bk}(r)$ and $P = \sum_b |\varphi_{bk}\rangle \langle \varphi_{bk}|$ is a projector onto the subspace spanned by the TB basis. Within tight-binding approximation the term $(H - PHP)\varphi_{bk}(r)$ is neglected because this vector is out of the TB subspace.

In practice, the starting point is the self adjoint matrix $H_{b'b}(k)$. The solutions of the Schrödinger equation are given as $\varphi_{bk}(r) = \sum_b c_{lb}(k) \varphi_{bk}(r)$ where the coefficients $c_{lb}(k)$ are determined as the eigenvectors of $H_{b'b}(k)$.

$$\sum_{b'} H_{b'b}(k) c_{lb'}(k) = E_{lk} c_{lb}(k)$$  (5.14)

The periodic part of $\varphi_{lk}(r)$ can be written as

$$u_{lk}(r) = \sqrt{\Omega} e^{-i k r} \varphi_{lk}(r).$$  (5.15)

Substituting into the original definition of the Berry matrix elements (5.7), we obtain

$$A_{ll'}(k) = i \sum_b c_{lb}(k) \nabla_k c_{lb'}(k) + \sum_{bb'} c_{lb}(k)^* c_{lb'}(k) \sum_{R} e^{-i k R} \int dr \varphi_b(r - R)^* \varphi_{b'}(r).$$  (5.16)
By introducing the notation $|k,l\rangle$ for the $L$-dimensional vector built up from the coefficients $c_{lb}(k)$, the matrix element can be rewritten as

$$A_{ll'}(k) = i\langle l,k|\nabla_k|l',k\rangle + \sum_{bb'} c_{lb}(k)^* c_{b'b}(k) \sum_{R} e^{-ikR} \int d\mathbf{r} \varphi_b(\mathbf{r} - \mathbf{R})^* \mathbf{r} \varphi_{b'}(\mathbf{r}) . \quad (5.17)$$

The second term is the matrix elements of the dipole operator taken between Wannier functions. These matrix elements are usually negligible due to the symmetry properties of atomic orbits or their well-localized behaviour. There are, however, a few cases when it is not true. For instance, if both $s$ and $p$ orbits of an atom are taken into account in the tight-binding approximation the matrix element of the dipole operator is not negligible. Nevertheless, in most cases (for example in graphene) the second term in (5.17) can be neglected and, hence,

$$A_{ll'}(k) = i\frac{\Omega}{\Omega} \int d\mathbf{r} u_{lk}(\mathbf{r})^* \nabla_k u_{l'k}(\mathbf{r}) \approx i\langle k,l|\nabla_k|k,l\rangle . \quad (5.18)$$

### 5.3 Two band system

Now we go on calculating the optical conductivity of two-band systems where the electron states are represented by two component vectors for which Eq. (5.18) is valid. Our motivation is that for frequencies lower than the bandwidth, only optical transitions between the two bands closest to the Fermi level are allowed. In this section we focus on electron systems at zero temperature with two bands where the lower band is fully occupied and the upper band is empty (half filling). It follows that optical transitions are allowed only from the lower band to the upper as illustrated in Fig. 5.1.

![Figure 5.1: Optical transitions in generic half-filled two-band system.](image)

The Hamiltonian of two band models is represented with a self-adjoint $2 \times 2$ matrix [56]. Assuming that it is independent of the spin the Hamilton operator can generally be written
\[ \hat{H}(\mathbf{k}) = \varepsilon_0(\mathbf{k}) \hat{I} + \varepsilon(\mathbf{k}) \tilde{n}(\mathbf{k}) \hat{\sigma} \]  

(5.19)

where \( \varepsilon_0(\mathbf{k}) \) and \( \varepsilon(\mathbf{k}) \geq 0 \) are real functions. The three-dimensional vector \( \hat{\sigma} \) is the pseudospin operator built up from the Pauli matrices given in Eq. (2.9) and \( \hat{I} \) is the \( 2 \times 2 \) identity matrix. The components of the three-dimensional unit vector \( \tilde{n}(\mathbf{k}) \) are real functions of the wavenumber.

Due to time reversal invariance of the Hamiltonian \( \varepsilon(-\mathbf{k}) = \varepsilon(\mathbf{k}) \), \( \varepsilon_0(-\mathbf{k}) = \varepsilon_0(\mathbf{k}) \) and \( \{n_x(-\mathbf{k}), n_y(-\mathbf{k}), n_z(-\mathbf{k})\} = \{n_x(\mathbf{k}), -n_y(\mathbf{k}), n_z(\mathbf{k})\} \). The energy spectrum of the two bands is \( E_{\pm}(\mathbf{k}) = \varepsilon_0(\mathbf{k}) \pm \varepsilon(\mathbf{k}) \) where the + and − signs correspond to the conductance and valance bands, respectively. Since \( \tilde{n} \) is a three-dimensional unit vector, it may be described by its azimuthal and polar angles which are also real functions of the wavenumber.

\[ n_x(\mathbf{k}) = \sin \vartheta(\mathbf{k}) \cos \varphi(\mathbf{k}) \]  

(5.20)

\[ n_y(\mathbf{k}) = \sin \vartheta(\mathbf{k}) \sin \varphi(\mathbf{k}) \]  

(5.21)

\[ n_z(\mathbf{k}) = \cos \vartheta(\mathbf{k}) \]  

(5.22)

Because of the time reversal properties of the Hamiltonian, \( \vartheta(\mathbf{k}) \) is an even function while \( \varphi(\mathbf{k}) \) is an odd function of the wavenumber. The eigenvectors can be written as

\[ |\mathbf{k}, +\rangle = \begin{pmatrix} \cos \frac{\vartheta(\mathbf{k})}{2} \\ \sin \frac{\vartheta(\mathbf{k})}{2} e^{-i \varphi(\mathbf{k})} \end{pmatrix} \quad |\mathbf{k}, -\rangle = \begin{pmatrix} \sin \frac{\vartheta(\mathbf{k})}{2} e^{i \varphi(\mathbf{k})} \\ -\cos \frac{\vartheta(\mathbf{k})}{2} \end{pmatrix} \]  

(5.23)

and are evidently determined by \( \tilde{n}(\mathbf{k}) \). It is worth mentioning that \( \langle \mathbf{k}, \pm | \hat{\sigma} | \mathbf{k}, \pm \rangle = \pm \tilde{n}(\mathbf{k}) \), i.e., the vector \( \tilde{n}(\mathbf{k}) \) determines the pseudospin of the electrons and holes. In Fig. 5.2, the electron and hole states are illustrated in the three-dimensional pseudospin space.

At half filling photons excite electrons from the valence band to the conduction band as illustrated in Fig. 5.1. These transitions determine the optical conductivity which is obtained as

\[ \text{Re} \sigma_{\alpha\beta}(\omega) = \frac{2e^2}{\hbar} \frac{\pi \omega}{\Omega} \sum_{\mathbf{k}} A_{\alpha,++}(\mathbf{k}) A_{\beta,--}(\mathbf{k}) \delta \left( \omega - \frac{2\varepsilon(\mathbf{k})}{\hbar} \right) \]  

(5.24)

for positive frequencies and \( \text{Re} \sigma_{\alpha\beta}(\omega < 0) = \text{Re} \sigma_{\alpha\beta}(|\omega|) \) for negative frequencies. We note that Eq. (5.24) is valid only at zero temperature. At finite temperature analytical results can be given only if \( \varepsilon_0(\mathbf{k}) = 0 \). In this case (5.24) has to be multiplied by \( \text{th}(\hbar \omega/4k_B T) \). If \( \varepsilon_0(\mathbf{k}) \)
Figure 5.2: Electron and hole states represented in the three-dimensional pseudospin space for a given \( k \).

is non-zero, the finite temperature formula is more complicated and cannot be determined in general. In the zero temperature expression, however, \( \varepsilon_0(k) \) does not play any role and only \( \varepsilon(k) \) and \( \vec{n}(k) \) are relevant.

In tight binding approximation, we use \( A_{-+}(k) = i\langle -,k|\nabla_k|+,k \rangle \) instead of Eq. (5.7), leading to

\[
A_{-+}(k) = e^{i\varphi(k)} \left[ \nabla_k \vartheta(k) + \sin \vartheta(k) \frac{\nabla_k \varphi(k)}{2} \right].
\]

(5.25)

Now we substitute (5.25) into (5.24) and take advantage of the time reversal properties of different quantities, namely \( \varepsilon(k) = \varepsilon(-k) \), \( \vartheta(k) = \vartheta(-k) \) and \( \varphi(k) = -\varphi(-k) \) and that the Brillouin zone is also inversion symmetric. After a few steps we get the following short expression for the optical conductivity [56].

\[
\text{Re} \sigma_{\alpha\beta}(\omega) = \frac{e^2 \pi |\omega|}{\hbar^2} \sum_k \frac{\partial \vec{n}_\alpha}{\partial k_\alpha} \frac{\partial \vec{n}_\beta}{\partial k_\beta} \delta \left( |\omega| - \frac{2\varepsilon(k)}{\hbar} \right)
\]

(5.26)

This result shows that the optical conductivity of two-band systems can be calculated by identifying the vector field \( \vec{n}(k) \) and the dispersion \( \varepsilon(k) \) in the Hamiltonian and then evaluating the sum over the Brillouin zone given in (5.26). The off-diagonal elements of the optical conductivity do not necessarily vanish and describe Faraday rotation if the symmetry group of the system is low enough.
Now we apply Eq. (5.26) to the case of graphene. The Hamiltonian of graphene is written as

\[
\hat{H}^{1LG}(k) = \hbar v_F (k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) = \hbar v_F k \begin{pmatrix} 0 & e^{-i\gamma} \\ e^{i\gamma} & 0 \end{pmatrix} \tag{5.27}
\]
in linear approximation for the valley corresponding to \( K \), see Eq. (2.12). We note that both valleys have to be taken into account in order to have a time reversal invariant model, which was a necessary condition in the derivation of Eq. (5.26). However, this symmetry also ensures that the contribution of the \( K' \) valley to the optical conductivity is the same as that of \( K \), therefore, the optical conductivity of the \( K \) valley simply has to be multiplied by the valley degeneracy of 2.

In Eq. (5.27), the spectrum and the vector \( \vec{n} \) read as

\[
\varepsilon(k) = \hbar v_F k \quad \vec{n}(k) = \begin{pmatrix} \cos \gamma \\ \sin \gamma \\ 0 \end{pmatrix}. \tag{5.28}
\]

It is worth to mention that the spectrum depends on the magnitude of the wavenumber only while the vector \( \vec{n} \) depends on the angle variable only. It follows that \( \nabla \vec{n} \) contains only derivatives with respect to the angle variable, \( \gamma \). These terms are all proportional to \( k^{-1} \).

Substituting into Eq. (5.26), we get the universal result

\[
\text{Re} \sigma_{\alpha\beta}^{1LG}(\omega) = \frac{1}{4} \frac{e^2}{\hbar} \delta_{\alpha\beta} \tag{5.29}
\]
if valley degeneracy is taken into account.

Let us now take another example, the chirally stacked multilayer graphene. As already mentioned in Chapter 2, the effective Hamiltonian of low energy states can be written as

\[
\hat{H}^{\text{multi}LG}(k) = C k^M \begin{pmatrix} 0 & e^{-iM\gamma} \\ e^{iM\gamma} & 0 \end{pmatrix} \tag{5.30}
\]
where \( M \) is the number of layers. Of course, \( M = 1 \) corresponds to monolayer graphene. The dispersion relation and the pseudospin vector are

\[
\varepsilon(k) = C k^M \quad \vec{n}(k) = \begin{pmatrix} \cos(M\gamma) \\ \sin(M\gamma) \\ 0 \end{pmatrix}. \tag{5.31}
\]
Notice again that the pseudospin vector is the function of the polar angle only. By taking into account both valleys, the optical conductivity is then obtained as

$$\text{Re} \: \sigma_{\alpha \beta}^{\text{multiLG}}(\omega) = \frac{M e^2}{4 \hbar} \delta_{\alpha \beta}.$$  \hspace{1cm} (5.32)

which is independent of the frequency. We note that the low energy model of multilayer graphene (5.30) is time reversal invariant only if both valleys are taken into account.

In the case of monolayer graphene the result (5.29) was argued to be a consequence of the structure of the Dirac cones and the linear spectrum. In the next section we will show that the two-dimensionality and scale invariance of the system are important instead and the universal frequency dependence can be found in a wide class of two-band systems.

5.4 Scale invariant systems

Since the optical conductivity (5.26) cannot be calculated for generic two band systems, we restrict our investigation to a class of two-band systems in which the frequency dependence of the optical conductivity can be evaluated analytically. Before defining the class of scale invariant systems, we introduce several notations.

We use spherical coordinates in momentum space, i.e., $k$ denotes the magnitude and $\{\gamma\}$ stands for the set of angle variables of the wavenumbers. If the dimension of the system is $d$ the set $\{\gamma\}$ consists of $d - 1$ angle variables $\{\gamma_1, \gamma_2, \ldots, \gamma_{d-1}\}$. The gradient in momentum space can be written as

$$\nabla_k = e_k \frac{\partial}{\partial k} + \frac{1}{k} \sum_{j=1}^{d-1} c_j(\{\gamma\}) e_j \frac{\partial}{\partial \gamma_j}$$

where $e_k$ and $e_j$ are unit vectors corresponding to the spherical coordinates $k$ and $\gamma_j$, respectively. Here $c_j$ are coefficients of the Jacobian. Note that if the gradient acts on a function which depends on angle variables only, the derivative is propotional to $k^{-1}$.

Now, we focus on two-band systems which can be described by the Hamilton operator with the following properties. We do not consider $\varepsilon_0(k)$ because, as we have seen in the previous section, it does not influence the zero temperature optical conductivity. Additionally, we assume that the Hamiltonian depends on the magnitude of the momentum only through the dispersion and this dependence is power-law, i.e.,

$$\varepsilon(k) = C(\{\gamma\}) k^z$$  \hspace{1cm} (5.33)
where $z$ is the dynamic exponent and $C(\gamma) > 0$. In this case $\vec{n}(k) = \vec{n}(\gamma)$ is a function of angle variables only.

This assumption has lots of consequences. First, it follows that the conductance and valance bands touch each other at the Fermi level, i.e., there is no energy gap between them as shown in Fig. 5.3. Second, the system is invariant under dilatations which act on spacetime as $r \to br$ and $t \to b^z t$ where $b > 0$ is the scaling parameter. This also means that there is no characteristic energy or length scale in these systems. Third, the eigenvectors depend solely on angle variables so the direction of the pseudospin is determined by the direction of the momentum only. Since this feature is a kind of generalization of the chirality of neutrinos and electrons in graphene, from now on, we may also refer to systems with the above characteristics as general chiral systems. Note that monolayer graphene and chirally stacked multilayer graphene are both general chiral systems.

The density of states in general chiral systems is a power-law function of the energy as illustrated in Fig. 5.3 and

$$
\rho(\varepsilon) = \frac{\kappa}{\pi} \varepsilon^{\frac{d}{z}-1} \\
\kappa = \int \frac{d\gamma}{(2\pi)^{d-1}} C(\gamma)^{-\frac{d}{z}}
$$

where the notation $d\{\gamma\}$ stands for the integration with respect to all angle variables and the Jacobian determinant is also incorporated.

In order to calculate the optical conductivity one has to determine the derivatives $\partial \vec{n}/\partial k_\alpha$. Since $\vec{n}(\gamma)$ is a function of angle variables only, this derivative is always proportional to $k^{-1}$. In the thermodynamic limit the summation in Eq. (5.26) becomes an integral over the momentum space. This integral can be factorized into an integral with respect to angle variables and an integral with respect to $k$. The latter can be carried out analytically in the
case of general chiral systems and also determines the frequency dependence of the optical conductivity as

\[ \text{Re} \sigma_{\alpha\beta}(\omega) = \frac{e^2}{\hbar} \frac{d}{4z} \kappa \left( \frac{\hbar |\omega|}{2} \right)^{\frac{d-2}{2}} \]

where \( \kappa \) is the coefficient of the density of states (5.34) and \( K_{\alpha\beta} \) is a dimensionless factor defined as

\[ K_{\alpha\beta} = \kappa^{\frac{d-2}{d}} \int \frac{d\{\gamma\}}{(2\pi)^{d-1}} C(\{\gamma\}) \sum_{jj'=1}^{d-1} c_j(\{\gamma\})e_{j,\alpha}\frac{\partial \vec{n}}{\partial \gamma_j} c_{j'}(\{\gamma\})e_{j',\beta}\frac{\partial \vec{n}}{\partial \gamma_{j'}} \]

which also describes the possible anisotropy of the system.

We note that in certain cases (for example in monolayer and chirally stacked multilayer graphene) Eq. (5.35) has to be multiplied by valley degeneracy.

Since neither \( \kappa \) nor \( K_{\alpha\beta} \) depend on the frequency, the optical conductivity has universal \( |\omega|^{(d-2)/z} \) frequency dependence which is the main result of this chapter. Using Kramers-Kronig relations, the imaginary part of the conductivity can be obtained and also shows universal behaviour at low frequencies, \( \text{Im} \sigma(\omega) \sim \text{sgn}(\omega)|\omega|^{(d-2)/z}. \) In a two-dimensional system Eq. (5.35) always provides a frequency-independent result. This means that in the case of graphene two-dimensionality and scale invariance (or in other words, the chiral nature of quasiparticles) are responsible for the universal behaviour.

In one dimension there are no angle variables so the unit vector \( \vec{n} \) does not depend on the wavenumber which means that its derivative vanishes. It follows that in one-dimensional general chiral systems the optical conductivity is identically zero for finite frequency.

The result (5.35) is universal in the sense that the microscopic details do not influence the frequency dependence but are incorporated in prefactors only. The universal behaviour can be understood on the basis of dilatation invariance. Under dilatations, defined as \( r \to b r \) and \( t \to b^z t \), the current density operator scales as \( j \to b^{1-d-z} j \). Using the Kubo formula in Eq. (5.5), one can easily see that the optical conductivity scales as \( \sigma(b, \omega) = b^{2-d} \sigma(1, b^z \omega) \). The dilatation invariance demands \( d\sigma/db = 0 \), leading to

\[ (2 - d)\sigma(b, \omega) + z\omega \frac{\partial \sigma(b, \omega)}{\partial \omega} = 0 \quad \Rightarrow \quad \frac{\partial (\ln \sigma)}{\partial (\ln \omega)} = \frac{d - 2}{z}. \]

This results in \( \sigma(\omega) \sim |\omega|^{(d-2)/z} \) but says nothing about the prefactors.

Dynamic scaling analysis is a very powerful tool to explore the frequency dependence of the optical conductivity in the vicinity of the critical point of phase transitions[57, 58, 59].
Exactly at the critical temperature $T_{c}$, the system is scale invariant and power-law frequency dependence with the exponent $(d - z - 2)/z$ has been found in Ref. [57]. In quantum phase transitions one may use the effective dimension $d_{\text{eff}} = d + z$ instead of $d$ which leads to the same frequency dependence as in Eq. (5.35). It follows that in two-dimensional quantum critical systems, the optical conductivity is also frequency-independent [58].

The scaling argument can be applied to other physical quantities. For example, the static polarization function of general chiral systems depends on the wavenumber as $\chi(q) \sim q^{d-z}$ in agreement with Eq. (3.51) or Ref. [60]. Note that the scale invariance is closely related to the fact that there is no characteristic energy in the system. If an energy scale appears, for example due to gap-opening, Eq. (5.35) is not valid any more and the frequency dependence will be influenced by microscopic details, for example, the way how the gap has been formed.

In Chapter 4 we studied the antiferromagnetic phase transition in monolayer graphene. In the ordered phase an energy gap opens and the mean-field Hamiltonian is given by

$$\hat{H}_{\text{AF}}^{\text{monoLG}}(k) = \begin{pmatrix} \Delta & \hbar v_F k e^{-i\gamma} \\ \hbar v_F k e^{i\gamma} & -\Delta \end{pmatrix}.$$ (5.38)

for one valley, see Eq. (4.12). The eigenenergies and the pseudospin vectors are identified as

$$\varepsilon(k) = \sqrt{\Delta^2 + \hbar^2 v_F^2 k^2} \quad \vec{n}(k) = \frac{1}{\sqrt{\Delta^2 + \hbar^2 v_F^2 k^2}} \begin{pmatrix} \hbar v_F k \cos \gamma \\ \hbar v_F k \sin \gamma \\ \Delta \end{pmatrix}.$$ (5.39)

Substituting into Eq. (5.26), the optical conductivity is obtained as

$$\Re \sigma_{\text{AF},\alpha\beta}^{\text{monoLG}}(\omega) = \frac{e^2}{4\hbar} \delta_{\alpha\beta} \left[ \left( \frac{2\Delta}{\hbar \omega} \right)^2 + 1 \right] \Theta(\hbar |\omega| - 2\Delta)$$ (5.40)

where $\Theta(x)$ is the Heaviside function ensuring that optical transitions are prohibited for frequencies smaller than $2\Delta$. Eq. (5.40) does not exhibit universal frequency dependence which is clearly the consequence of the appearing energy scale $\Delta$. As approaching the critical point, $\Delta \to 0$ and at the critical point the frequency dependence becomes universal as

$$\Re \sigma_{\text{AF}}^{\text{monoLG}}(\omega; \Delta \to 0) = \frac{e^2}{(4\hbar)}.$$

### 5.5 Conclusion

We presented analytic derivation of low frequency optical conductivity of two-band systems based on Kubo formalism. As a result, we obtained universal frequency dependence in systems
which are invariant under dilatations and, hence, do not have characteristic energy scale. Scale invariance is closely related to the fact that the pseudospin is determined by the direction of the momentum only. This property may be regarded as some kind of chirality in a very general sense. The exponent of the frequency dependence is determined solely by the dynamical exponent and the dimension of the system as

\[ \text{Re} \sigma(\omega) \sim |\omega|^\frac{\nu-2}{z}. \] (5.41)

In two dimensions the optical conductivity is independent of the frequency for any dynamic exponent in any scale invariant system. These results imply that the universal behaviour of the optical conductivity in monolayer graphene is not a consequence of the linear dispersion, but the scale invariance and the two-dimensionality of the system. The results of this chapter are published in Ref. [61].

The universal frequency dependence of the optical conductivity is in accordance with dynamical properties of critical systems, which are also invariant under dilatations.

These results, however, account for dynamical properties within linear response theory only. Dynamics of a system driven far away from equilibrium is a fascinating field of physics and such non-equilibrium processes are the subject of recent investigations. In the next chapter, we will study non-equilibrium properties of interacting one-dimensional systems (two-dimensional cases are far more complicated).
Chapter 6

Non-equilibrium dynamics in one-dimensional interacting systems

Beside graphene, ultra cold atomic systems have also attracted lots of interest. By confining atoms in a magnetic or optical trap and cooling them with proper setup of lasers, one can achieve realization of various number of many body models, such as the Bose Hubbard model or the Luttinger model [12, 13]. The advantage of these systems is that their parameters, e.g. the strength of the interaction, can be modified artificially in the experiment. By tuning the parameters of the system, interesting phenomena, for example, superfluid-insulator transition can be observed.

In cold atomic systems, time-dependent processes are also observable triggering tremendous number of theoretical works studying non-equilibrium dynamics of correlated many-body systems[62]. The coupling between the atoms and the environment is usually very weak leading to an almost perfectly closed quantum system. Hence, the time evolution of the system is governed by the time dependent Schrödinger equation. This enables us to investigate interesting phenomena, such as quantum thermalization, Bloch oscillations or relaxation processes after driving the system out of equilibrium with a quantum quench[63, 64].

One of the most fascinating issue is the description of the steady state the system reaches waiting long time after a quantum quench. In generic quantum system, the state is determined by the time-dependent density matrix whose time evolution is governed by the von Neumann equation. During the quantum quench, $0 < t < \tau$ where $\tau$ is the quench duration, one of the parameters in the Hamiltonian changes following a slow or fast quench protocol leading
to an inhomogeneous von Neumann equation which is usually very difficult to solve. After
the quench, the time evolution is much simpler, since it is governed by the time-independent
final Hamiltonian $\hat{H}(\tau)$ which, however, does not necessarily commute with the instantaneous
density operator $\hat{\rho}(\tau)$.

In general, the density operator shows no thermalization since its eigenvalues do not
change during the unitary time evolution and, hence, the entropy is constant as a function
of time. In integrable systems, where the number of integrals of motion is macroscopic, the
absence of thermalization is demonstrated also by that the conserved quantities do not relax
to their thermal equilibrium value [63]. In this case, the steady state can be described by
the so-called diagonal ensemble which is determined by the diagonal matrix elements of the
density operator, $\hat{\rho}(\tau)$, in the eigenrepresentation of the final Hamiltonian $\hat{H}(\tau)$. To be more
precise, let us introduce the eigenstates of the final Hamiltonian as $H(\tau)|\Psi_n\rangle = E_n|\Psi_n\rangle$. In
this representation the density operator at $t = \tau$ can be written in the form of

$$\hat{\rho}(\tau) = \sum_{nm} \rho_{nm} |\Psi_n\rangle \langle \Psi_m|$$

(6.1)

where the matrix elements are defined as

$$\rho_{nm} = \langle \Psi_n | \hat{\rho}(\tau) | \Psi_m \rangle.$$  

(6.2)

The further time evolution is governed by the time-independent final Hamiltonian $\hat{H}(\tau)$ leading to

$$\hat{\rho}(t > \tau) = \sum_{nm} \rho_{nm} e^{i(E_m - E_n)t} |\Psi_n\rangle \langle \Psi_m|.$$ 

(6.3)

In the long time limit, the expectation value of physical quantities are determined by the time
averaged density operator

$$\bar{\rho}(t > \tau) = \sum_n \rho_{nn} |\Psi_n\rangle \langle \Psi_n| := \hat{\rho}_{DE}$$

(6.4)

where all non-diagonal elements vanish if there are no degenerate states. In the case of
degenerate states not only diagonal elements but also diagonal blocks remain as illustrated
below.

\[
\hat{\rho}_{\text{DE}} = 
\begin{pmatrix}
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & \Box & \Box & 0 \\
0 & \Box & \Box & 0 \\
0 & \Box & \Box & 0 \\
\end{array}
& 0 & 0 & \Box \\
0 & \Box & 0 & 0 \\
0 & \Box & 0 & 0 \\
0 & \Box & 0 & 0 \\
\end{pmatrix}
\]

The diagonal ensemble is sufficient to deduce the expectation value and the whole distribution of constants of motion at any instant and that of all physical quantities in the steady state but says nothing about relaxation processes. The relaxation due to dephasing may be characterized by the time-dependent fidelity or in other words the Loschmidt echo. This quantity measures the overlap between the initial and the time-evolved states and provides an insight to the relaxation processes without reference to any physical quantities.

In non-equilibrium physics, analytical calculations are usually very complicated, therefore, one usually focuses on one-dimensional systems and so do we in this chapter where we analyze the dynamical properties of the Luttinger model. The Luttinger model describes the universality class of many one-dimensional interacting systems at equilibrium. One goal of the present chapter is to determine the diagonal ensemble describing the steady state the system reaches after a generic quantum quench.

How the system reaches this steady state, is another interesting question and will be studied in terms of the Loschmidt echo in Sec. 6.4.

In Sec. 6.5, we focus on the statistics of final energy which is directly observable in cold atomic systems by repeating the procedure of releasing atoms from the trap and measuring their energy many times. We note that if the initial temperature is zero, the final energy equals the work done on the system during the quench. This is because the initial energy is well-defined and is eventually zero in the Luttinger model. At finite temperature, however, the initial energy is a random variable and, hence, the work done differs from the initial energy motivating us to study the work statistics separately in the case of finite initial temperatures.
6.1 Luttinger model

One-dimensional strongly correlated systems often form a Luttinger liquid, made of bosonic sound-like collective excitations, regardless to the statistics of the original system. For instance, in the case of one-dimensional interacting electrons the particle-hole excitations near the Fermi level behave as bosonic quasiparticles and the model can be described as a Luttinger liquid. In the vicinity of the Fermi level, the spectrum of electrons can be considered as a linear function of the momentum, therefore, the elementary excitations also possess linear dispersion. In this dissertation we do not derive of the Luttinger model from the interacting electron system, i.e. the bosonization, but only pronounce the resulting Hamiltonian as the starting point of this chapter. For more details, see for example Ref. [65]. Thus, bosonization leads to the quadratic Hamiltonian

\[ \hat{H} = \hat{H}_0 + \hat{V} \]  

\[ \hat{H}_0 = \sum_{q > 0} \hbar v_F |q| \left( b_q^+ b_q + \frac{1}{q} b_{q-q} b_{-q} \right) \]  

\[ \hat{V} = \sum_{q > 0} \hbar \delta v |q| \left( b_q^+ b_q + b_{-q}^+ b_{-q} \right) + g(q) \left( b_q^+ b_{-q} + b_q b_{-q} \right) \]

where \( \hat{H}_0 \) is the kinetic energy in the original fermionic language while \( \hat{V} \) corresponds to the interaction of the fermions where only relevant scattering processes are taken into account [65]. In Eq. (6.5), \( b_q \) is the annihilation operator of the bosonic quasi-particles and \( \hbar v_F |q| \) is the noninteracting dispersion with \( v_F \) being the original Fermi velocity of the fermions which is renormalized by \( \delta v \) due to interaction. From now on, the dispersion of the kinetic energy with renormalized velocity will be denoted by \( \omega(q) = \omega_0(q) + \delta \omega(q) = \hbar (v_F + \delta v)|q| \). The interesting part of the interaction describes pair creation or annihilation of bosons. The interaction strength is given as \( g(q) = g_2 |q| e^{-R_0 q} \) where we have introduced \( R_0 \) as the finite range of the interaction which also regularizes integrals without introducing an ultraviolet cut-off.

Note that the wavenumbers \( q > 0 \) are good quantum numbers and the problem simplifies to two coupled oscillators whose frequency is \( \omega_0(q) \) in the non-interacting case. The quadratic Hamiltonian is can be diagonalized by Bogoliubov transformation as

\[ \hat{H} = E_{GS} + \sum_{q > 0} \Omega(q) \left( d_q^+ d_q + d_{-q}^+ d_{-q} \right) \]  

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where
\[ d_q = \frac{\sqrt{\omega(q) + \Omega(q)} b_q + \sqrt{\omega(q) - \Omega(q)} b_{-q}^+}{\sqrt{2\Omega(q)}} \]  \hfill (6.9)
\[ d_{-q}^+ = \frac{\sqrt{\omega(q) + \Omega(q)} b_{-q}^+ + \sqrt{\omega(q) - \Omega(q)} b_q}{\sqrt{2\Omega(q)}} \]  \hfill (6.10)
are the annihilation operators of the new bosonic quasi-particles and

\[ \Omega(q) = \sqrt{\omega(q)^2 - g(q)^2} \]  \hfill (6.11)

is the new spectrum. The ground state energy is given as \( E_{GS} = \sum_{q>0}(\Omega(q) - \omega(q)) < 0 \) and the ground state itself can be written as

\[ |GS\rangle = \prod_{q>0} \sqrt{\frac{2\Omega(q)}{\omega(q) + \Omega(q)}} e^{-\frac{\omega(q) - \Omega(q)}{\omega(q) + \Omega(q)} b_q^+ b_{-q}} |\Psi_0\rangle \]  \hfill (6.12)

where \( |\Psi_0\rangle \) is the vacuum of the \( b \)-bosons.

We note that the two-oscillator model is symmetric under \( q \leftrightarrow -q \). It follows that the difference of the occupation number operators in the \( q \) and \(-q\) modes are left unchanged during the Bogoliubov transformation, \( d_q^+ d_q - d_{-q}^+ d_{-q} = b_q^+ b_q - b_{-q}^+ b_{-q} \).

Now we turn to non-equilibrium dynamics of the Luttinger model when the interaction \( \hat{V} \) is switched on following a time-dependent quench protocol.

### 6.2 Time evolution during quantum quenches

Although the Luttinger model describes the equilibrium properties of the interacting system, it is not entirely clear how it can be extended to non-equilibrium processes. In an out-of-equilibrium situation, additional processes, which are termed irrelevant in equilibrium, are inevitably present in lattice models and can still play an important role. To understand the applicability of the Luttinger model in non-equilibrium situation, several lattice models have been tested and investigated by comparing numerically exact calculations with analytical results using bosonization [66, 67, 68, 69]. These combined numerical and analytical studies indicate that the Luttinger model provides a good description of the steady state.

The non-equilibrium model we investigate throughout this chapter is given by the time-dependent Hamiltonian

\[ \hat{H}(t) = \hat{H}_0 + Q(t)\hat{V}, \]  \hfill (6.13)
where \( Q(t) \) is the quench protocol which vanishes for \( t < 0 \) and equals 1 for \( t > \tau \).

In experiments, energy exchange between the system and the environment is negligible apart from the energy change due to the quench. The coupling between the system and the reservoir is so small, that the relaxation time of thermalization is much longer than the time-scale of the measurement. Hence, the system is regarded as a closed quantum system and its time evolution is determined by the von Neumann equation. The time dependence can be transferred to the Bogoliubov coefficients defined through the time dependent creation and annihilation operators

\[
b_{\pm q}(t) = u_q(t) b_{\pm q} + v_q^*(t) b_{\mp q}^\dagger ,
\]

where the dynamics of the coefficients is determined from Heisenberg’s equation of motion,

\[
\text{i} \hbar \partial_t b_q = [H, b_q] ,
\]

leading to

\[
\text{i} \hbar \partial_t \begin{pmatrix} u_q(t) \\ v_q(t) \end{pmatrix} = \begin{pmatrix} \omega(q, t) & g(q, t) \\ -g(q, t) & -\omega(q, t) \end{pmatrix} \begin{pmatrix} u_q(t) \\ v_q(t) \end{pmatrix} .
\]

The initial conditions are given as \( u_q(0) = 1 \) and \( v_q(0) = 0 \). During the whole time evolution \(|u_q(t)|^2 - |v_q(t)|^2 = 1 \) is satisfied. We note that the differential equation given in Eq. (6.15) can be solved exactly in very special cases only. For example, in the simple case of a sudden quench, when \( \tau \to 0 \), \( u_q(\tau) = 1 \) and \( v_q(\tau) = 0 \). When the quench duration is finite and \( Q(t) \) is a linear function of the time, the model resembles the Landau-Zener model and, hence, the solution can be given in terms of parabolic cylinder functions. Nevertheless, in Secs. 6.3 and 6.4, we do not specify \( Q(t) \) and describe the steady state for arbitrary quench protocol. In Secs. 6.5 and 6.6, we investigate the simple case of a sudden quench only.

### 6.3 Density operator and diagonal ensemble

In general, the density operator of a quantum system provides the complete description of a given state. In experiments, however, the density matrix cannot be observed directly and information about the quantum state can be gained only by measuring different physical quantities. In theory, first we focus on the density operator and then derive the expectation value of physical quantities.

During the whole time evolution the system is decoupled with respect to the quantum numbers \( q > 0 \), as seen in Eq. (6.13). In this section we restrict our investigation to a single
$q > 0$ mode, i.e. we study the model of two coupled oscillators corresponding to $q$ and $-q$ with the same frequencies $\Omega(q)$. The results can easily be generalized to all channels by taking the product of the density operators of all modes. We also drop the subscript $q$ and the indices $q$ and $-q$ are replaced by $+$ and $-$, respectively (e.g. $d_q$ will henceforth be denoted with $d_+$). In the reduced Hilbert space, the basis is spanned by the occupation number eigenstates $|n_+, n_-\rangle$ in which the number of $d_\pm$ bosons is $n_\pm$.

Let us consider that the system is initially prepared in the finite temperature thermal equilibrium state given by

$$\hat{\rho}_0 = \frac{e^{-\beta \hat{H}_0}}{Z_0} \quad Z_0 = \text{Tr} \left[ e^{-\beta \hat{H}_0} \right]$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature. In the reduced two-oscillator model

$$\hat{\rho}_0 = \frac{e^{-\beta \omega_0 (b_+^+ b_+ + b_-^+ b_-)}}{z_0} \quad z_0 = \text{Tr} \left[ e^{-\beta \omega_0 (b_+^+ b_+ + b_-^+ b_-)} \right] = (1 - e^{-\beta \omega_0})^{-2}$$

In the forthcoming calculation, results for zero initial temperatures can be obtained simply by taking the $\beta \to \infty$ limit. At zero temperature, the thermal equilibrium is the pure ground state described by a single wavefunction, $|\Psi_0\rangle$, while at finite temperature the quantum state is mixed.

During the quench, the time evolution is highly non-trivial because of the explicit time-dependence of the Hamiltonian. Although the differential equation (6.15) cannot be solved analytically, the density operator at $t = \tau$ can be expressed in terms of the time-dependent Bogoliubov coefficients, $u(\tau)$ and $v(\tau)$. Right at the end of the quench, the time-evolved density operator is given by

$$\hat{\rho}(\tau) = \hat{U}(\tau) \hat{\rho}_0 \hat{U}(\tau)$$

where $\hat{U}(t)$ is the time evolution operator, defined for example through $\hat{U}(t)^+ b_q \hat{U}(t) = b_q(t)$. The exponent of $\hat{\rho}_0$ can be expressed in terms of $b_\pm(\tau)$ by using the inverse transformation of (6.14). In the resulting expression, the operators $b_\pm(\tau)$ simply have to be replaced by $b_\pm$ under the action of $\hat{U}(\tau)$, leading to

$$\hat{\rho}(\tau) = \frac{1}{z_0} e^{\beta \omega_0 ((|u(\tau)|^2 + |v(\tau)|^2)(b_+^+ b_+ + b_-^+ b_-) - 1 - 2v(\tau) u(\tau)^* b_+ b_- - 2u(\tau)^* v(\tau) b_+^+ b_-^+)}.$$
After performing a Bogoliubov transformation defined in Eq. (6.9), the density operator can be rewritten as

$$\hat{\rho}(\tau) = \frac{1}{z_0} e^{\beta \omega_0 \left(1 - a(\tau) 2\hat{K}_0 - c(\tau) \hat{K}_- - c(\tau)^* \hat{K}_+ \right)}$$

(6.20)

where

$$a(\tau) = \frac{\omega}{\Omega} \left( 1 + 2 |v(\tau)|^2 \right) + \frac{g}{\Omega} \text{Re}(u(\tau)^* v(\tau))$$

(6.21)

$$c(\tau) = -\frac{g}{\Omega} (1 + 2 |v(\tau)|^2) + 2i \text{Im}(u(\tau)v(\tau)^*) - \frac{2\omega}{\Omega} \text{Re}(u(\tau)v(\tau)^*)$$

(6.22)

and we have introduced the quadratic operators

$$\hat{K}_0 = \frac{d_+ d_+ + d_- d_-}{2}$$

$$\hat{K}_+ = d_+ d_-$$

$$\hat{K}_- = d_+ d_- = \hat{K}_+$$

(6.23)

with the bosonic operators $d_\pm$ diagonalizing the final Hamiltonian. Note that $\hat{K}_0$ does not change the number of bosons while $\hat{K}_+$ ($\hat{K}_-$) creates (annihilates) a pair of $d_+$ and $d_-$ bosons. These operators also obey the commutation relations of the $su(1,1)$ algebra,

$$[\hat{K}_0, \hat{K}_\pm] = \pm \hat{K}_\pm$$

$$[\hat{K}_+, \hat{K}_-] = 2\hat{K}_0,$$

(6.24)

and they all commute with the difference occupation number operator, $\Delta \hat{n} = \hat{n}_+ - \hat{n}_- = d_+^+ d_- - d_-^+ d_+$. Later, these commutation properties will help us to work with the exponential of these operators.

Note that in Eq. (6.20), all information about the quench is incorporated into the real $a(\tau)$ and the complex $c(\tau)$ coefficients satisfying $a(\tau)^2 - |c(\tau)|^2 = 1$. This property implies that $|a(\tau)| \geq 1$ and because of the initial conditions of the Bogoliubov coefficients, $u(\tau = 0) = 1$, $a(\tau) \geq 1$ strictly holds. This quantity is also closely related to the expectation value of the occupation number in the final state

$$n(\tau) := \text{Tr}[\hat{\rho}(\tau) \hat{n}_\pm] = \text{Tr}[\hat{\rho}_0 \hat{n}_\pm(\tau)] = a(\tau)n_0 + \frac{a(\tau) - 1}{2}$$

(6.25)

where $n_0 = (e^{\beta \omega_0} - 1)^{-1}$ is the mean occupation number in the initial state. Note that due to inversion symmetry the expectation values $\text{Tr}[\hat{\rho}(\tau) \hat{n}_+]$ and $\text{Tr}[\hat{\rho}(\tau) \hat{n}_-]$ are the same.

The inequality $a(\tau) \geq 1$ indicates that on average there is a net boson production during the quench no matter how the interaction is switched on. This property is a consequence
of the bosonic nature of quasi-particles. Moreover, the higher the initial temperature is, the more bosons are produced during the quench, since

\[ n(\tau) - n_0 = (a(\tau) - 1) \left( n_0 + \frac{1}{2} \right) \geq 0 \quad \text{increases with } T \]

These results refer to the expectation value of the occupation numbers but their whole distribution can also be given by determining the probabilities \( \langle n_+, n_- | \hat{\rho}(\tau) | n_+, n_- \rangle \) where \( |n_+, n_-\rangle \) are the occupation number eigenstates. Since these are the eigenstates of the final Hamiltonian as well, the \( \langle n_+, n_- | \hat{\rho}(\tau) | n_+, n_- \rangle \) matrix elements also determine the diagonal ensemble which provides a full description of the steady state and the expectation value of any integrals of motion. In the two-oscillator model the constants of motion are \( \hat{n}_+, \hat{n}_- \), their arbitrary products and linear combinations.

Off-diagonal elements, such as \( \langle n_+, n_- | \rho(t > \tau) | n'_+, n'_- \rangle \), have harmonic time dependence given by \( e^{i\Omega(q)(n_+ + n_- - n'_+ - n'_-)t} \) as we have mentioned in the introduction. These matrix elements are important only if the time evolution of a non-preserved quantity is studied. For example, in the next section the fidelity will be such a quantity since \( \hat{H}_0 \) is not an integral of motion after the quench. In the long run, however, contribution of the off-diagonal matrix elements to the expectation value of physical quantities vanishes due to dephasing unless there are degenerate energy states. In our model, \( |n_+, n_-\rangle \) and \( |n'_+, n'_-\rangle \) are degenerate if \( n_+ + n_- = n'_+ + n'_- \) but matrix elements are non-zero only with \( n_+ - n_- = n'_+ - n'_- \) since \( [\hat{\rho}(\tau), \Delta \hat{n}] = 0 \). Hence, the diagonal blocks corresponding to degenerate subspaces are diagonal themselves.

Thus, the diagonal ensemble is given by the matrix elements

\[ \rho(n_+, n_-) := \langle n_+, n_- | \hat{\rho}(\tau) | n_+, n_- \rangle, \quad (6.27) \]

which also yield the probability of having \( n_+ \) and \( n_- \) bosons in the + and – oscillators. We note that \( \rho(n_+, n_-) = \rho(n_-, n_+) \) is physically expected because both the initial Gibbs ensemble and the time-dependent Hamiltonian are invariant under \( q \leftrightarrow -q \).

The generating function of the occupation number distribution \( (6.27) \) is defined as

\[ f(\xi_+, \xi_-) := \sum_{n_+, n_-=0}^{\infty} e^{i(\xi_+ n_+ + \xi_- n_-)} \rho(n_+, n_-) = \text{Tr} \left[ \hat{\rho}(\tau) e^{i(\xi_+ \hat{n}_+ + \xi_- \hat{n}_-)} \right]. \quad (6.28) \]
The expectation value of integrals of motion can be calculated by taking the derivatives of \( f(\xi_+ + \xi_-, \xi_+ - \xi_-) \) with respect to \( \xi_+ \) and \( \xi_- \), for example \( \langle \hat{n}_+ \rangle = -i \partial_{\xi_+} f(\xi_+ + \xi_-) \) \( |_{\xi_+ = 0, \xi_- = 0} \). We will see in Section 6.5 that Eq. (6.28) is also very useful in determining the probability distribution of the total energy as well.

Now, we obtain the generating function \( f(\xi_+ + \xi_-, \xi_+ - \xi_-) \) for an arbitrary quench protocol and arbitrary initial temperature analytically. The key point of the calculation is to derive a single exponential from \( \hat{\rho}(\tau) e^{i(\xi_+ \hat{n}_+ + \xi_- \hat{n}_-)} \). Taking advantage of the commutation properties of the operators \( \hat{K}_0, \hat{K}_\pm \) and \( \Delta \hat{n} \), the generating function is derived analytically as

\[
 f(\xi_+ + \xi_-) = \left[ 1 + n(\tau) \left( 1 - e^{i(\xi_+ + \xi_-)} \right) + \Delta n_0^2 \left( e^{i\xi_+} - 1 \right) \left( e^{i\xi_-} - 1 \right) \right]^{-1} 
\]

(6.29)

where \( \Delta n_0^2 = n_0 + n_0^2 = e^{\beta \omega_0} (e^{\beta \omega_0} - 1)^{-2} \) is variance of the initial boson number and \( n(\tau) \) is the expectation value of the occupation number after the quench (see (6.25) or Ref. [70]). Details of the calculation can be found in Appendix A. The function in Eq. (6.29) is symmetric under \( \xi_+ \leftrightarrow \xi_- \) in accordance with \( \rho(n_+, n_-) = \rho(n_-, n_+) \).

The generating function (6.29) behaves universally in the sense that, no matter how the interaction is switched on, the final boson number distribution is solely determined by its expectation value. Any information about the quench protocol is incorporated into one single number which is the real \( a(\tau) \) coefficient defined in (6.21).

The diagonal matrix elements can be obtained by Fourier transforming Eq. (6.29). This is carried out analytically by introducing the complex variables \( z_\pm = e^{-i\xi_\pm} \). The complex integrals give the matrix elements as

\[
 \rho(n_+, n_-) = \frac{\Delta n_0^{2(n_+ - n_-)} (n(\tau) - \Delta n_0^2)^{n_-}}{(1 + n(\tau) + \Delta n_0^2)^{n_+ + 1}} \sum_{l=0}^{n_-} \frac{\binom{n_-}{l} \binom{n_+ + l}{n_-}}{(n(\tau) - \Delta n_0^2)^l (1 + n(\tau) + \Delta n_0^2)^l} \Delta n_0^4 l 
\]

(6.30)

for \( n_+ \geq n_- \). The opposite case is obtained from \( \rho(n_+, n_-) = \rho(n_-, n_+) \). We emphasize again that Eq. (6.30) is exact for arbitrary quench protocol and initial temperature. One can easily check that in the absence of an interaction quench, i.e. when \( n(\tau) = n_0 \), the \( \rho(n_+, n_-) \) distribution simplifies to the initial thermal distribution,

\[
 \rho(n_+, n_-; \text{no quench}) = \frac{n_0^{n_+ + n_-}}{(1 + n_0)^{n_+ + n_- + 2}} = \frac{1}{z_0} e^{-\beta \omega_0 (n_+ + n_-)} 
\]

(6.31)

which is illustrated in Fig. 6.1. In the initial thermal state the random variables \( n_+ \) and \( n_- \) are independent and completely uncorrelated, \( \text{Corr}(n_+, n_-) = 0 \).
Figure 6.1: Joint probability distribution of initial boson numbers in the two-oscillator model. For the plot, \( n_0 = 4 \) was chosen.

Now, let us analyze Eq. (6.30) in the presence of an interaction quench but with zero initial temperature. In this limit, \( n_0 \to 0 \) and only the \( l = 0 \) term is finite in the sum of Eq. (6.30), leading to

\[
\rho(n_+, n_-) = \delta_{n_+, n_-} \frac{n(\tau)^{n_+}{}_{(1 + n(\tau))}^{n_+ + 1}}{}
\]

where the final occupation number is now simply given by \((a(\tau) - 1)/2\). These particles are all excited during the quench and were not present in the initial state. The number of bosons in the \( +q \) and \(-q \) modes are the same which stems from the fact that the difference \( \hat{n}_+ - \hat{n}_- = d_+^* d_+ - d_-^* d_- = b_+^* b_+ - b_-^* b_- \) is preserved during the time evolution and its expectation value is zero in the initial state. The steady state described by (6.32) is highly non-thermal because the boson numbers in the \( q \) and \(-q \) channels are completely correlated.

For finite initial temperature, the difference \( n_+ - n_- \) may be nonzero and, therefore, \( \rho(n_+, n_- \neq n_+) \) elements show up in the final state as well. Diagonal elements of the density matrix are illustrated in Fig. 6.2 with different initial temperatures.

At low temperatures or for high frequencies \((\beta \omega_0 \gg 1)\) the occupation number \( n_0 \) is exponentially small and \( \Delta n_0^2 \approx n_0 \approx e^{-\beta \omega_0} \) to leading order. Matrix elements up to first order in \( n_0 \) are non-vanishing only if \( n_+ = n_- \) or \( n_+ = n_- \pm 1 \), and the corrections to the zero temperature case are given by

\[
\rho(n_+, n_-) = \frac{2(a(\tau) - 1)^{n_+}}{(a(\tau) + 1)^{n_+ + 1}} \begin{cases} 
1 - 2n_0 & \text{if } n_+ = n_- \\
2n_0n_\pm & \text{if } n_+ = n_- \pm 1
\end{cases}
\]

which is still non-thermal because of the strong correlation between \( n_+ \) and \( n_- \).
Figure 6.2: Diagonal matrix elements of the density operator \( \langle n_+, n_- | \hat{\rho}(\tau) | n_+, n_- \rangle \). In the figures \( n_+ \) and \( n_- \) are measured on the horizontal and the vertical axes. The quantity \( a(\tau) \), which characterizes the quench protocol and is independent from the temperature, is 2 for all figures. The temperature varies such that the initial occupation number is a) \( n_0 = 0 \) zero temperature b) \( n_0 = 1 \) c) \( n_0 = 30 \) high temperature. Colors do not represent the same values in different figures and only illustrate the structure of diagonal matrix elements.

At high temperatures or for low frequencies (\( \beta \omega_0 \ll 1 \)) the initial occupation number is large (\( n_0 \gg 1 \)). If \( n_0 \gg a(\tau) \) also holds, the elements of the density matrix for large \( n_+ \) and \( n_- \) are written as

\[
\rho(n_+, n_-) \approx \frac{1}{n_0^2} e^{-(n_+ + n_-) a(\tau) n_0},
\]

which resemble to a thermal density matrix. However, the random variables \( n_+ \) and \( n_- \) are correlated even at very high temperatures. The correlation is obtained by using the generating function (6.29) as

\[
\text{Corr}(n_+, n_-) = 1 - \frac{n_0 + n_0^2}{n(\tau) + n(\tau)^2}
\]

which monotonically decreases as the initial temperature increases but saturates at \( 1 - a(\tau)^{-2} \).

Note that the random variables are uncorrelated if the \( a(\tau) = 1 \) which is possible in the case of adiabatic quench only. Fig. 6.3 shows the temperature dependence of the correlation.

We emphasize again that only a single \( q > 0 \) mode was considered in this section. All the modes should be taken into account when certain physical quantities, e.g. total energy, are evaluated.
Figure 6.3: Correlation of the random variables $n_+$ and $n_-$ as a function of the initial temperature for a given quench protocol. The variables are less correlated for higher initial temperatures but even at very high temperatures they are correlated if the quench is non-adiabatic.

6.4 Loschmidt echo

In the previous section we determined the diagonal ensemble by calculating all the diagonal matrix elements of the density operator. The result (6.30) allows one to evaluate the expectation value of any physical quantity in the steady state but tells nothing about relaxation of the system and how the steady state is reached. In this section, we calculate the Loschmidt echo which provides a deep insight to the time evolution and relaxation of the system without reference to any particular physical quantity.

The Loschmidt echo, or sometimes called fidelity, measures the overlap of the time evolved and initial density operators [71, 72]. Since the initial Hamiltonian is not a constant of motion after the quench, the initial density operator does not commute with the final Hamiltonian and, hence, the fidelity has explicit time-dependence [73].

At zero temperature, both the initial and the time evolved states are pure states described by a single wavefunction and the fidelity is defined as

$$ F(t) = |\langle \Psi_0 | \Psi(t) \rangle| $$

(6.36)

where $|\Psi_0\rangle$ is the ground state of the initial Hamiltonian and $|\Psi(t)\rangle = \hat{U}(t) |\Psi_0\rangle$ is the time evolved state.

Generalization of Eq. (6.36) to finite initial temperatures is, however, not obvious because there exist many possible metrics of density operators leading to the same zero temperature
limit \(6.36\). In quantum information theory, the overlap of quantum states is defined by means of the so-called Uhlmann fidelity \([74, 71, 75]\)

\[
F_U(t) = \text{Tr} \left[ \sqrt{\rho_0^{1/2} \hat{\rho}(t) \rho_0^{1/2}} \right].
\]  
(6.37)

The fidelity is symmetric to the exchange of the density matrices and \(0 \leq F_U(t) \leq 1\) always holds where the latter relation becomes equality in the case of identical density operators. The Uhlmann fidelity is related to the Bures metric in which the angle between the two density matrices is given by \(\arccos F_U(t)\). Since the density matrices are normalized to unity, their angle can be used to quantify their distance. In the zero temperature limit, the Uhlmann fidelity simplifies to

\[
F_U(T = 0; t) = |\langle \Psi_0 | \Psi(t) \rangle| \quad \text{as required.}
\]

For finite initial temperature, the trace in Eq. (6.37) has to be evaluated in the following way. Similarly to the derivation of \(f(\xi_+, \xi_-)\) in Appendix A, one has to derive a single exponential instead of \(\hat{\rho}_0^{1/2} \hat{\rho}(t) \hat{\rho}_0^{1/2}\) by using the commutational properties of \(\hat{K}_{0,q}\) and \(\hat{K}_{\pm,q}\). This can be done by using a faithful representation of the \(su(1,1)\) algebra as presented in Appendix A. Then, by diagonalizing the exponent of the single exponential and halving the eigenvalues due to the square root in (6.37), the fidelity is obtained as

\[
\ln F_U(t) = \sum_{q>0} \ln \frac{\cosh(\beta \omega_0(q)) - 1}{\sqrt{1 + |u_q(t)|^2 \sinh^2(\beta \omega_0(q)) - 1}}
\]
(6.38)

where \(u_q(t)\) is the Bogoliubov coefficient defined in Eq. (6.14). With zero initial temperature, this simplifies to

\[
\ln F_U(T = 0; t) = - \sum_{q>0} \ln |u_q(t)|.
\]
(6.39)

The resulting expression in Eq. (6.38) shows that the Loschmidt echo depends remarkably on the initial temperature and is exact for arbitrary temperature, interaction strength and quench protocol. Moreover, it can be shown analytically that higher initial temperature results in less fidelity, i.e. during the time evolution the quantum state gets "farther" from the initial state – in the sense of Bures metric – if there are more bosons initially. This property is related to the fact that for higher initial temperature more bosons are created on average during the quench.

In the rest of this section, we investigate the Uhlmann fidelity in the special case of a sudden quench \((\tau \to 0)\). In this limit, the Bogoliubov coefficient is obtained as

\[
u_q(t) = \cos(\Omega(q)t) - i \frac{\omega(q)}{\Omega(q)} \sin(\Omega(q)t)
\]
(6.40)
for $t > 0$. The time dependence of the Uhlmann fidelity is evaluated numerically and plotted in Figure 6.4.a showing that higher initial temperature induces lower fidelity. As a function of time, the fidelity decreases monotonically but saturates to a non-zero value. The steady value is reached for times much larger than $\beta$ or $\tau_0$ being the time-scale corresponding to the finite range of the interaction $R_0 = v_F \tau_0$. In the numerical calculation, the velocity renormalization is neglected because we are interested in interaction effects coming from a finite $g_2$. Figure 6.4.b shows the long time limit of the Uhlmann fidelity as a function of $g_2/v_F$.

\begin{align*}
\ln F_U(t) &= \sum_{q>0} \frac{g^2}{\omega_0^2} \sin^2(\omega_0 t) \left\{ 1 + \frac{\tau_0}{\beta} Z\left(\frac{\tau_0}{2\beta}\right) + \text{Re}\left(\frac{i\tau_0}{t - i\tau_0} - \frac{\tau_0}{\beta} Z\left(\frac{\tau_0}{2\beta} - \frac{it}{2\beta}\right)\right) \right\}
\end{align*}

where $\alpha = |E_{ad}|\tau_0$ is the so-called orthogonality exponent with $E_{ad} = -Lg_2^2/(16\pi\tau_0^2v^3)$ being the ground state energy of the final Hamiltonian within perturbation theory. In the formulas, $L$ is the length of the sample and

\begin{align*}
Z(x) &= \psi\left(\frac{3}{4} + x\right) - \psi\left(\frac{1}{4} + x\right) \quad (6.42)
\end{align*}
with $\psi(x)$ being the digamma function. In the long time limit, $t \gg \tau_0$ and $t \gg \beta$, the second term in Eq. (6.41) vanishes and

$$
\ln F_U(t \to \infty) = -\alpha \left[ 1 + \frac{\tau_0}{\beta} Z \left( \frac{\tau_0}{2\beta} \right) \right].
$$

(6.43)

At low temperatures, the long time value ($t \gg \beta \gg \tau_0$) of the Loschmidt echo is obtained as

$$
\ln F_U(t \to \infty) = -\alpha - \frac{1}{16} \left( \frac{g_2}{v} \right)^2 \frac{LT}{v}
$$

(6.44)

showing that the fidelity is exponentially suppressed for non-zero initial temperatures. The temperature dependent term possesses a universal prefactor in the Luttinger liquid sense, namely that it is independent of the high energy cutoff, $1/\tau_0$.

We note that even in the long time limit, $t \ll L/v$ is required. For larger times, comparable to $L/v$, quantum revival occurs which is always present in finite quantum systems.

In this section we have determined the Loschmidt echo characterizing the overlap between the time evolved and initial states. The Uhlmann fidelity decreases monotonically in a non-oscillating way as the time evolves and reaches a steady value for times $t \approx \beta, \tau_0$. The expectation value of any non-preserved physical quantities is expected to exhibit similar relaxation.

We have also seen that higher initial temperature results in less fidelity. This statement was proven analytically for arbitrary interaction strength and quench protocol.

### 6.5 Probability distribution of total energy after a sudden quench

Now we turn back to characterizing the steady state by determining the statistics of the final total energy which could be observed directly in cold atom experiments. Repeating the procedure of releasing the system from the trap and measuring its energy many times is expected to lead to the probability distribution function of the total energy. The total energy in the final state is a random variable even at zero temperature because the initial ground state evolves to a linear combination of eigenstates of the final Hamiltonian. At finite temperature the initial energy is already random and so is the final energy.

Since the energy is preserved after the quench, its distribution does not change while the steady state is reached. Therefore, it is sufficient to determine the probability distribution
function, $P(E)$, right at $t = \tau$. The generating function of $P(E)$ is defined as

$$G(\lambda) = \int_{-\infty}^{\infty} dE e^{i\lambda E} P(E).$$

(6.45)

Denoting by $|n\rangle$ the eigenstates of the final Hamiltonian, $\hat{H}$, the generating function can be rewritten as

$$G(\lambda) = \int_{-\infty}^{\infty} dE e^{i\lambda E} \sum_n \langle n | \hat{\rho}(\tau) | n \rangle \delta(E - E_n) = \text{Tr} \left[ \hat{\rho}(\tau) e^{i\lambda \hat{H}} \right].$$

(6.46)

We note that in the zero temperature and sudden quench limit the generating function is closely related to the Loschmidt echo since

$$G(T = 0; \lambda) = \langle \Psi_0 | e^{i\lambda \hat{H}} \Psi_0 \rangle$$

(6.47)

as a function of $-\lambda$ coincides with the Loschmidt echo as a function of time. At finite temperature, however, no such relation exists.

The final Hamiltonian $\hat{H}$ is a linear combination of $\hat{n}_q = d_+^q d_q$ and $\hat{n}_{-q} = d_+^{-q} d_{-q}$, hence, the generating function can be expressed in terms of $f(\xi_+, \xi_-)$ defined in Eq. (6.28) as

$$\ln G(\lambda) = i\lambda E_{ad} + \sum_{q>0} \ln f(\lambda \Omega(q), \lambda \Omega(q)) =
\begin{align*}
&= i\lambda E_{ad} - \sum_{q>0} \ln \left[ 1 + n_q(\tau) \left( 1 - e^{2i\lambda \Omega(q)} \right) + \Delta n_{0,q}^2 \left( e^{i\lambda \Omega(q)} - 1 \right)^2 \right]
\end{align*}$$

(6.48)

where $n_q(\tau)$ is the expectation value of the occupation number after the quench and $\Delta n_{0,q}^2$ is the variance of the initial boson number. In Eq. (6.48), $E_{ad}$ is the ground state energy of the final Hamiltonian and the first term results in a shift of the probability distribution function only.

Since the sum over $q$ in Eq. (6.48) cannot be performed analytically, we consider weak interaction quenches and that $\tau \to 0$ and we also disregard the velocity renormalization. Within perturbation theory for small values of $g_2/v$, the occupation number is given by

$$n(\tau = 0, q) = n_0(q) + \frac{g(q)^2}{4\omega_0(q)^2} \left( n_0(q) + \frac{1}{2} \right)$$

(6.49)

in the final state up to second order in $g_2/v$. Substituting into Eq. (6.48), the sum over wavenumber can be evaluated leading to

$$\ln G(\lambda) = \frac{i\lambda}{\beta - i\lambda} \ln Z_0(\beta) + i\lambda E_{ad} \left[ 1 + \left( \frac{2\tau_0}{\beta - i\lambda} \right)^2 \zeta \left( 2, 1 + \frac{2\tau_0}{\beta - i\lambda} \right) \right] + E_{ad} \tau_0 h \left( \frac{\beta}{\tau_0}, \frac{\lambda}{\tau_0} \right)$$

(6.50)
where
\[
\begin{aligned}
    h \left( \frac{\beta}{\tau_0}, \frac{\lambda}{\tau_0} \right) &= 1 - \frac{1}{(z^*)^2} 
    \left[ (1 - z) \psi \left( \frac{1 - z}{z^*} \right) + (1 + z) \psi \left( \frac{1 + z}{z^*} \right) - 2 \psi \left( \frac{1}{z^*} \right) \right]
    \\
    z &= \frac{\beta + i \lambda}{2 \tau_0}.
\end{aligned}
\]  

In Eqs. (6.50) and (6.51), \( \zeta(n, x) = \sum_{k=0}^{\infty} (k + x)^{-n} \) is the Hurwitz zeta function and \( \psi(x) \) is the digamma function. Within perturbation theory
\[
E_{ad} = -\frac{L}{16 \pi v_F \tau_0} \left( \frac{g_2}{v_F} \right)^2 \frac{1}{\tau_0}. 
\]  

We note that expanding the logarithm of the generating function with respect to \( g_2/v \) corresponds to the expansion of the cumulants.

In order to calculate the probability distribution function, we have to Fourier transform the generating function Eq. (6.50). The function \( \ln G(\lambda) \) has poles on the lower complex semiplane only which ensures that for energies lower than the ground state energy \( E_{ad} \), the integral of the Fourier transformation can be closed on the upper semiplane and, hence, results in zero. This, of course meets physical expectations, namely the energy of the system cannot be lower than the ground state energy.

Now, let us investigate two simple cases when the generating function (6.50) can be Fourier transformed analytically and will also play important role later.

First, we examine the zero initial temperature case. In this limit \( h(\beta/\tau_0 \to \infty, \lambda/\tau_0) = \lambda/(i \tau_0 + \lambda) \) and the generating function simplifies to
\[
\ln G(T = 0; \lambda) = i \lambda E_{ad} - \frac{\lambda}{i \tau_0 + \lambda} \alpha 
\]  

where \( \alpha = |E_{ad}| \tau_0 \) is the orthogonality exponent. This dimensionless parameter is proportional to the system size and also determines the shape of the distribution while \( \tau_0 \) defines the scale of the energy only. The Fourier transform of Eq. (6.53) can be obtained analytically and results in
\[
P(T = 0; E) = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i \lambda E + \ln G(T=0; \lambda)} = 
\]
\[
= e^{-\alpha} \delta(E - E_{ad}) + e^{-\alpha} e^{-\tau_0(E - E_{ad})} \sqrt{\frac{\alpha \tau_0}{E - E_{ad}}} I_1 \left( 2 \sqrt{\alpha \tau_0 (E - E_{ad})} \right) 
\]  

where \( I_1(x) \) is the modified Bessel function of the first kind. The detailed calculation can be found in Appendix B. The resulting function (6.54) is the zeroth order noncentral chi-squared
distribution with the noncentrality parameter $2\alpha$. The probability distribution function is plotted in Fig. 6.5 for different values of $\alpha$. For small systems, $\alpha$ is small (Fig. 6.5.a), most of the probability weight is carried by the Dirac delta centered at $E_{ad}$ corresponding to the vacuum-to-vacuum process or in other words the adiabatic transition. The continuous part of the distribution decays exponentially as $\exp(-\tau_0(E - E_{ad}))$.

For large systems, when $\alpha$ is large (Fig. 6.5.c), the Dirac delta peak is exponentially suppressed and the continuous part carries almost all the probability weight and forms a sharp peak around $E = 0$, i.e. the energy of the initial state. The continuous peak is sharp in the sense that the width, scaling as $\sim \sqrt{L}$, is negligible compared to the ground state energy, which scales as $\sim L$. This behaviour meets the requirement of normal systems in standard statistical mechanics. In the large system limit, the continuous peak is described by the non-Gaussian function

$$P(T = 0; E) \approx \frac{1}{2\sqrt{\pi} (E - E_{ad})^{3/2}} e^{-\left(\sqrt{\alpha} - \sqrt{\tau_0 E + \alpha}\right)^2}.$$  

(6.55)

In the intermediate region, a crossover between the two limiting cases can be observed in Fig. 6.5.b.

We note that if the initial state is the ground state of the initial Hamiltonian, the total energy of the final state equals the work done on the system during the quench. Therefore, the probability distribution function in Eq. (6.54) provides statistics of work as well. At finite temperature, however, these statistics do not coincide.

Figure 6.5: Probability distribution function of the final energy in the sudden quench limit for different system sizes, $\alpha \sim L/(v\tau_0)(g_2/v)^2$.  

The other, analytically manageable case is the unquenched case \((g_2 = 0)\) at finite temperature when the final state just coincides with the initial thermal equilibrium state. The generating function reads as

\[
\ln G(g_2 = 0; \lambda) = -\frac{\lambda}{i\beta + \lambda} \ln Z_0 \tag{6.56}
\]

which leads to another noncentral chi-squared distribution with the noncentrality parameter \(2 \ln Z_0\),

\[
P(g_2 = 0; E) = \frac{e^{-\beta E}}{Z_0} \left[ \delta(E) + \sqrt{\frac{L\pi}{6E v}} I_1 \left(2\sqrt{\frac{L\pi}{6v}} E\right) \right], \tag{6.57}
\]

which is equal to the Boltzmann factor \(\exp(-\beta E)/Z_0\) multiplied by the total energy density of states of a one-dimensional Bose gas with linear dispersion.

The distribution function (6.57) can be analyzed in the same way as it has been done in the case of the zero temperature statistics. For small systems, when \(\ln Z_0\) is small, the Dirac-delta carries most of the probability weight and the continuous part contributes an exponentially decaying tail only. For large systems, when \(\ln Z_0\) is large, almost all the spectral weight is carried by a non-Gaussian sharp peak centered at \(\langle E \rangle = (\ln Z_0)/\beta \sim T^2\) and of width \(\Delta E = \sqrt{2\ln Z_0/\beta} \sim T^{3/2}\).

Now we turn to the more complicated situation of a small interaction quench with finite initial temperature. The generating function of the energy statistics can be obtained analytically only at low temperature \(\beta \gg \tau_0\). In the sudden quench limit, it reads as

\[
\ln G(\lambda; \beta \gg \tau_0) = -\frac{\lambda}{i\beta + \lambda} \ln Z_0 + i\lambda E_{\text{ad}} - \frac{\lambda}{i\tau_0 + \lambda} \alpha \tag{6.58}
\]

which is the sum of Eqs. (6.53) and (6.56) indicating that the probability distribution function is the convolution of Eq. (6.54) and Eq. (6.57). These two noncentral chi-squared distributions consist of a Dirac delta part and a continuous part and, therefore, so does their convolution. The weight of the Dirac delta after convolution is \(\exp(-\alpha)/Z_0\) which is again the probability of the vacuum-to-vacuum process.

The continuous part of the probability distribution function after convolution is plotted in Fig. 6.6 for different system sizes and temperatures. For small systems (\(\alpha\) is small, see Fig. 6.6.a), most of the spectral weight is carried by the Dirac-delta at zero temperature. With increasing temperature, one part of the Dirac delta stays at \(E_{\text{ad}}\) while another part evolves to a finite-width peak centered around \((\ln Z_0)/\beta\).
In the thermodynamic limit (large system with $\alpha \gg 1$, see Fig. 6.6.c) the zero temperature distribution function consists of a finite-width peak at about $E = 0$ and a Dirac delta at the adiabatic ground state energy with a small probability weight. At finite temperature the finite-width is shifted to $\langle E \rangle(T) = (\ln Z_0)/\beta$ and broadens as $\Delta E(T) = \sqrt{2\alpha/\tau_0^2 + 2(\ln Z_0)/\beta^2}$. At low temperatures
\[
\frac{\Delta E(T) - \Delta E(0)}{\Delta E(0)} \sim T^3
\] (6.59)
which is clearly a consequence of the non-equilibrium situation because at equilibrium $\Delta E(T) \sim T^{3/2}$ was found.

We note that in the strict thermodynamic limit, the width of the distribution is negligible compared to its position because $(\Delta E(T) - \Delta E(0))/\langle E \rangle(T) \approx \sqrt{2\tau_0/(\sqrt{\alpha}\beta)} \sim L^{-1/2}$.

Finite temperature effects presented in this section could be observed directly by measuring $P(E)$ but, to my best knowledge, no experiment has been reported so far.

### 6.6 Statistics of work

In the previous section the probability distribution of final total energy was investigated. We have already mentioned that with zero initial temperature - when the system is initially prepared in the ground state with zero energy - the final energy equals the work done on the system during the quench. At finite temperature, however, the initial energy is random with probabilities determined by the Gibbs ensemble indicating that the work statistics and that of the total energy differ from each other

Measuring the work statistics requires in principle two energy measurements[76, 77], one before and one after the time dependent protocol, though in the zero temperature case, the first one could be omitted[78]. At finite temperature, both measurements are required and, as a consequence, the work itself cannot be considered as an observable[79]. Even so, there are some suggestions how the statistics could be measured by coupling the system of interest to a qubit[80, 81, 68].

In this section we investigate the probability distribution function of work, $\tilde{P}(W)$. Since in the initial thermal equilibrium state the system may have arbitrarily large positive energy, the distribution function of work has no lower bound. Another interesting feature of the work statistics is that for generic quantum quenches, the distribution function obeys the so-called
Figure 6.6: Probability distribution function of total energy following a sudden quench. In each figure the blue dashed curve corresponds to zero temperature. The analytic result consists of a Dirac delta (blue dashed arrow) and a continuous part. Green and yellow curves show the continuous part of the total energy distribution function at temperatures $\beta = 30\tau_0$ and $\beta = 10\tau_0$. The orthogonality exponent varies as: a) $\alpha = 0.2$ small system b) $\alpha = 4$ c) $\alpha = 20$ large system. For all system sizes the distribution is shifted in positive direction and broadened as the temperature increases. For all figures $g_2/v = 0.1$ was chosen.

Jarzynski equality [77],

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F} \quad (6.60)$$

where $\Delta F = F(\tau) - F_0$ is the difference of the free energy before and after the quench.
The generating function of the distribution of work is obtained as [79]

\[ \tilde{G}(\lambda) = \int_{-\infty}^{\infty} dW e^{i\lambda W} \tilde{P}(W) = \text{Tr} \left[ \hat{\rho}_0 e^{-i\lambda \hat{H}_0} e^{i\lambda \hat{H}_H(\tau)} \right], \]  

where

\[ \hat{H}_H(\tau) = e^{-i\hat{H}_0 \tau} \hat{H} e^{i\hat{H}_0 \tau} \]  

is the final Hamiltonian in Heisenberg picture. The generating function can be rewritten by means of the generating function of the total energy \( G(\lambda, \beta) \) as

\[ \tilde{G}(\lambda, \beta) = \frac{Z_0(\beta + i\lambda)}{Z_0(\beta)} G(\lambda, \beta + i\lambda). \]  

By substituting Eq. (6.48) into this formula, we would get a very complicated formula which is very hard to work with. Therefore, we consider weak interaction strength and treat it as a perturbation. Using Eq. (6.50) yields

\[ \ln \tilde{G}(\lambda) = i\lambda E_{ad} \left( 1 + 8 \frac{\tau_0^2}{\beta^2} \left( 2, 1 + \frac{2\tau_0}{\beta} \right) \right) + E_{ad} \tau_0 h \left( \frac{\beta + i\lambda}{\tau_0}, \frac{\lambda}{\tau_0} \right) \]  

up to second order in \( g_2/v \) where the function \( h \) was defined in Eq. (6.51) and may now be rewritten as

\[ h \left( \frac{\beta + i\lambda}{\tau_0}, \frac{\lambda}{\tau_0} \right) = 1 + 2 \left( \frac{2\tau_0}{\beta} \right)^2 \left[ 1 - \frac{\beta + 2i\lambda}{2\tau_0} \psi \left( \frac{2\tau_0 - 2i\lambda}{2\tau_0} \right) + \left( 1 + \frac{\beta + 2i\lambda}{2\tau_0} \right) \psi \left( \frac{2\tau_0 + 2i\lambda}{\beta} \right) \right] \]  

with \( \psi(x) \) being the digamma function. The generating function in Eq. (6.64) is valid only in the sudden quench limit but for arbitrary temperature. Due to the singularities of the digamma, \( \ln \tilde{G}(\lambda) \) has poles on both complex semiplanes in accordance with the absence of lower bound in the probability distribution function. It can be proven that Eq. (6.64) satisfies the Jarzynski equality, \( \langle e^{-\beta W} \rangle = \tilde{G}(\lambda = i\beta) = Z(\tau)/Z_0 \) where \( Z(\tau) = \text{Tr} \left[ e^{-\beta \hat{H}} \right] \) is the partition function of the final Hamiltonian.

By using Eq. (6.64), the cumulants of the distributions can be obtained analytically but the shape of the distribution can be determined by numerical Fourier transformation only. The numerical results are shown in Fig. 6.7 for different system sizes and initial temperatures.

In the small system limit, the zero temperature probability distribution function consists of a Dirac delta with large probability weight and an exponentially decaying tail (see Fig. 6.7.a).
Figure 6.7: Probability distribution function of work statistics following a sudden quench. In each figure the blue dashed curve shows the zero temperature case with the blue arrow representing the Dirac delta part of the distributions. Green, yellow and red solid curves correspond to temperatures $\beta = 30\tau_0$, $\beta = 10\tau_0$ and $\beta = 4\tau_0$, respectively. The orthogonality exponent varies as a) $\alpha = 0.2$ small system, b) $\alpha = 4$ c) $\alpha = 20$ large system. a) In the small system limit most of the probability weight is carried by the Dirac delta part at zero temperature. At finite temperature this broadens to a finite width peak. c) In the large system limit the distribution function consists of a single peak which slightly broadens as the temperature increases. b) In the intermediate region one can notice the broadening of the Dirac delta part and the continuous part simultaneously, i.e., the features of small and large system are combined in this region.

At finite temperature the Dirac-delta disappears and deforms to a broadened, negatively skewed peak lying on the exponential tail.

In the thermodynamic limit the only change is that the zero temperature peak slightly
broadens (see Fig. 6.7.c). The width of the peak varies as

\[
\frac{\Delta W(T) - \Delta W(0)}{\Delta W(0)} = \frac{4\pi^2}{3}(\tau_0 T)^3,
\]

according to analytical results. This means that significant broadening could be noticeable at higher temperatures only.

Due to the fact that the system remains in its initial state in the sudden quench limit, the expectation value of work is found to be zero \( \langle W \rangle_{SQ} = 0 \) irrespectively of the system size.

### 6.7 Conclusion

We have theoretically studied quantum quenches in the Luttinger model when the initial state is prepared at thermal equilibrium. The steady state has been described by the diagonal ensemble, i.e., by deriving exact analytical expressions for the diagonal matrix elements of the time evolved density operator. The result in Eq. (6.30) is valid for arbitrary interaction strength, quench protocol and initial temperatures. Surprisingly, the occupation number distribution depends on the quench protocol only through the expectation value \( n(\tau) \). We have shown that this expectation value is always larger than that in the initial state, \( n_0 \), and their difference is larger for higher initial temperature. We have also seen that at low temperatures or for high frequency modes, which are poorly occupied, the density matrix has a non-thermal structure due to the correlation between the \( n_+ \) and \( n_- \) channels. At higher temperatures or for lower frequencies, however, the density matrix shows thermal features and the correlation of the random variables \( n_+ \) and \( n_- \) decreases but it saturates at a nonzero value. This implies that the system does not behave thermally even at very high temperatures.

To characterize the relaxation of the system, the time evolution of the Uhlmann fidelity (Loschmidt echo) has been studied. As the time evolves, the Loschmidt echo relaxes to a non-zero value which is exponentially suppressed for large systems and for finite initial temperatures. The results suggest that non-preserved quantities follow similar relaxation.

Finite temperature effects in the statistics of final total energy and work done on the system during the quench have also been investigated in the sudden quench limit. It is worth mentioning again that these two distributions coincide at zero temperature but differ from each other if the initial temperature is finite. In the latter case, the initial energy is not well defined but can take arbitrarily large value. From this we also conclude that the work
distribution function has no lower bound. Within perturbation theory and at low temperature
the distribution function of total energy is found to be the convolution of initial energy and
zero temperature work distributions. Numerical results show that the distribution is shifted
and broadened due to finite temperature for both the thermodynamic and small system limits.
In small systems, however, the broadening is more robust. The finite temperature effects in
the statistics of work depend remarkably on the system size as well. In the small system
limit, significant rearrangement may be observed with increasing temperature, while in the
thermodynamic limit, the peak of the distribution broadens only slightly. These effects could
possibly be observed experimentally, using the setups suggested in Refs. [68, 80, 81]. The
results presented in this chapter are published in Ref. [82]
Chapter 7

Summary and thesis statements

In this dissertation we have studied several properties of two fascinating low-dimensional systems: graphene and cold atomic systems. The understanding of electronic properties of graphene is crucial in its potential future applications. In Chapter 3, we have investigated the Friedel oscillation around a well localized impurity, and determined the short wavelength pattern of the change in the local density of states and in electron density. We showed that a resolution of the STM tip worse than the atomic scale could lead to cancellation of the leading $r^{-2}$ term in the density change, which would agree with the conventional behaviour in a two-dimensional electron gas, and leaving the next-to-leading correction decaying as $r^{-3}$.

In the case of undoped graphene, the density change has non-oscillating, $r^{-3}$ behavior which is consistent with the electron susceptibility behaving as $\chi(q) \sim q$ indicating very weak intrinsic screening.

We have also studied effects of the Coulomb interaction on the electronic structure. Within mean-field approximation, the critical behaviour of Mott transition has been presented in the case of half-filled monolayer graphene. We have generalized the model to arbitrary power-law density of states $\rho(\varepsilon) \sim |\varepsilon|^r$, and determined the critical exponents of a second order quantum phase transition as a function of $r$. The critical coupling was found finite if $r > 0$ and zero in the $-1 < r \leq 0$ regime. The results imply that the unconventional critical behaviour in monolayer graphene can be explained by the linear energy dependence of the density of states and, of course, make predictions on the critical behaviour of other systems with power law density of states.

The universal frequency dependence of the optical conductivity is, however, not the conse-
quence of the linear behaviour of the density of states or the dispersion relation but is closely related to the chiral nature of quasi-particles and the two-dimensionality of the system. The optical conductivity of generic scale invariant two-band systems was found to depend on the frequency as $|\omega|^{(d-2)/2}$ at zero temperature. The results are in accordance with the dynamical properties of systems at the critical point of second order quantum phase transitions.

Dynamical properties of one-dimensional interacting systems have also been investigated in a non-equilibrium situation, i.e., when the strength of the interaction is switched on following a time dependent protocol. We determined the diagonal ensemble which provides a full description of the steady state and allows one to calculate the expectation value and the whole distribution of any constants of motion. Relaxation processes have been characterized by the time dependent Loschmidt echo which was found to be smaller for higher initial temperature for arbitrary quench protocol. This property is a consequence of the fact that the net boson production during the quench increases as the initial temperature rises. In experiments, the steady state is probed by measuring physical quantities such as the energy of the system. Here, we presented how the finite initial temperature influences the probability distribution function of the total energy and the statistics of work done on the system during the quantum quench.

Below the thesis statements are listed.

1. I investigated the atomic scale spatial variations of the Friedel oscillation in monolayer graphene. In the presence of a well localized impurity, I obtained the change in the local density of states and in the electron density within Born approximation. Far from the impurity, the latter shows long wavelength oscillating behavior with an envelope decaying as $r^{-2}$. By taking into account the atomic orbitals and intervalley scattering, I showed that the leading correction vanishes in an STM experiment with spatial resolution worse than three unit cells. In the absence of intervalley scattering, a resolution worse than one unit cell already leads to cancellation leaving us the next-to-leading $r^{-3}$ correction. The results are published in Ref. [28].

2. I studied the critical behavior of an antiferromagnetic quantum phase transition in undoped monolayer graphene within mean-field approximation. The critical exponents differ from that of the conventional Landau theory. The resulting unconventional critical behaviour was explained by generalizing the model to systems with arbitrary power law density of states.
I derived how the critical exponents of a quantum phase transition depend on the density of states exponent, $r$, within mean-field theory. As a result, I found significant $r$-dependence in the $-1 < r < 2$ regime with singular behavior in the limit of constant density of states ($r = 0$). In the $r \geq 2$ region, the critical exponents do not depend on the density of states exponent and coincide with their conventional value in Landau theory. The results are published in Ref. [38].

3. Using the Kubo formula, I derived analytical expressions for the optical conductivity of generic two-band systems whose quasi-particles possess a pseudospin degree of freedom. I showed that if the pseudospin is determined only by the direction of the particle’s momentum, i.e. the particles are chiral in a general sense, the optical conductivity exhibits universal power law frequency dependence with the exponent $(d - 2)/z$ where $d$ is the number of spatial dimensions of the system and $z$ is the dynamical exponent. The results are published in Ref. [61].

4. In the Luttinger model, I studied the diagonal ensemble which provides a full description of the steady state after a quantum quench and also coincides with the joint distribution of boson numbers in the momentum channels of the final state. The distribution was analytically obtained for arbitrary quench protocol, interaction strength and for arbitrary initial temperature. For a given channel, the result shows universal behavior in the sense that all information about the quench protocol is incorporated into the expectation value of the boson number. All higher moments are already determined by the expectation value. I showed that for higher initial temperatures, the boson numbers in the $q$ and $-q$ channels are less correlated but are never uncorrelated unless the quench is adiabatic. I found that for higher initial temperatures more bosons are produced during the quench. The results are published in Ref. [82].

5. I investigated the finite temperature effects in the statistics of total energy and work done in the Luttinger model after a sudden interaction quench. After deriving the generating function of the distributions analytically within perturbation theory, the probability distribution functions were evaluated by numerical Fourier transformation. The shape of the distribution depends remarkably on the system size. For small systems, the distributions are significantly deformed as the initial temperature increases. For large system, the total energy distribution is shifted to positive direction, while the expectation value of the work done on
the system remains at zero and no significant deformation was found. I showed that the variance of the distributions behaves as $\sim T^3$ at low temperatures. The results are published in Ref. [82].

Acknowledgements

I would like to express my thanks to my supervisor, Prof. Attila Virosztek, for guiding and helping me with stimulating discussion and helpful advices during my doctoral work. His comments greatly helped me writing my Ph. D. dissertation.

I am also grateful to Dr. Balázs Dóra for valuable discussions and for fruitful cooperation.
Appendix A

Generating function of the occupation number distribution after quantum quench

The generating function of the occupation number probability distribution is defined as

\[ f(\xi_+, \xi_-) = \text{Tr} \left[ \hat{\rho}(\tau) e^{i(\xi_+ \hat{n}_+ + \xi_- \hat{n}_-)} \right] \] (A.1)

where \( \hat{\rho}(\tau) \) is the exact time evolved density operator after the quench which was obtained as

\[ \hat{\rho}(\tau) = \frac{1}{z_0} e^{\beta\omega_0(1-a(\tau)2\hat{K}_0-c(\tau)\hat{K}_- -c(\tau)^*\hat{K}_+)} \] (A.2)

in Eq. (6.20) where the coefficients are given by

\[ a(\tau) = \frac{\omega}{\Omega}(1 + 2|v(\tau)|^2) + 2\frac{g}{\Omega}\text{Re}(u(\tau)^*v(\tau)) \] (A.3)

\[ c(\tau) = -\frac{g}{\Omega}(1 + 2|v(\tau)|^2) + 2i\text{Im}(u(\tau)v(\tau)^*) - \frac{2\omega(\tau)}{\Omega}\text{Re}(u(\tau)v(\tau)^*) \] (A.4)

Here, \( u(\tau) \) and \( v(\tau) \) are the Bogoliubov coefficients defined in Eq. (6.14). In Eqs. (A.3) and (A.4), \( \omega(\tau) \) is the non-interacting energy with renormalized velocity, \( g \) is the interaction strength and \( \Omega = \sqrt{\omega(\tau)^2 - g^2} \) is the eigenenergy of the final Hamiltonian. For arbitrary quench protocol, \( a(\tau)^2 - |c(\tau)|^2 = 1 \) holds true. The other exponential under the trace in Eq. (A.1) is rewritten as

\[ e^{i(\xi_+ \hat{n}_+ + \xi_- \hat{n}_-)} = e^{-i\xi + i\Delta \xi \hat{n} e^i\xi 2\hat{K}_0} \] (A.5)
where we have introduced $\xi = (\xi_+ + \xi_-)/2$ and $\Delta \xi = (\xi_+ - \xi_-)/2$. Using a faithful representation of $su(1, 1)$ algebra [83, 84], one can derive a single exponential which equals the product $\hat{\rho}(\tau)e^{i(\hat{\xi}_+ n_+ + \xi_- n_-)}$. The generators of the $su(1, 1)$ algebra may be faithfully represented by

$$2\hat{K}_0 \rightarrow \sigma_z \quad \hat{K}_\pm \rightarrow (\pm \sigma_x + i \sigma_y)/2 \quad (A.6)$$

where $\sigma_x$, $\sigma_y$ and $\sigma_z$ are the $2 \times 2$ Pauli matrices.

The single exponent then can be diagonalized by standard Bogoliubov transformation. After diagonalization,

$$\hat{\rho}(\tau)e^{i(\xi_+ \hat{n}_+ + \xi_- \hat{n}_-)} = \frac{e^{-i\xi + \beta \omega_0}}{z_0} e^{i \Delta \xi \Delta - \ln(B + \sqrt{B^2 - 1})(1 + \hat{n}_+ + \hat{n}_-)} \quad (A.7)$$

where

$$B = \cos \xi \cosh(\beta \omega_0) - ia(\tau) \sin \xi \sinh(\beta \omega_0), \quad (A.8)$$

and $\hat{n}_\pm = \hat{d}_\pm^+ \hat{d}_\pm$ is the occupation number operator after Bogoliubov transformation and $\Delta \hat{n} = \hat{n}_+ - \hat{n}_-$. The annihilation operator is expressed with the new annihilation and creation operators as

$$d_\pm = \frac{\hat{d}_\pm + \gamma \hat{d}_\mp^+}{\sqrt{1 - |\gamma|^2}}, \quad (A.9)$$

$$\gamma = \frac{\sqrt{B^2 - 1} + i \sin \xi \cosh(\beta \omega_0) - a(\tau) \cos \xi \sinh(\beta \omega_0)}{c(\tau)e^{-i\xi} \sinh(\beta \omega_0)}. \quad (A.10)$$

Substituting Eq. (A.7) into Eq. (A.1), the generating function is obtained as

$$f(\xi_+, \xi_-) = \left[ 1 + n(\tau) \left( 1 - e^{i(\xi_+ + \xi_-)} \right) + \Delta n_0^2 \left( e^{i \xi_+} - 1 \right) \left( e^{i \xi_-} - 1 \right) \right]^{-1} \quad (A.11)$$

where $\Delta n_0^2 = e^{\beta \omega_0} (e^{\beta \omega} - 1)^{-2}$ is the variance of the initial boson number and $n(\tau) = \text{Tr} [\hat{\rho}(\tau) \hat{n}_\pm] = (a(\tau)(2n_0 + 1) - 1)/2$ the expectation value of the occupation number after the quench. Note that $f(\xi_+, \xi_-)$ is a $2\pi$-periodic function of its variables and $f(\xi_+, \xi_-) = f(\xi_-, \xi_+)$. The latter implies that $\rho(n_+, n_-) = \rho(n_-, n_+)$.
Appendix B

Derivation of $P(E)$ at zero temperature

In this Appendix we present the Fourier transformation of the zero temperature generating function

$$\ln G(T = 0; \lambda) = i\lambda E_{\text{ad}} - \frac{\lambda}{i\tau_0 + \lambda} \alpha$$  \hspace{1cm} (B.1)

which has a singularity at $-i\tau_0$ being on the lower complex semiplane. By introducing $W = E - E_{\text{ad}}$, the probability distribution function is given by

$$P(E) = \lim_{R \to \infty} \int_{-R}^{R} \frac{d\lambda}{2\pi} e^{-i\lambda W - \frac{\lambda}{i\tau_0 + \lambda} \alpha}$$  \hspace{1cm} (B.2)

Now we close the path of the integration on one of the complex semiplanes. If $W < 0$, the path is closed on the upper semiplane where there are no singularities and we obtain $P(E) = 0$ in this region. If $W > 0$, the bath is closed on the lower semiplane leading to

$$P(E) = \lim_{R \to \infty} \left[ \oint_{\mathcal{C}_R} \frac{d\lambda}{2\pi} e^{-i\lambda W - \frac{\lambda}{i\tau_0 + \lambda} \alpha} - \int_{\mathcal{K}_R} \frac{d\lambda}{2\pi} e^{-i\lambda W - \frac{\lambda}{i\tau_0 + \lambda} \alpha} \right]$$  \hspace{1cm} (B.3)

where $\mathcal{K}_R$ corresponds to the semicircle on the lower semiplane and of the radius $R$, as illustrated in Fig. B.1. The closed loop $\mathcal{C}_R$ includes $\mathcal{K}_R$ and the $[-R; R]$ interval of the real axis. In the second term the integral variable takes large values for which the integrand simplifies to $\exp(-i\lambda W - \alpha)$. The path of the integral in the first term can be deformed to arbitrary loop with clockwise orientation as long as the singularity at $\lambda_0 = -i\tau_0$ stays inside.
One may choose the unit circle around \( \lambda_0 \) denoted by \( C_{\lambda_0} \). The probability distribution function is rewritten as

\[
P(E) = \oint_{C_{\lambda_0}} \frac{d\lambda}{2\pi} e^{-i\lambda W - \frac{\lambda}{\tau_0 + \alpha}} - e^{-\alpha} \lim_{R \to \infty} \int_{K_R} \frac{d\lambda}{2\pi} e^{-i\lambda W} = \\
= \oint_{C_0} \frac{d\lambda}{2\pi} e^{-i(\lambda-\tau_0)W - \frac{\lambda-\tau_0}{\lambda}} + e^{-\alpha} \lim_{R \to \infty} \int_{-R}^{R} \frac{d\lambda}{2\pi} e^{-i\lambda W}
\]

(B.4)

where \( C_0 \) stands for the clockwise unit circle around the origin of the complex plane. The integral in the second term provides a Dirac-delta while the first term yields a modified Bessel function of the first kind as

\[
P(E) = e^{-\alpha} e^{-\tau_0 W} \sqrt{\frac{\alpha \tau_0}{W}} I_1 \left( 2\sqrt{\alpha \tau_0 W} \right) + e^{-\alpha} \delta(W).
\]

(B.5)

Figure B.1: Integral path on the complex plane.
Bibliography


