Structure factors of S=1/2 spin chains and magnetism at the edges of graphene ribbons

by

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

Doctor of Philosophy

in

THE FACULTY OF GRADUATE AND POSTDOCTORAL STUDIES
(Physics)

The University Of British Columbia
(Vancouver)

September 2014

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Abstract

In this thesis we study two different one dimensional systems. The first project is on the transverse dynamical structure factors of the XXZ spin chain and the second project is on magnetism of zigzag edges of graphene nano-ribbons.

In chapter 2, we apply field theory methods, first developed to study x-ray edge singularities, to interacting one-dimensional systems in order to include band curvature effects and study edge singularities at arbitrary momentum. We point out that spin chains with uniform Dzyaloshinskii-Moriya interactions provide an opportunity to test these theories since these interactions may be exactly eliminated by a gauge transformation that shifts the momentum. However, this requires an extension of these x-ray edge methods to the transverse spectral function of the XXZ spin chain in a magnetic field.

In chapter 3, by considering the Hubbard model in the weak coupling limit, $U \ll t$, for bearded as well as zigzag edges, we argue for existence of magnetic edges. We first present an argument based on Lieb’s theorem. Then, projecting the Hubbard interactions onto the flat edge band, we prove that the resulting one-dimensional model has a fully polarized ferromagnetic ground state. We also study excitons and the effects of second neighbor hopping as well as a potential energy term acting on the edge only, proposing a simple and possibly exact phase diagram with the magnetic moment varying smoothly to zero. Finally, we consider corrections of second order in $U$, arising from integrating out the gapless bulk Dirac excitations.
Preface

This thesis is based almost entirely on notes written by myself during my PhD program. In addition some sections are based on notes written by my research supervisor Ian Affleck, and also publications authored by me and my supervisor. The concept and scope of the research was developed collectively by myself and my supervisor. All the analytical and numerical calculations in this thesis were conducted by me but heavily influenced by significant consultation with my supervisor.

Chapter 2, is the study of transverse dynamical structure factors of XXZ spin chains. Most of this chapter is contained in the following paper: H. Karimi, I. Affleck, Physical Review B, 84, 174420 (2011).

A version of chapter 3 has been published. H. Karimi, I. Affleck, Physical Review B, 86, 115446 (2012). This chapter contains more detailed version of calculation and longer introductory sections, which all written by me.
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<tbody>
<tr>
<td>RG</td>
<td>renormalization group</td>
</tr>
<tr>
<td>ESR</td>
<td>Electron Spin Resonance</td>
</tr>
<tr>
<td>LL</td>
<td>Luttinger liquid</td>
</tr>
<tr>
<td>DSF</td>
<td>dynamical structure factor</td>
</tr>
<tr>
<td>DMRG</td>
<td>Density Matrix Renormalization Group</td>
</tr>
<tr>
<td>NNN</td>
<td>next nearest neighbour</td>
</tr>
<tr>
<td>DM</td>
<td>Dzyaloshinskii-Moriya</td>
</tr>
<tr>
<td>ARPES</td>
<td>Angle-Resolved Photoemission Spectroscopy</td>
</tr>
<tr>
<td>STM</td>
<td>Scanning Tunneling Microscope</td>
</tr>
<tr>
<td>ZZ</td>
<td>zigzag-zigzag</td>
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<tr>
<td>ZB</td>
<td>zigzag-bearded</td>
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Acknowledgments

First and foremost, I would like to express my deepest gratitude to my research supervisor Prof. Ian Affleck, for his excellent guidance, caring and patience, encouraging and helping me to experience diverse field of Condensed Matter Physics. Thanks also for funding me for all these years.

I would like to thank my supervisory committee, Prof. Mark Van Raamsdonk, Prof. Marcel Franz and Prof. Robert Kiefl for their criticism of my research, constructive feedback and guidance. Special thanks to Mark Van Raamsdonk for helping me to develop my background in high energy physics during my M.Sc program.

To the University of British Columbia (UBC) for giving me the opportunity to discover Vancouver, and funding me through the Graduate Entrance Fellowship, International Partial Tuition Scholarship, the PhD Tuition Fee Award and University Four Year Fellowship.

I will always be grateful to my parents for their everlasting encouragement and support and believing in me. Of my friends and colleagues, I could write at length how each provided their own unique brand of fellowship and support.

Finally, I would like to thank Elham, my best friend and beloved partner for her love and creating the best moments of life for me, whom I can not express the debt of gratitude I owe her.
Chapter 1

Introduction

One dimensional interacting quantum systems, due to strong quantum fluctuations in one dimension, have very interesting and unusual many body effects. For example because of strong quantum fluctuations, continuous symmetries can not be broken spontaneously; as a result there is no long range order in the system. The order parameter is ill-defined and conventional phase transitions (Landau picture), based on breakdown of continuous symmetries, are absent in such systems. Although there is no long range order in such systems, we could still define a form of "quasi long-range" ordering for these systems and study different phases and phase transitions in one dimension.

One dimensional quantum systems are not only relevant in theoretical realm. One dimensional spin chains, where in some three dimensional compounds due to lattice structure, exchange interaction in one direction is higher than other directions [1, 2] are one example of extensively studied experimentally quantum systems. Also edge states of some two dimensional systems such as Graphene with zigzag edges [3] or Quantum Hall systems [4] and 2D Topological Insulators [5], are well localized near the edges and are effectively one dimensional. Study of quantum system require understanding of both its ground state, to study phase transitions, and correct description of excitations of the system to address dynamical properties, such as spectral functions which are measurable in photo emission spectroscopy or dynamical structure factors which can be probed by inelastic neutron scattering experiments or Electron Spin Resonance (ESR).
In this thesis we study two different one dimensional quantum systems, in one project we study the dynamical structure factors of spin chains and in the other we focus on ground state properties and try to prove theoretically and understand the magnetic properties of edge states of Graphene with zigzag edges.

1.1 Anisotropic spin chain, XXZ model

The anisotropic spin chain, XXZ model is one of the most studied one dimensional quantum systems. The Hamiltonian description of this model is given by

\[ H = J \sum_j [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z - h S_j^z], \]

where \( J \) is the exchange coupling, \( \Delta \) represents anisotropy in exchange interaction which could be present due to lattice structure, the last term is just the Zeeman term due to presence of magnetic field which could be applied experimentally. For general values of \( \Delta \) the system only has \( U(1) \) symmetry and the well defined quantum number is total spin along the \( z \)-direction \( S^z = \sum_j S_j^z \). The special case of \( \Delta = 1 \) and \( h = 0 \) is called Heisenberg spin chain [6] which has \( SU(2) \) symmetry and has been studied extensively.

The phase diagram of XXZ spin chain is well understood by using combination of theoretical methods [7] and also using analytic and numeric solutions of powerful methods such as Bethe ansatz [8-10]. Although the spin can take any integer or half-integer values, we only focus for the case of \( S = 1/2 \) spin chain. In general the anisotropy in spin chain compounds is very weak and \( \Delta \approx 1 \), but there are many artificial systems whose effective Hamiltonian description could be mapped to XXZ Hamiltonian with arbitrary values of \( \Delta \), for example ultra cold bosonic atoms trapped in optical lattices [11] or Josephson junction arrays [12].

By using Bethe ansatz methods the phase diagram of XXZ model as function of \( \Delta \) and \( h \) is known exactly. The limiting case of \( \Delta \to -\infty \) and \( \Delta \to \infty \) are the limiting ferromagnetic and anti-ferromagnetic Ising chain, respectively. In these cases the system is gapped and the excitations are the domain-walls.

The range of \( \Delta \) which is more relevant is the case of \(-1 < \Delta \leq 1\), which is the
critical line. In this regime the system is gapless and also it does not have long-range order. The other two cases are both gapped. When $\Delta > 1$ we have gapped system and ground state is in Neel phase; when $\Delta < -1$ the ground state is in the ferromagnetic phase.

Although the ground state and also the spectrum of excitations can be derived by using Bethe ansatz solutions, finding the dynamical quantities such as spin-spin structure factors is very difficult. The reason is calculating the correlation functions requires working with very large number of complicated wavefunctions, which number grows exponentially as $2^N$, where $N$ is the number of sites. As a result development of a field theoretical approach to study the spin chain systems and in general, one dimensional quantum system is very useful to study the correlations and dynamical structure functions.

1.2 Luttinger liquid

By using Jordan-Wigner transformation [2] the spin-1/2 XXZ model could be mapped to interacting one dimensional spinless fermion model. Thus in principle any theoretical methods relevant to study interacting fermion model could be used to understand the spin chains.

In two and three dimensions the Landau theory of fermi liquid is general method to study the interacting models. In this picture the excitations of the interacting system are quasi-particles with some renormalized velocity and effective mass. But in one dimension strong quantum fluctuations lead to breakdown of Fermi liquid theory[13].

The equivalent theoretical framework of Fermi liquid theory in one dimension is Luttinger liquid (LL) and bosonization method [2,7,9,14]. The Luttinger Liquid is the low energy fixed point of the one dimensional electron systems [15]. In this approach first the dispersion is linearized near the Fermi points $\pm k_F$. As we are only interested in low energy description of the system we only keep excitations near the fermi energy. It also could be shown that higher order band curvature terms of the dispersion are irrelevant in renormalization group (RG) sense. Then
by using bosonization method [16] we represent the fermionic fields in terms of some bosonic fields. Using bosonization representation the kinetic part of fermion models maps to kinetic part of the bosonic picture.

But the important difference is that the interaction part of fermionic model which usually has four fermion operator, maps to a quadratic term in bosonic representation which means we could include the interaction effects exactly, not perturbatively. The resulting non-interacting bosonic Hamiltonian is called the Luttinger Hamiltonian [17] which only has two parameters in it. The first one is the velocity of the bosonic excitations, and the second one is called “stiffness”.

\[ H_{LL} = \frac{v}{2\pi} \left[ K (\partial_x \theta)^2 + \frac{1}{K} (\partial_x \phi)^2 \right] \]  

(1.2)

By using the dictionary of bosonization and Jordan-Wigner transformation we could represent the spin operators in terms of bosonic fields; when the corresponding bosonized Hamiltonian is non-interacting, the spin-spin correlations can be found [18]. And it turns out that spin-spin correlations decay with a power law, as function of distance, which confirms the non-existence of long range order and the exponent of the decay only depends on Luttinger parameter \( K \).

As a result it is crucial to find a relation between the parameters of Luttinger model, \( v \) and \( K \), in terms of the parameters of microscopic model, \( \Delta, J \) and \( h \). For the special case of \( h = 0 \) it is possible to find an exact analytical equation for \( K \) and \( v \) in terms of \( \Delta \) and \( J \). But for general case of non-zero magnetic field it is possible, by using Bethe ansatz equations [9], to find numerically the Luttinger parameter for any value of anisotropy.

We should mention that the bosonization method is asymptotically exact as we approach the Fermi point, or excitations with \( q \to 0 \). Although it is a powerful method to address many theoretical questions using it to find the dynamical quantities at finite momentum \( q \neq 0 \) gives not very exact results [19].

For example let’s look at dynamic structure factor, which is the imaginary part of retarded density-density correlation function. The Fourier transform of density operator at momentum \( q \) consists of particle-hole excitations with total momentum \( q \). \( \rho(q) = \sum p \, c_{q+p}^\dagger c_p \). Then by using Lehmann representation it could be shown that
dynamical structure factor at momentum $q$ and frequency $\omega$, could be represented by

$$S(\omega, q) = \sum_\alpha \delta(\omega - E_p^{(\alpha)}(q)),$$

(1.3)

where the summation is over all possible configuration of particle-hole excitations with momentum $q$, and the energy of that excitation is given by $E_p^{(\alpha)}(q)$.

Thus if we linearize the dispersion relation of fermions, with velocity $v_F$, the energies of all the possible particle-hole excitations are exactly the same, $E_p^{(\alpha)}(q) = v_F q$, Fig. 1.1. This means that the dynamical structure factor (DSF) is only delta function peak at zero temperature, and going to finite temperature leads to symmetric Lorentzian broadening of it. But by using neutron scattering experiments is was pointed out that the DSF has asymmetric double peak structure at finite temperatures which is in contradiction to bosonization result[20].

We could see that if we include the band curvature of the dispersion then the energies of the particle-hole excitations not only depends on the total momentum but also on the position of the particle and the hole. For example in Fig. 1.1 we see that the energy of a particle-hole excitation for a hole near fermi point is smaller than for the case where the particle is near the fermi point. As a result of this, the DSF is not a delta function peak and has structure even at zero temperature. This is an important observation, it tells us that the DSF is non-zero only at some energy interval $\omega_L(q) < \omega < \omega_U(q)$, where $\omega_{L/U}(q)$ are the threshold lower and upper frequencies of particle-hole excitation for fixed $q$, and DSF has non-zero width given by $\delta\omega = \omega_U - \omega_L$ even at zero temperature. Although in general including the interaction terms will lead to many more p-h excitations and as a result to some tails and smearing of the sharp feature of the DSF, but non-zero width and asymmetric shape of DSF remains intact.

1.3 Beyond the Luttinger Liquid paradigm

As we mentioned in previous section, in order to fully understand the dynamical structure factors at finite momentum we need to include the effects of higher order band curvature effects. Although these higher order terms are irrelevant in renormalization group sense for asymptotic theory as $q \to 0$, they could be in-
Figure 1.1: Energy of particle-hole excitations for fixed values of total momentum $q$, but for different particle and hole momenta. Fig a the energy for non-linear dispersion. It is clear that the energy depends on the momentum of particle or hole. Fig b is the energy for linearized dispersion; the energy is independent of the momentum of particle or hole.
cluded perturbatively in the study of finite momentum DSFs. But it turns out that
the study of these band curvature terms is not a trivial task and they cause some
infrared divergences in perturbation analysis, specially near the thresholds \[21, 22\].

In bosonization approach the interactions were treated exactly while the ap-
proximation was linearized dispersion. Using different approach, Pustilnik et al.
\[23\] studied dynamical structure factors by keeping the non-linearity of the disper-
sion intact while doing perturbation in the interaction. Although perturbations lead
to logarithmic divergences in all orders, using methods developed for X-ray edge
singularities in metals \[24\], these divergences could be managed in consistent way.
The results were quite astonishing. Pustilnik et al. found that dynamical structure
factors have power law singularities near the threshold energies while the singu-
larity exponents had momentum dependencies. The momentum dependencies of
exponents in this approach has no equivalent counterpart in linearized bosoniza-
tion and Luttinger Liquid theory. Further study of that approach \[25–30\] lead to
development of nonlinear Luttinger liquid theory.

Although this approach is perturbative in terms of interaction, the resulting
field-theoretical model could be used as a phenomenological framework to study
the DSF of a general one-dimensional system at finite momentum. Among all one
dimensional interacting systems, the more attractive ones are those which are ex-
actly solvable by Bethe ansatz. For this class of models it is possible to find the
parameters of the phenomenological nonlinear Luttinger liquid model for any inter-
action strength \[22\]. Combination of this new approach with Bethe ansatz for ex-
actly solvable models leads to nontrivial tests of this approach, which could be done
using numerical methods such as Density Matrix Renormalization Group (DMRG)
\[31\].

1.4 Magnetism at the edges of graphene ribbons

Graphene is a two dimensional allotrope of Carbon which has many interesting
electronic properties. In graphene the Carbon atoms are arranged in honeycomb
lattice Fig. 1.2 The \( sp^2 \) hybridization of the atomic \( s \) orbital with two \( p \) orbitals
leads to trigonal planar structure, and to the formation of so called $\sigma$ bond between the neighboring carbon atoms, with distance equal to 1.42Å. This $\sigma$ band is responsible for holding the carbon atoms in two dimensions and the robustness of graphene. The remaining $p$ orbital is perpendicular to plane of this planar structure and the resulting covalent bond between $p$ orbitals of the neighboring atoms lead to the formation of $\pi$ band, which is responsible for many low-energy electronic and transport properties of graphene.

The first theoretical study of the band structure of graphene was done by P. R. Wallace in 1946 [32]; he showed the unusual semimetallic behavior of it. The more systematic study of the low-energy excitations of graphene leads to its most interesting properties. Simple tight-binding study of the dispersion of graphene
shows that the dispersion vanishes linearly at two inequivalent points, these point are so called Dirac points.

Semenoff [33] showed that the low energy excitations near these two points are massless chiral, Dirac fermions. Quite interestingly these excitations were propagating like massless fermions but with fermi velocity which is about 1/300 of velocity of light.

In addition to interesting properties of excitations of bulk graphene, it turns out that graphene with some specific boundary conditions has very interesting properties too. Again by using simple tight-binding model it could be shown that a semi-infinite graphene sheet with zigzag boundary, or edge, supports zero energy states. More importantly it could be shown that these zero energy modes are localized near the zigzag edge. As these edge modes have zero energy and have flat energy band Fig. 3.3a then it’s quite natural to expect that even weak interactions could have drastic effects on the ground state of these zero modes.

Mean field theoretical study of these edge states for graphene with electron-electron interactions, Hubbard interaction [34, 35], revealed that the edge states are spin polarized. In this work we first give an argument based on Lieb’s theorem that the turning on the Hubbard interaction could lead to the magnetization of the edge modes. Then by projecting out the bulk excitations we find an effective Hamiltonian which describes the edge modes and then try to prove the magnetism of it’s ground state rigorously.

1.5 Overview

In this thesis we study two different one dimensional systems. The first one is the study of transverse spin dynamical structure factors $S^{+−}(q, ω)$ of XXZ model. The goal is to study the shape of DSFs and to derive analytical expressions for singularity exponents near the threshold frequencies. Pereira et al. [22] extensively studied the DSF for longitudinal spin, $S^{zz}(q, ω)$, here we use same approach to study the transverse spin structure factors. Transverse structure factors are more complicated than the longitudinal spin structure factors. The reason is that in doing the Jordan-Wigner transformation the transverse spins are non-local in terms of fermion operators and even for non-interacting regime still there is no exact re-
sult for dynamical correlation functions. Transverse spin structure factors could be measured either by neutron scattering measurements in general, or using Electron Spin resonance experiments for special class of spin chains with lower symmetry which supports uniform Dzyaloshinskii-Moriya (DM) [36, 37] interaction.

In chapter 2 we first describe a possible experimental realization for the measurement of transverse spin structure factors by using ESR for special class of samples to test the theoretical predictions. The reason for using ESR is that it is more accurate while neutron scattering measurements resolutions is not enough to see the singularity features for small momentum. Then we use bosonization approach and treat the band curvature terms perturbatively, and will show that this approach leads to divergences near the threshold frequencies which means unreliability of bosonization method for the study of singularity exponents.

By using the beyond bosonization method we find the singularity exponents and the shape of transverse structure factors for the XXZ model. Similar to the longitudinal case we find momentum dependence in the singularity exponents. One important and nontrivial test of our result would be to look at the SU(2) symmetric case, since in that case symmetry implies that both transverse and longitudinal structure factors have to be same; we see that our result for singularity exponents are in agreement with the results of longitudinal case [22].

In chapter 3 we study a completely different one dimensional system: graphene edge states. It is well known that the tight binding description of graphene with zigzag edges supports zero energy modes. By looking at the wave function of these modes it turns out that they are well localized at the zigzag edges. Fujita et al. [34] studied the graphene ribbons with zigzag edges with Hubbard interaction by using mean field methods and quite astonishing they found that for any interaction strength the edges are spin polarized.

In that chapter by using the projection method [35] we study the effective Hamiltonian of the edge modes, which we expect to become valid in the weakly interacting limit of the Hubbard model. We show rigorously that the ground state of the projected Hamiltonian is ferromagnetic and as a result the edges are spin polarized. Then we include the effect of unavoidable nearest neighbor hopping terms and study the stability of ferromagnetic state of the edge as function of next nearest neighbor hopping strength, and we show that the fully polarized state remains
intact for some range of next nearest neighbour (NNN) hopping term and having passed some critical value the polarization gradually decreases.

Then in final section we take into account the effect of bulk excitations. Integrating out the bulk excitations leads to higher order interactions. The important result of doing so is that it leads to long range anti-ferromagnetic exchange interaction between two edges of a graphene ribbon. This means that for a graphene ribbon with both edges in zigzag shape each edge is spin polarized and the total spins of the edges are coupled anti-ferromagnetically. Another effect of integrating out the bulk excitation is to have higher order interaction correction to the projected Hamiltonian. By studying these correction we see that they even make the magnetism of the edges more robust.
Chapter 2

Spectral functions and Dzyaloshinskii-Moriya interactions in XXZ spin chains

2.1 introduction

One dimensional (1D) interacting systems exhibit unusual correlation effects dominated by strong quantum fluctuations. Fortunately, an array of powerful theoretical methods exists to study this physics, which is finding many experimental realizations. One powerful method is based on bosonization [2, 7, 9, 14] leading to the Luttinger liquid concept. Traditionally these methods are based on low energy effective field theory and only apply to the low energy excitations occurring near certain wave-vectors (such as $q = 0$). In the case of fermion models they begin by linearizing the dispersion relation near the Fermi energy and ignoring irrelevant band curvature effects. However, in the last few years, these bosonization methods have been significantly extended by using techniques first developed to study X-ray edge singularities [22, 23, 25, 27, 29].

This has shown that band curvature effects, while formally irrelevant in the renormalization group sense [38], can nonetheless have important effects on line-shapes of spectral functions even at low energy. Perhaps even more importantly, by
combining these techniques with Bethe ansatz methods, it has become possible to make exact predictions of critical exponents at arbitrary momentum [27, 29]. That is, spectral functions are predicted to have the form

\[ S(q, \omega) \rightarrow A[\omega - \omega_L(q)]^{-\eta} \]

near singular energies \( \omega_L(q) \) for arbitrary \( q \) where both \( \omega_L(q) \), which is not small, and the exponents \( \eta(q) \) are determined exactly using the Bethe ansatz. Recently, this approach has been extended to also obtain the amplitudes of correlation functions, \( A \), using the Bethe ansatz [39]. This new approach has been applied to a number of systems including fermions and bosons moving in the continuum [23, 25–27], the fermion spectral function for a tight binding model [22] and the longitudinal spectral function of the XXZ S=1/2 spin chain in a magnetic field [28, 29] with Hamiltonian:

\[
H = J \sum_{i=1}^{N} \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) - h \sum_i S_i^z
\]  

(2.1)

The longitudinal and transverse spectral function are given by:

\[
S_{zz}(q, \omega) = \frac{1}{N} \sum_j \int_{-\infty}^{\infty} dt e^{-i q j + i \omega t} \langle S_j^z(t) S_0^z(0) \rangle
\]

\[
S_{ss'}(q, \omega) = \frac{1}{N} \sum_j \int_{-\infty}^{\infty} dt e^{-i q j + i \omega t} \langle S_j^s(t) S_0^{s'}(0) \rangle
\]  

(2.2)

We set the lattice spacing \( a = 1 \), and \((s, s') = (+, -) \) and \((-+, +) \). For non-zero \( h \), \( S^{+-} \) and \( S^{-+} \) are different. In principle, at arbitrary \( q \), neutron scattering experiments would normally measure a sum of \( S^{zz} \) and the transverse spectral functions. The high neutron fluxes available at the Spallation Neutron Source may eventually make such experimental confirmation possible, here we explore another route.

Quasi 1D magnetic compounds that do not have link parity symmetry (reflection about the midpoint of a link) will generally have magnetic Hamiltonians containing anti-symmetric Dzyaloshinskii-Moriya [36, 37] interactions:

\[
\delta H = \sum_j \vec{D}_j : (\vec{S}_j \times \vec{S}_{j+1}).
\]  

(2.3)

The two standard cases are staggered \( \vec{D}_j = (-1)^j \vec{D} \) and uniform interaction \( \vec{D}_j = \)
\( \vec{D} \). Staggered DM interactions are invariant under site-parity (reflection about a site) but violate symmetry of translation by one site. On the other hand, uniform DM interactions have no parity symmetry whatsoever but respect full translation invariance. We restrict our further discussion to the case where \( \vec{D}_j \propto \hat{z} \) so that the DM vector is parallel to the easy (or hard) axis of the symmetric exchange interactions, a situation which is sometimes dictated by symmetry.

With this configuration, it is possible to eliminate the DM interactions exactly by a gauge transformation, yielding the standard XXZ model of Eq. (2.1) with modified parameters. This approach was used to study staggered DM interactions in Ref. [40, 41] and the theory was applied to a number of real materials. Here we consider the case of uniform DM interactions, \( \vec{D}_j = \hat{z}D \) and choose \( D > 0 \). To show this transformation, it is more convenient to write the interacting Hamiltonian in terms of \( S^\pm \), as the magnetic field is in the same direction as DM interaction, without loss of generality we could ignore the Zeeman term.

\[
H + \delta H = \frac{1}{2} \sum_{i=1}^N ((J + iD)S_i^+ S_{i+1}^- + (J - iD)S_i^- S_{i+1}^+ + 2J\Delta_{eff} S_i^z S_{i+1}^z) \quad (2.4)
\]

In this case by defining a gauge transformation, local rotations around \( z \)-direction, as follow:

\[
\tilde{S}_j^+ = e^{-i\alpha_j} S_j^+ \quad \tilde{S}_j^z = S_j^z \quad (2.5)
\]

where

\[
\alpha = \tan^{-1} \left( \frac{D}{J} \right) \quad (2.6)
\]

the Hamiltonian Eq. (2.4) transforms to standard XXZ Hamiltonian:

\[
H = \sum_i \left( \tilde{S}_i^z \tilde{S}_{i+1}^z + \tilde{S}_i^\pm \tilde{S}_{i+1}^\mp + \Delta_{eff} \tilde{S}_i^\pm \tilde{S}_{i+1}^\pm \right) \quad (2.7)
\]
where the new exchange coupling and anisotropy parameters are given by

\[ J = \sqrt{J^2 + D^2}, \quad \Delta_{\text{eff}} = \Delta \cos(\alpha). \]  (2.8)

The electron spin resonance (ESR) adsorption intensity, in standard Faraday configuration, is proportional to the transverse spectral function at \( q = 0 \), since the wave-vector of microwave photons is much less than the inverse lattice spacing. After the gauge transformation, the ESR intensity is therefore proportional to \( S^{+-} \) and \( S^{-+} \), for the Hamiltonian of Eq. (2.1) at \( q = \alpha \). [By using circularly polarized microwave radiation both \( S^{+-}(\alpha, \omega) \) and \( S^{-+}(\alpha, \omega) \) could be measured separately]. Thus the edge singularities predicted by X-ray edge methods at a non-zero wave-vector \( \alpha \) given by Eq. (2.6) are directly measured by ESR. ESR on spin chain compounds with uniform DM interactions therefore would provide a powerful probe of the new bosonization predictions. Quasi-1D spin-1/2 antiferromagnetic insulators containing DM interactions with a uniform component include Cs$_2$CuCl$_4$ [42, 43] and KCuGaF$_6$ [44]. This provides a strong motivation to extend the X-ray edge methods to study edge singularities in the transverse spectral functions of the XXZ chain in a magnetic field.

In the next section we review results on the transverse spectral function using standard bosonization and then show that band curvature effects (in the equivalent fermion model) render these results invalid close to edge singularities. In Sec. 2.3 we apply X-ray edge methods to the model obtaining new results on the leading edge singularities. In Sec. 2.4 sub-dominant singularities are discussed. Section 2.5 discusses ESR with uniform DM interactions, based partly on the results of Sec. 2.3. Sec. 2.6 contains conclusions and open questions.

### 2.2 Spectral function of the XXZ spin chain

The XXZ \( S = 1/2 \) model of Eq. (2.1) is equivalent to an interacting spinless fermion model by the Jordan-Wigner transformation:

\[ S^+_i = c^\dagger_i c_i - \frac{1}{2}, \]
\[ S^-_i = (-1)^i \exp(i\pi \sum_{k<j} c^\dagger_k c_k) c_j. \]  (2.9)
The Hamiltonian (2.1) is transformed to

\[ H = \frac{-J}{2} \sum (c_i^\dagger c_{i+1} + h.c.) - h \sum c_i^\dagger c_i \]
\[ + J \Delta \sum (c_i^\dagger c_i - \frac{1}{2}) (c_{i+1}^\dagger c_{i+1} - \frac{1}{2}). \]  

(2.10)

Note the factor of \((-1)^j\) in the second line of Eq. (2.9) is necessary for the first term in the fermionic Hamiltonian, Eq. (2.10), to have the standard minus sign. \( h \) is the chemical potential of the fermionic model with \( h = 0 \) corresponding to half-filling. For the non-interacting case \( \Delta = 0 \), the Hamiltonian is just a free fermion model and by going to momentum space

\[ c_p = \frac{1}{\sqrt{N}} \sum c_j e^{ipj} \]

where \( p = 2\pi n/N \) for periodic boundary conditions, the energy spectrum of non-interacting fermion model is found to be

\[ H = \sum (-J \cos(p) - h) c_p^\dagger c_p. \]  

(2.11)

For non-interacting case and using fermionic representation the longitudinal spectral function is given by

\[ S^{zz}(\omega, q) = \frac{1}{N} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle n_q(t)n_q(0) \rangle \]  

(2.12)

where \( n_q = \sum_j e^{iqj} n_j = \sum_p c_p^\dagger c_{p+q} \). To find an analytical result for longitudinal spectral function, it is more convenient to use Lehmann representation of Eq. (2.12), as follow

\[ S^{zz}(\omega, q) = \frac{2\pi}{N} \sum |\langle 0|n_q|\alpha \rangle|^2 \delta(\omega - E_\alpha - E_\Omega) \]  

(2.13)

where \( |\alpha \rangle \) is an eigenstate with energy \( E_\alpha \) and \( E_\Omega \) is the energy of the ground state. By using the fact that the system is non-interacting and doing some straightforward
algebra the final result for spectral function is

\[ S^{zz}(\omega, q) = \frac{\theta(\omega - \omega_L(q))\theta(\omega_U(q) - \omega)}{\sqrt{(2J \sin q/2)^2 - \omega^2}}. \tag{2.14} \]

We see that \( S^{zz} \) is non-zero only in finite frequency range for a fixed momentum \( q \); the lower and upper thresholds for \( k_F < \pi/2 \) are given by

\[ \omega_U(q) = 2J \sin \frac{|q|}{2} \sin(k_F + \frac{|q|}{2}) \]
\[ \omega_L(q) = 2J \sin \frac{|q|}{2} \sin(k_F - \frac{|q|}{2}) \tag{2.15} \]

and for \( k_F = \pi/2 \)

\[ \omega_U(q) = 2J \sin \frac{|q|}{2} \]
\[ \omega_L(q) = J \sin |q| \tag{2.16} \]

From Eq. (2.14), it is easily seen that the support of \( S^{zz} \), for \( \Delta = 0 \), is restricted to the interval \([\omega_L, \omega_U]\). The nature of these lower and upper thresholds is different for zero and non-zero magnetic field. For non-zero magnetic field and \( k_F < \pi/2 \) the lower threshold is given by creating one deep hole with momentum \( q \), whereas the upper threshold is achieved by excitation of one high-energy electron with momentum \( q \). But for zero magnetic field, \( k_F = \pi/2 \), particle-hole symmetric case, the lower threshold is achieved either by creating one deep hole or one high energy electron but higher threshold is given by symmetric particle hole excitation around Fermi point with momentum of each \( q/2 \).

In contrast to the longitudinal spectral function, even for \( \Delta = 0 \) and having the entire spectrum at hand, finding the transverse spectral function is a very difficult problem. The reason for this complication is the complicated form of the transverse spin operators, which have the string operator in their fermionic form Eq. (2.9). The equal time transverse correlation function, in this case, is known exactly[45] but less is known about dynamical correlations. The non-local nature of string operator is such that we can not even evaluate simply the lower and upper threshold
for $S^{-+}$ and $S^{+-}$. By applying $S^+_j$ to the vacuum, the exponential factor of it will allow creation of any number of particle hole excitations

$$S^+_j |0\rangle = \exp(i\pi \sum_{j<i} c^+_j c^+_i) |0\rangle = \sum_n \frac{(i\pi \sum_{j<i} c^+_j c^+_j)^n}{n!} c^+_i |0\rangle$$

So it is obvious that potentially $S^{-+}(\omega, q)$ could be non-zero for fixed $q$ and any $\omega$. However, in general, we expect an infinite number of progressively weaker singularities, extending down to zero energy, similar to the case of the longitudinal structure function in a non-zero magnetic field [22]. After reviewing the standard bosonization method in next section and its results for spin structure factors in section 2.2.2, we look at the effects of irrelevant band curvature operators in section 2.2.3.

### 2.2.1 Bosonization of interacting fermion model

In this part we first review the bosonization method and how to map a field theory from fermionic representation to bosonic form. The bosonization is powerful method to study interacting one dimensional models. The essence of the approach is to study low-energy properties of a system; thus we only need to keep the low energy excitation. So let’s see how it works.

Having done the Jordan-Wigner transformation, the fermionic model description of the spin model is given by

$$H = \frac{-J}{2} \sum_i (c^+_i c^+_{i+1} + h.c.) - \hbar \sum_i c^+_i c_i$$

$$+ J\Delta \sum_i (c^+_i c_i - \frac{1}{2})(c^+_{i+1} c_{i+1} - \frac{1}{2})$$

(2.17)

As we discussed in section 2.2 for $\Delta = 0$, this is just free fermion model and the ground state has all states filled up to momentum $\pm k_F$, with $k_F = \cos^{-1}(h/J)$. To find the low-energy description of Eq. (2.17) we only include the excitations around the two Fermi points Fig. 2.1 and linearize the energy dispersion near these
Figure 2.1: The band structure of non-interacting fermion model. To find low energy field theory of interacting model we only keep excitation within the cutoff $\Lambda_F$.

points

$$c_j \equiv \Psi(x) \approx \psi_R(x)e^{ik_Fx} + \psi_L(x)e^{-ik_Fx}$$

$$\varepsilon_{\pm k_F+q} = \pm v_F q + \frac{q^2}{2m} + \cdots$$ (2.18)

where $\psi_{R/L}$ are slowly varying fields, which represents excitations near $\pm k_F$. $v_F = J\sin k_F$ is velocity of the excitations, $m = (J\cos k_F)^{-1}$ is the effective mass at Fermi level and $\cdots$ are higher order band curvature terms.
The continuum model representation of Hamiltonian 2.17 is

\[ H_0 = \int dx : \psi_R^\dagger(x) v_F(-i\partial_x) \psi_R(x) + \psi_L^\dagger(x) v_F(-i\partial_x) \psi_L(x) : \]

(2.19)

where we have dropped higher derivative terms, as they are irrelevant in the sense of renormalization group. Similarly we could write the interaction part of Hamiltonian 2.17 in terms of continuum field as follow

\[ H_{int} = \Delta J \int dx : \Psi^\dagger(x)\Psi(x) : \Psi^\dagger(x+a)\Psi(x+a) : \]

\[ = \Delta J \int dx \rho_R(x)\rho_R(x+a) + \rho_L(x)\rho_L(x+a) + e^{2k_F a} \rho_R^\dagger(x)\rho_L(x)\rho_L^\dagger(x+a)\rho_R(x+a) + h.c.] \]

(2.20)

where \( \rho_{R/L} \equiv \psi_R^\dagger \psi_{R/L} \) are the density of right mover and left mover excitations. For general value of \( k_F \) the last term of above equation, so called Umklapp scattering term, is oscillatory and in low-energy theory we can ignore it. But for the case of half-filling, \( k_F = \pi/2 \), which corresponds to zero magnetic field regime it is non-oscillatory and we should include it in the study of the Hamiltonian.

The bosonization of the Hamiltonian \( H_0 + H_{int} \) is performed by expressing the fermionic operators \( \psi_{R/L} \) in terms of some bosonic fields as follow

\[ \psi_R(x) \approx \frac{\eta}{\sqrt{2\pi\alpha}} e^{-i\sqrt{2\pi} \phi_R(x)} \]

\[ \psi_L(x) \approx \frac{\eta}{\sqrt{2\pi\alpha}} e^{i\sqrt{2\pi} \phi_L(x)} \]

(2.21)

where \( \alpha = k_F^{-1} \) is a short distance cutoff, \( \phi_{R/L}(x) \) are right and left component of bosonic field and \( \eta \) is called Klein factor, which is introduced to ensure the correct anti-commutation relation for fermionic fields. The commutation relation for the
bosonic fields are

\[
\left[ \phi_R, \phi_L \right] = \frac{i}{2}
\]

\[
\left[ \phi_R(x), \phi_L(y) \right] = \pm \frac{i}{2} \text{sign}(x-y) \tag{2.22}
\]

The fields \( \phi_R/L \) could be expressed in terms of a bosonic field \( \tilde{\phi} \) and its dual field \( \tilde{\theta} \) as follow

\[
\tilde{\phi} = \frac{\phi_L - \phi_R}{\sqrt{2}}
\]

\[
\tilde{\theta} = \frac{\phi_L + \phi_R}{\sqrt{2}} \tag{2.23}
\]

with commutation relation given by \( [\tilde{\phi}(x), \partial_y \tilde{\theta}(y)] = i \delta(x-y) \). By using bosonized representation of fermionic operators it is easy to show that the right and left densities are proportional to derivatives of bosonic operators:

\[
\rho_{R/L} \approx \pm \frac{1}{\sqrt{2\pi}} \partial_x \phi_{R/L} \tag{2.24}
\]

and total density is given by

\[
n(x) = \Psi^\dagger(x)\Psi(x) \approx \sigma + \frac{1}{\sqrt{\pi}} \partial_x \tilde{\phi} + \frac{1}{\pi \alpha} \cos \left( \sqrt{4\pi \alpha} \tilde{\phi} - 2k_F x \right)
\]

\[
\tag{2.25}
\]

where \( \sigma = k_F/\pi \) gives filling fraction, \( \sigma = 1/2 \) corresponds to half-filling. Similarly we could find the bosonized version of the kinetic part of Hamiltonian 2.19 as follow

\[
H_0 = \int dx \, iv_F \left( : \psi_R^\dagger \partial_x \psi_R - \psi_L^\dagger \partial_x \psi_L : \right)
\]

\[
= \frac{v_F}{2} \int dx \left[ (\partial_x \tilde{\phi})^2 + (\partial_x \tilde{\theta})^2 \right] \tag{2.26}
\]
and bosonized representation of terms in interaction part Eq. (2.20) are

\[
\begin{align*}
\rho_{R/L}(x)\rho_{R/L}(x+a) &= \frac{1}{2\pi}(\partial_x \phi_{R/L})^2 \\
\rho_{R}(x)\rho_{L}(x+a) &= -\frac{1}{2\pi} \partial_x \phi_{R} \partial_x \phi_{L}
\end{align*}
\]

\[
\begin{align*}
\psi_{R}^{\dagger}(x)\psi_{L}(x)\psi_{L}^{\dagger}(x+a)\psi_{R}(x+a) &= \\
&= \cos k_{F} \left( \partial_{x} \phi_{R} - \partial_{x} \phi_{L} \right)^{2} + \frac{\sin k_{F}}{3\sqrt{2\pi}} \left( \partial_{x} \phi_{R} - \partial_{x} \phi_{L} \right)^{3} + \cdots \quad (2.27)
\end{align*}
\]

where \( \cdots \) are higher order more irrelevant terms in the sense of renormalization group, but the have important effect on spectral functions near the singular points as discussed in 2.2.3. By ignoring all the irrelevant and highly oscillatory terms the final form of low-energy bosonic Hamiltonian is given by

\[
H = \frac{v_{F}}{2} \int dx \left\{ \left( 1 + \frac{g_{4}^{2}}{2\pi v_{F}} \right) \left[ \partial_{x} \phi_{R} + \partial_{x} \phi_{L} \right]^{2} - \frac{g_{2}^{2}}{\pi v_{F}} \partial_{x} \phi_{R} \partial_{x} \phi_{L} \right\} \quad (2.28)
\]

where \( g_{2} = g_{4} = 2J\Delta(1 - 2\cos(2k_{F})) \). The Hamiltonian (2.28) could be written in the following form known as Luttinger Liquid Hamiltonian

\[
H_{LL} = \frac{v}{2} \int dx \left[ K \left( \partial_{x} \theta \right)^{2} + \frac{1}{K} \left( \partial_{x} \phi \right)^{2} \right] \quad (2.29)
\]

where \( v \) is the renormalized velocity and \( K \) is the Luttinger parameter, and are given by

\[
\begin{align*}
v &= v_{F} \sqrt{\left( 1 + \frac{g_{4}^{2}}{2\pi v_{F}} \right)^{2} - \left( \frac{g_{2}}{2\pi v_{F}} \right)^{2}} \approx v_{F} \left( 1 + \frac{2\Delta}{\pi} \sin k_{F} \right) \\
K &= \sqrt{\frac{2\pi v_{F} + g_{4} - g_{2}}{2\pi v_{F} + g_{4} + g_{2}}} \approx 1 - \frac{2\Delta}{\pi} \sin k_{F} \quad (2.30)
\end{align*}
\]

The expressions for \( v \) and \( K \), in terms of microscopic model (2.17) are valid only for \( \Delta \ll 1 \). For zero magnetic field there is an exact expression for velocity and
Luttinger parameter, derived from Bethe ansatz calculations [9]

\[ v = J \frac{\pi \sqrt{1 - \Delta^2}}{2 \arccos \Delta}, \quad K = \left[ 2 - 2 \arccos(\Delta) / \pi \right]^{-1}. \] (2.31)

For non-zero magnetic field, away from half-filling, there is no analytic expression for \( v \) and \( K \), but they could be found by using numerical methods to solve Bethe ansatz equations.

As we see the bosonization method is a powerful method to study one dimensional interacting systems, to study the new bosonic model we only need to know two parameters, velocity \( v \) and the Luttinger parameter \( K \). By evaluating these two parameters either explicitly or by using numerical methods all the physical properties of the system could be expressed in terms of them.

### 2.2.2 Spectral function of XXZ spin chain using bosonization

As mentioned before, calculating the dynamical correlations for XXZ model is very difficult, and is one of the most studied problems of one dimensional spin chains. By using field theory methods known as bosonization\([2, 7, 9, 14]\) we could get some information about low-energy effective description of these correlations. Here we review the results of bosonization for the transverse spectral function of the XXZ Hamiltonian Eq. (2.1).

To use bosonization approach for finding the spectral functions of XXZ model, we need to write the spin operators in terms of the bosonic fields. From Jordan-Wigner transformation we have a relation between spin operators and fermion operators; by using the result of previous section we could find an expression for spin operators in terms of bosonic fields.

As we see from Eq. (2.9) the easy one is \( S_j^z \):

\[ S_j^z \approx m + : \psi_L^\dagger \psi_L : + : \psi_R^\dagger \psi_R : + (\psi_L^\dagger \psi_R^\dagger + \text{h.c.}) \]

\[ = m + \sqrt{\frac{K}{\pi}} \partial_x \phi + C \cos \left( \sqrt{4\pi K} \phi + (2\pi m + \pi)x \right) \] (2.32)

where \( : \ldots : \) denotes normal ordering and \( m = \langle S_h^z \rangle \) is the magnetization, which is
related to the Fermi wave-vector by the exact relation:

$$2k_F = 2\pi m + \pi$$ (2.33)

For weak fields,

$$m \to K h / (\pi v).$$ (2.34)

$C_j$ is a non-universal constant. To obtain the low energy representation of $S_j^+$ from Eq. (2.9) we use:

$$\Psi_{R/L} \propto e^{-i \sqrt{\pi/K} \theta \pm i \sqrt{\pi K} \phi}$$ (2.35)

We also approximate the exponential of the Jordan-Wigner string operators using:

$$i \pi \sum_{l<j} c_l^+ c_j \approx i \pi \int_{-\infty}^{j} dy (k_F + \sqrt{K/\pi} \phi)^\pm i \sqrt{\pi K} \phi(j) = N + i \pi k_F j + i \sqrt{\pi K} \phi(j)$$ (2.36)

where $N$ is just a constant. Following the standard bosonization approach [7] we have ignored the oscillating term in $c_j^+ c_j$ in the exponential of the Jordan-Wigner string operator, but we will consider it in the next sub-section. Note that $\exp[i \sum_{j<i} c_j^+ c_j]$ is Hermitian, taking eigenvalues $\pm 1$. On the other hand, the exponential of the continuum limit operator in Eq. (2.36) is not Hermitian. To deal with this problem the standard approach [7] is to instead take the continuum limit of $\cos[\pi \sum_{l<j} c_l^+ c_j]$:}

$$\cos[\pi \sum_{l<j} c_l^+ c_j] \approx e^{i \pi k_F j} e^{i \sqrt{\pi K} \phi(j)} + h.c.$$ (2.37)

Substituting these low energy limit formulas into the second of Eq. (2.9) gives:

$$S_j^+ \propto (-1)^j e^{-i \sqrt{\pi/K} \theta} \left[ e^{i k_F j} e^{i \sqrt{\pi K} \phi} + e^{-i k_F j} e^{-i \sqrt{\pi K} \phi} \right] \times \left[ e^{i k_F j} e^{i \sqrt{\pi K} \phi} + e^{-i k_F j} e^{-i \sqrt{\pi K} \phi} \right] = e^{-i \sqrt{\pi/K} \theta} \left[ C(-1)^j + C_- \cos(2\pi m x + \sqrt{4\pi K} \phi) \right]$$ (2.38)

where $C$ and $C_-$ are two other non-universal constants. It can be seen from Eqs. (2.32) and (2.38) that the applied magnetic field induces a shift in momenta of
both transverse and longitudinal spin operators, but in different ways. For the longitudinal operator, it shifts only the staggered part but for transverse spin it shifts only the uniform part. This shift is small for weak fields where the approximation of ignoring band curvature is valid.

Let us focus on transverse structure function near $q \approx 0$ for weak fields. At zero temperature we have

\[ \langle S_j^+(t)S_0^- (0) \rangle \propto e^{-iHx} \frac{1}{(vt + x - i\epsilon)^2 + 2\eta} \epsilon^{iHx} \]

where $x = j, H$ and $\eta$ are given by

\[ H = \frac{2\pi m}{K} \]
\[ \eta = \frac{(1 - 2K)^2}{8K} \]

obeying $\eta < 1/8$ for $|\Delta| < 1$, and $\epsilon$ is a positive quantity of order the lattice spacing. By taking the Fourier transform, the spectral function $S^{+-}$ is

\[ S^{+-}(q, \omega) \propto \theta(\omega - \nu|q + H|) \left( \frac{\omega + \nu(q + H)}{\omega - \nu(q + H)} \right)^{1 + 2\eta} \left( \frac{\omega - \nu(q - H)}{\omega + \nu(q - H)} \right)^{1 - 2\eta} \]

Note that the first term has a diverging threshold at $\omega = \nu(q + H)$ for $q + H > 0$ and a vanishing threshold at $\omega = -\nu(q + H)$ for $q + H < 0$. The second term is the parity transform ($q \rightarrow -q$) of the first. Diverging and vanishing thresholds are indicated by solid and dotted lines in Fig. [2.2a]. Note that, two diverging thresholds occur in $S^{+-}(q, \omega)$ for $|q| < H$ which cross each other at $q = 0$ but that there is only one diverging thresholds for $|q| > H$. $S^{-+}$ is obtained from $S^{+-}$ by the transformation $H \rightarrow -H$. (Recall that we are assuming $H > 0$.)
Figure 2.2: Singular points of zero temperature transverse spin spectral function of XXZ model, predicted by bosonization. The solid lines indicate diverging singularities and dashed line the vanishing singularities.
\begin{equation}
S^{+\pm}(q, \omega) \propto \theta(\omega - v|q - H|) \left( \frac{\omega + v(q - H)}{\omega - v(q - H)} \right)^{1+2\eta} \left( \frac{\omega - v(q + H)}{\omega + v(q + H)} \right)^{1-2\eta}
\end{equation}

Its diverging and vanishing thresholds are shown in Fig. [2.2b]. Note that, for \( S^{+\pm} \), no diverging thresholds occur for \( |q| < H \) and a single diverging threshold occurs for \( |q| \approx H \) and also near \( q \approx \pi \).

For ESR applications we will be especially interested in the case \( \Delta \) slightly less than 1 and small \( H \) corresponding to \( K \) slightly greater than 1/2 and thus \( \eta \ll 1 \). Then it is important to note that the \( \eta \) dependence of the constant factor in \( S^{+\pm} \) is \( \propto \sin^2(2\pi\eta)\Gamma(-1-2\eta)\Gamma(1-2\eta) \) [46], which vanishes linearly with \( \eta \); here \( \Gamma \) is Euler’s Gamma function. To study the line shape at \( H = 0 \) and \( \eta \rightarrow 0 \), we take into account that this expression for \( S(q, \omega) \) is only valid for a finite range of \( \omega, v|q| < \omega < \Lambda \) for an upper cutoff \( \Lambda \), of order \( J \) or less. We then use the fact that

\begin{equation}
\lim_{\eta \rightarrow 0} \int_{vq}^{\Lambda} \frac{2\eta \theta(\omega - vq)}{(\omega - vq)^{1-2\eta}} = \lim_{\eta \rightarrow 0} \Lambda^{2\eta} = 1.
\end{equation}

Therefore we have

\begin{equation}
\lim_{\eta \rightarrow 0} 2\eta \theta(\omega - vq) / (\omega - vq)^{1-2\eta} = \delta(\omega - vq)
\end{equation}

and thus the term with a diverging threshold approaches

\begin{equation}
S(q, \omega) \propto v|q|\delta(\omega - vq). \quad (\eta \rightarrow 0).
\end{equation}

For a fixed momentum \( q \) and small \( \eta \), \( S(q, \omega) \) as function of \( \omega \) is depicted in Fig. [2.3]. Here we show only one term with a diverging threshold. It is zero for frequencies such that \( \omega < vq \), and it has a local minima at point \( \omega^* \) given by

\begin{equation}
\omega^* = \sqrt{\frac{1 - \eta}{\eta}vq} \approx \frac{vq}{\sqrt{\eta}}.
\end{equation}

So for \( \eta \approx 0.1 \) we get \( \omega^* \approx 3vq \). We should also be careful about the cases of very small anisotropy; from Eq. (2.44) we see that for fixed momentum \( q \), as
Figure 2.3: Zero temperature transverse spectral function $S^{+-}(\omega, q)$ predicted by bosonization for fixed $q$. a) shows transverse spectral function for zero magnetic field and b) is for non-zero magnetic field with $q < H$. 
anisotropy gets smaller and smaller \( \omega^\ast \) becomes larger and larger, so it seems that we are getting out of the region where bosonization is trustworthy. The results of bosonization are reliable below some cutoff \( \Lambda \); then the consistency relation \( \omega^\ast < \Lambda \) will gives us a restriction on momentum \( q \) such that we must have \( vq < \sqrt{\eta} \Lambda \).

In fact, as shown above \( S^{+-} \) and \( S^{--} \) are a sum of two terms each with a separate threshold for all \( q \neq 0 \). Depending on which spectral function we look at and the value of \( q \), these thresholds can be both diverging, both vanishing or one diverging, one vanishing. The various shapes of \( S(q, \omega) \) are sketched in Fig. [2.4]. In the special case \( q = 0 \), there is a single term of diverging threshold type.

\[ S \]

\[ S \]

\( q \) \( \sim \) \( H \) for \( S^{+-} \)

\( H \) \( \sim \) \( |q| \) for \( S^{+-} \)

\( q \) \( \sim \) \( H \) for \( S^{--} \)

\( H \) \( \sim \) \( |q| \) for \( S^{--} \)

**Figure 2.4:** Various shapes of singularities of \( S^{+-} \) and \( S^{--} \) for different range of momentum \( q \), with \( |q|, H \ll 1 \), predicted by bosonization.
For the transverse Green’s function at $q \approx \pi$ we have

\[
\langle S^+(x,t)S^-(0) \rangle \approx \langle S^-(x,t)S^+(0,0) \rangle \\
\propto e^{i\pi x} \frac{1}{(vt-x-i\epsilon)^{1/4K}(vt+x-i\epsilon)^{1/4K}}
\]

where $x = j$. By taking the Fourier transform we obtain the transverse spectral function near $q = \pi$:

\[
S^+(q, \omega) \approx S^-(q, \omega) \propto \frac{\theta(\omega - v|q - \pi|)}{(\omega^2 - v^2(q - \pi)^2)^{1-1/4K}}
\]

So we see that the singularity exponent for staggered part is $1 - 1/4K$, which is different than the exponent for uniform part. Now there is a single diverging threshold at $\omega = v|q - \pi|$ for either sign of $q - \pi$ for both $S^{+ -}$ and $S^{- +}$. It seems natural to assume that the diverging thresholds of $S^{+ -}$ and $S^{- +}$ starting at $q = \pm H$ can be interpolated to the diverging thresholds terminating at $q = \pi$. Such an assumption goes beyond the standard bosonization approach which is restricted to $q$ near 0 and $\pi$ (and to small $H$) but we shall see in section 2.3, using X-ray edge methods, that this interpolation is correct.

However we will also find that the exponents of the diverging thresholds that are predicted by standard bosonization: $1 - 2\eta$ near $|q| = H$ and $1 - 1/(4K)$ near $q = \pi$ are both incorrect, as are the exponents of the vanishing thresholds.

### 2.2.3 Effect of irrelevant band curvature operators

In previous sub-section we reviewed the prediction of bosonization for the singularity exponent of transverse spectral functions. In this section by including the effect of band curvature operators we show that the predictions of naive bosonization for singularity exponents are not reliable.

In bosonization approach we treat the interactions exactly but we linearize the dispersion around Fermi points and neglect the effects of higher order band curvature terms. By power counting these terms are irrelevant in low energies and renormalize to zero, but as discussed in [28], the effect of these operators is important near the singular thresholds for longitudinal spectral function. We will show
that the same argument works for transverse spectral function. In this section we look at the effect of these terms to lowest order for $h \neq 0$.

As shown in [28, 38] by including the effect of band curvature corrections the Hamiltonian becomes

$$\mathcal{H} = \mathcal{H}_{LL} + \delta \mathcal{H}$$

(2.47)

where $\mathcal{H}_{LL}$ is Luttinger Liquid Hamiltonian and $\delta \mathcal{H}$ is given by

$$\delta \mathcal{H} = \frac{\sqrt{2\pi}}{6} \int dx \{ \eta_- \left[ (\partial_x \phi_L)^3 - (\partial_x \phi_R)^3 \right] 
+ \eta_+ \left[ (\partial_x \phi_L)^2 \partial_x \phi_R - (\partial_x \phi_R)^2 \partial_x \phi_L \right] \}$$

(2.48)

Where to first order in $\Delta$ we have

$$\eta_- \approx \frac{1}{m} \left( 1 + \frac{2\Delta}{\pi} \sin k_F \right)$$

$$\eta_+ \approx -\frac{3\Delta}{\pi m} \sin k_F$$

where $m = (J \cos k_F)^{-1}$ is the effective mass of Fermi excitations. For weak interaction we can neglect $\eta_+$ and only include the effect of $\eta_-$ term in Eq. (2.48).

Now let us evaluate the transverse spectral function using perturbation theory in $\delta \mathcal{H}$. By ignoring terms proportional to $\eta_+$ which mixes right and left operators, in general we are looking for the following kind of imaginary time correlation functions

$$G_{\nu \overline{\nu}}(x, \tau) = G_R(x, \tau)G_L(x, \tau)$$

$$G_R(x, \tau) = \langle e^{i\sqrt{2\pi \nu} \phi_R(x, \tau)} e^{-i\sqrt{2\pi \nu} \phi_R(0, 0)} \rangle$$

$$G_L(x, \tau) = \langle e^{i\sqrt{2\pi \overline{\nu}} \phi_L(x, \tau)} e^{-i\sqrt{2\pi \overline{\nu}} \phi_L(0, 0)} \rangle$$

(2.49)

Where $\nu$ and $\overline{\nu}$ could be written explicitly in terms of Luttinger parameter, $K$, but for the following discussion we do not need their explicit form. The first order
correction from perturbation Eq. (2.48) modifies the correlation function to

\[
G_{\nu \bar{\nu}}(x, \tau) = G^{(0)}(0) - \frac{i\eta - \sqrt{2\pi}}{6} \int dz d\tau' \langle e^{i\sqrt{2\pi}\nu \phi_R(x, \tau)} (\partial_z \phi_R(z, \tau'))^3 e^{-i\sqrt{2\pi}\nu \phi_R(0,0)} G^{(0)}_L(x, \tau) + \frac{i\eta - \sqrt{2\pi}}{6} \int dz d\tau' \langle e^{i\sqrt{2\pi}\bar{\nu} \phi_L(x, \tau)} (\partial_z \phi_L(z, \tau'))^3 e^{-i\sqrt{2\pi}\bar{\nu} \phi_L(0,0)} G^{(0)}_R(x, \tau) \rangle 
\]  

(2.50)

To evaluate the correlation function Eq. (2.50), we focus on corrections to \( G_R(x, \tau) \); calculations for \( G_L(x, \tau) \) are exactly the same.

So we have

\[
G_R(x, \tau) = G^{(0)}_R(x, \tau) - \frac{i\eta - \sqrt{2\pi}}{6} \int dz d\tau' \langle e^{i\sqrt{2\pi}\nu \phi_R(x, \tau)} (\partial_z \phi_R(z, \tau'))^3 e^{-i\sqrt{2\pi}\nu \phi_R(0,0)} G^{(0)}_L(x, \tau) \rangle
\]  

(2.51)

In diagrammatic way the non-zero contributions are depicted in Fig. [2.5].

\[\text{Figure 2.5: The relevant Feynman graphs which contribute to correlation in first order of perturbation.}\]
So the non-zero correction is given by

\[
\delta G_R \propto \int dzd\tau' \langle e^{i\sqrt{\frac{2}{\pi\nu}\phi_R(x, \tau)}} (\partial_z \phi_R(z, \tau'))^3 e^{-i\sqrt{\frac{2}{\pi\nu}\phi_R(0,0)}} \rangle 
\]

\[
= \int dzd\tau' \int \sum_{n,m} \frac{(i\sqrt{2\pi\nu})^n(-i\sqrt{2\pi\nu})^m}{n!m!} \langle \phi_R(x, \tau)^n(\partial_z \phi_R(z, \tau'))^3 \phi_R(0,0)^m \rangle 
\]

\[
\delta G_R = \int dzd\tau' \sum_{m,n} 3nm(m-1) \frac{(i\sqrt{2\pi\nu})^n(-i\sqrt{2\pi\nu})^m}{n!m!} 
\]

\[
\times \langle \phi_R(x, \tau)^n(\partial_z \phi_R(z, \tau'))^m \phi_R(0,0)^m \rangle^2 
\]

(2.52)

In going from second line to third line, we have used Wick’s theorem, and the factor $3nm(m-1)$ comes from the all possible number of contraction of fields. Thus we have

\[
\delta G_R \propto -3i\sqrt{(2\pi\nu)^3} G_R^{(0)}(x, \tau) \times 
\]

\[
\int dzd\tau' \langle \phi_R(x, \tau) \partial_z \phi_R(z, \tau') \rangle \langle \partial_z \phi_R(z, \tau') \phi_R(0,0) \rangle^2 
\]

(2.53)

Now by using the fact that

\[
< \partial_z \phi_{R,L}(x, \tau) \phi_{R,L}(0,0) > = \frac{1}{2\pi} \frac{1}{v\tau + ix} 
\]

(2.54)

we can write Eq.\ 2.53 as

\[
\delta G_R \propto 3i\sqrt{(2\pi\nu)^3} G_R^{(0)}(x, \tau) \int dzd\tau' \frac{1}{v(\tau' - \tau) - i(z - x)(v\tau' - iz)^2} \frac{1}{(v\tau - ix)^2} 
\]

\[
= -12i\sqrt{(2\pi\nu)^3} \frac{1}{(v\tau - ix)(v\tau - i\nu)^2} \int d\tau' \frac{\text{sgn}(\tau') - \text{sgn}(\tau' - i\nu)}{(v\tau - i\nu)^2} 
\]

\[
= -12i\sqrt{(2\pi\nu)^3} \frac{t}{(v\tau - ix)^2 + v} 
\]

(2.55)
By replacing $v\tau \to ((v\tau - ix) + (v\tau + ix))/2$ we can write $\delta G_R$ as

$$\delta G_R \propto -\frac{6\pi i \sqrt{(2\pi v)^3}}{v} \left( \frac{1}{(v\tau - ix)^{1+\nu}} + \frac{v\tau + ix}{(v\tau + ix)^{2+\nu}} \right)$$

(2.56)

With exactly the same calculations we will get results for left moving fields as

$$\delta G_L \propto -\frac{6\pi i \sqrt{(2\pi v)^3}}{v} \left( \frac{1}{(v\tau + ix)^{1+\nu}} + \frac{v\tau - ix}{(v\tau - ix)^{2+\nu}} \right)$$

(2.57)

Now by plugging all these results into Eq. (2.50), the final form of the correlation function to first order is given by

$$G_{\nu \bar{\nu}}(x, \tau) = \frac{1}{(v\tau - ix)^\nu(v\tau + ix)^\bar{\nu}} \{ 1 - \frac{4\pi^2 \eta_- \sqrt{v^3}}{v} \left( \frac{1}{v\tau - ix} + \frac{v\tau + ix}{(v\tau - ix)^2} \right) 
+ \frac{4\pi^2 \eta_- \sqrt{v^3}}{v} \left( \frac{1}{v\tau + ix} + \frac{v\tau - ix}{(v\tau + ix)^2} \right) \}$$

(2.58)

Now by taking the Fourier transform of Eq. (2.58) and continuing to real frequencies, we have

$$G_{\nu \nu}(\omega, q) = (\omega - vq)^{\nu-1}(\omega + vq)^{\bar{\nu}-1} \{ 1 - \frac{4\pi^2 \eta_- \sqrt{v^3}}{v} (\omega - vq) \left( 1 + \frac{\omega - vq}{\omega + vq} \right) 
+ \frac{4\pi^2 \eta_- \sqrt{v^3}}{v} (\omega + vq) \left( 1 + \frac{\omega + vq}{\omega - vq} \right) \}$$

(2.59)

Where $\eta_- \approx 1/m$. It is easily seen from the last term of Eq. (2.59) that, as $\omega$ approaches $vq$, the perturbative corrections blow up like $q^2/m(\omega - vq)$. This is exactly the reason that bosonization fails near the threshold. We also see that for $|\omega - vq| \gg q^2/2m$, perturbative corrections become small and we get the naive bosonization results, so we showed that irrelevant operators potentially will change the singularity exponent of correlation functions near the threshold but their effect is negligible away from the threshold so they would not change the qualitative shape of correlation function found by bosonization. In the following section by using the X-Ray edge method we find the singularity exponents of transverse spectral functions.
2.3 X-Ray Edge method

In sub-section 2.2.2 by use of standard bosonization we found that the transverse spectral functions $S^{+-}(\omega, q)$, for $q$ near 0 has a diverging singularity with exponent $1 - 2\eta$. In sub-section 2.2.3 we argued that band curvature operators would change the result of bosonization for singularity exponents. In this section we will explore this question by extending bosonization using X-ray edge methods introduced in [22, 23, 27, 29]. We find that by use of these methods, transverse spectral functions have different critical exponents at singular energies than predicted by standard bosonization. We also point out the existence of large numbers of sub-leading singularities with vanishing intensities, similar to the ones found by standard bosonization.

We use the notation and results of [22] and we skip the details of derivations; interested readers should see [22, 29] and also Appendix A for most detailed calculations. In this approach we try to evaluate transverse spectral functions for fixed momentum $q$ by including the effect of a single high-energy particle or hole excitation. To do this we need to find relevant momenta of this excitation which contributes to the spectral functions at momentum $q$. In this section we find the effective Hamiltonian for these excitations, and also those relevant momenta.

Suppose that the momentum of this particle or hole excitation is $k$. (We will eventually use the notation $k_p$ for a particle and $k_h$ for a hole.) In X-Ray edge method we are interested in the high energy excitations near this momentum $k$ and also low-energy excitations around the fermi points Fig. 2.6. Thus we can write the fermion operator in the following form

$$c_j \approx \psi_R e^{ik_j} + \psi_L e^{-ik_j} + d e^{ik_j}. \quad (2.60)$$

Where $\psi_R, \psi_L$ and $d$ vary slowly on lattice scale. Then by linearizing the dispersion around the fermi points and bosonizing low energy fermions, and also linearizing the dispersion around high-energy particle or hole excitation, we have

$$\mathcal{H} = d^\dagger (\varepsilon - iu\partial_x) d + \frac{v}{2} \left[ (\partial_x \psi_L)^2 + (\partial_x \psi_R)^2 \right] + \frac{1}{\sqrt{2\pi K}} (\kappa_L \partial_x \psi_L - \kappa_R \partial_x \psi_R) d^\dagger d$$

Where

$$\mathcal{H} = d^\dagger (\varepsilon - iu\partial_x) d + \frac{v}{2} \left[ (\partial_x \psi_L)^2 + (\partial_x \psi_R)^2 \right] + \frac{1}{\sqrt{2\pi K}} (\kappa_L \partial_x \psi_L - \kappa_R \partial_x \psi_R) d^\dagger d$$

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Figure 2.6: In beyond Luttinger models, in addition to low energy excitations we also include the effect of a high-energy particle or a deep hole. In this case we have a hole at momentum $k$.

Here the chiral fields $\varphi_L$ and $\varphi_R$ are the transformed ones defined by:

\[
\phi = \frac{\varphi_L - \varphi_R}{\sqrt{2}} \quad \text{and} \quad \theta = \frac{\varphi_L + \varphi_R}{\sqrt{2}}.
\]

This Hamiltonian is described in [47,49] for Luttinger liquid coupled to an impurity. The parameters of above Hamiltonian are as follows; $\varepsilon$ is the energy of the high energy particle or hole and, for $\Delta = 0$, it is given by $\varepsilon = -2J(\cos k - \cos k_F)$. $u$ is the velocity of the heavy particle or hole and equals $J \sin k$ at $\Delta = 0$. $v$ and $K$ are
the boson velocity and Luttinger parameter, respectively. $v$ may be regarded as the Fermi velocity of the interacting fermion model. It is the only velocity appearing in the standard bosonization approach and plays the role of the “velocity of light” in the effective Lorentz invariant field theory. The velocity parameter $u$, describing the high energy particle or hole is an important new parameter in the X-ray edge approach. Finally $\kappa_{R,L}$ are the couplings between high energy fermion and bosonic fields and to first order in $\Delta$ are given by

$$\kappa_{R,L} = 2\Delta \left[ 1 - \cos(k_F \mp k) \right].$$

These coupling could be evaluated by Bethe ansatz calculations\cite{9} for any $\Delta, H$ and $k$. They are important for finding the singularity exponents. Note that, in general, $u, \varepsilon$ and $\kappa_{R,L}$ all depend on $k$ as well as $\Delta$ and $h$.

The Hamiltonian (2.61) looks complicated as it contains interactions between fermions and bosons. We can eliminate the interacting part of (2.61) by doing a unitary transformation given by

$$U = \exp \left[ -i \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi K}} (\gamma_R \phi_R + \gamma_L \phi_L) \tilde{d}^\dagger \tilde{d} \right]$$

(2.61)

Effect of unitary transformation on bosonic and fermionic fields is as follows

$$\partial_x \phi_{R,L} = \partial_x \tilde{\phi}_{R,L} \mp \frac{\gamma_{R,L}}{\sqrt{2\pi K}} \tilde{d}^\dagger(x) \tilde{d}(x)$$

$$d = \tilde{d} \exp \left[ -i \frac{1}{\sqrt{2\pi K}} (\gamma_R \phi_R + \gamma_L \phi_L) \right]$$

$$\phi_{R,L} = \phi_{R,L} \mp \frac{\gamma_{R,L}}{4\sqrt{2\pi K}} \tilde{N}(x)$$

where $\tilde{N}(x)$ is defined by:

$$\tilde{N}(x) = \int_{-\infty}^{\infty} \operatorname{sgn}(x-y) \tilde{d}^\dagger(y) \tilde{d}(y) dy.$$ (2.62)

It is easy to see that unitary transformation leaves $\tilde{d}^\dagger(x) \tilde{d}(x)$ invariant and we can decouple fermionic fields from the bosonic ones with appropriate choice of $\gamma_{R,L}$, given by

$$\gamma_{R,L} = \frac{\kappa_{R,L}}{v \mp u}$$

(2.63)
Having done the unitary transformation the Hamiltonian will look like

\[ \mathcal{H} = \frac{\nu}{2} \left[ (\partial_t \Phi_L)^2 + (\partial_t \Phi_R)^2 \right] + d^\dagger (\epsilon - iu \partial_x) d + \cdots \]  

(2.64)

Where \( \cdots \) means higher dimension irrelevant interactions that will be produced by doing unitary transformation and which we ignore.

We now consider the transverse Green’s function:

\[ S^{-+} = \langle S_j(t) S_0^+ (0) \rangle. \]

By doing Jordan-Wigner transformation, we have

\[ S^{-+}_j (t) = e^{\pi j} \langle c_j(t) \cos[\pi N_j(t)] \cos[\pi N_0(0)] c_0^\dagger (0) \rangle \]

where \( c_j(t) \) is approximated as in Eq. (2.60) and

\[ N_j(t) = \sum_{l<j} c_l^\dagger (t) c_l (t) \]

To obtain the transverse spectral function, \( S^{-+}(q, \omega) \) at a wave-vector \( q \) far from the low energy regions, \( \pm H, \pi \), the term that we are interested in is

\[ S^{-+}_j (t) = e^{\pi j} e^{ik_p j} \langle d(j,t) \cos[\pi N_j(t)] \cos[\pi N_0(0)] d_0^\dagger (0,0) \rangle. \]  

(2.65)

We see that \( d \) must be chosen to be a particle operator and we have consequently labeled its momentum \( k_p \). Note that we have written the Jordan-Wigner string operator in manifestly Hermitian cos form, as in Sec. 2.2.2. Now we decompose
into c-number, non-oscillatory and oscillatory parts

\[
N_j(t) = \frac{k_F}{\pi} j + \tilde{n}(j,t) + m(j,t)
\]

\[
\tilde{n}(x,t) = \int_{x-E}^{x} dy : \psi_R^\dagger(y,t) \psi_R(y,t) : + : \psi_L^\dagger(y,t) \psi_L(y,t) : + d^\dagger(y,t) d(y,t)
\]

\[
m(x,t) = \int_{x-E}^{x} \left\{ \psi_R^\dagger(y,t) d(y,t) e^{i(k_F-k_p)y} + \psi_L^\dagger(y,t) d(y,t) e^{i(k_F+k_p)y} + \psi_L^\dagger(y,t) \psi_R(y,t) e^{2ik_Fy} + h.c. \right\}
\]

\[
\propto \left( \frac{1}{i(k_p-k_F)} \psi_R^\dagger(x',t) e^{-ik_Fx} + \frac{1}{i(k_F+k_p)} \psi_L^\dagger(x',t) e^{ik_Fx} \right) d(x',t) e^{ik_p x}
\]

\[
+ \frac{1}{2ik_F} \psi_L^\dagger(x',t) \psi_R(x',t) e^{2ik_Fx} + h.c.
\]

Where \( \epsilon \rightarrow 0^+ \), \( x' \equiv x - \epsilon \) and in the third line we used the fact that both \( \psi \) and \( d \) are slowly varying fields and most of the contribution of the integral comes from limiting point \( x - \epsilon \). At this point we will set the rapidly oscillating term, \( m(x,t) \), to zero. This will give the dominant divergent singularity in the transverse spectral function. By Taylor expanding in powers of \( m(x,t) \) we obtain various vanishing singularities as well as unimportant renormalizations of the amplitude of the divergent singularity, as we discuss in Sec IV. We may then decompose \( \tilde{n}(x,t) \) into its commuting high energy and Fermi surface part.

\[
\tilde{n}(x,t) \equiv n(x,t) + n_d(x,t)
\]

\[
n(x,t) \equiv \int_{x-E}^{x} : \psi_R^\dagger(y,t) \psi_R(y,t) : + : \psi_L^\dagger(y,t) \psi_L(y,t) :
\]

\[
n_d(x,t) \equiv \int_{x-E}^{x} d^\dagger(y,t) d(y,t) dy.
\]

Because all the \( d \) operators in \( \tilde{n}(x,t) \) are at points \( y < x \), we have

\[
[\tilde{n}(x,t), d(x,t)] = 0
\]

and thus we may drop the \( n_d \) terms leaving:

\[
S_j^{++}(t) \propto e^{i(k_Fx_j)} \langle \cos[k_F j + \pi n(j,t)] d(x,t) d^\dagger(0,0) \cos[\pi n(0,0)] \rangle
\]

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Following Eq. (2.36) this becomes:

\[ S_j^+ (t) \propto e^{i(k_F + \pi)j} \langle \cos[k_F j + \sqrt{\pi K} \phi(j,t)]d(j,t)d^\dagger(0,0) \cos[\sqrt{\pi K} \phi(0,0)] \rangle. \]

Note that we have treated the Jordan-Wigner string operator in precisely the same approximation as in the standard bosonization approach. We now make the unitary transformation of Eq. (2.62) so that the fermion and bosons are decoupled. Noting that \( \tilde{N}(x,t) \) annihilates the vacuum this leaves:

\[ S_j^+ \propto \langle \tilde{d}(x,t) \cos[k_F x + \sqrt{\pi K} \tilde{\phi}(x,t)]e^{\frac{i}{\sqrt{2\pi}}[\pi \phi_R(x,t) + \pi \phi_L(x,t)]}e^{\frac{i}{\sqrt{2\pi}}[\pi \phi_R(0,0) + \pi \phi_L(0,0)]} \cos[\sqrt{\pi K} \tilde{\phi}(0,0)]d^\dagger(0,0)e^{i(k_F - \pi)x} \]

Separating the fermionic and bosonic factors, this becomes:

\[ S_j^+ (t) = S^{0-+}(x,t)\langle \tilde{d}(x,t)d(0)\rangle \]  

(2.66)

where \( x = j \),

\[ S^{0-+}(x,t) = e^{i(\pi + k_F)x}I_-(x,t) + e^{i(\pi + k_F)x}I_+(x,t) \]

(2.67)

and

\[ I^+_R(x,t) = \langle e^{-i\sqrt{2\pi v_F^R} \phi_R(x) + i\sqrt{2\pi v_F^L} \phi_L(x)}e^{i\sqrt{2\pi v_F^R} \phi_R(0) - i\sqrt{2\pi v_F^L} \phi_L(0)} \rangle \]

\[ I^+_L(x,t) = (\frac{\epsilon}{\epsilon + i v_F - i x})^{v_R^+} (\frac{\epsilon}{\epsilon + i v_F + i x})^{v_L^+} \]

\[ I^-_R(x,t) = \langle e^{i\sqrt{2\pi v_F^R} \phi_R(x) - i\sqrt{2\pi v_F^L} \phi_L(x)}e^{-i\sqrt{2\pi v_F^R} \phi_R(0) + i\sqrt{2\pi v_F^L} \phi_L(0)} \rangle \]

\[ I^-_L(x,t) = (\frac{\epsilon}{\epsilon + i v_F - i x})^{v_R^+} (\frac{\epsilon}{\epsilon + i v_F + i x})^{v_L^+} \]  

(2.68)
Where \( \epsilon \) is of order of the lattice spacing and \( v^\pm_{R,L} \) are defined as follow

\[
v^\pm_R = \frac{1}{4} \left( \frac{\gamma_R}{\pi \sqrt{K}} \pm \sqrt{K} \right)^2 \]

\[
v^\pm_L = \frac{1}{4} \left( \frac{\gamma_L}{\pi \sqrt{K}} \mp \sqrt{K} \right)^2 .
\]  

(2.69)

At zero magnetic field we have \( \gamma_{R,L}/\pi = 1 - K \),\(^\text{[29]}\) independent of momentum, so the results will simplify to

\[
v^\pm_R = \frac{1}{4K} (1 - K \pm K)^2 \]

\[
v^\pm_L = \frac{1}{4K} (1 - K \mp K)^2 .
\]  

(2.70)

Having done the unitary transformation, the \( \bar{d} \) fields act as free particle so we have

\[
\langle \bar{d}(x,t)\bar{d}^\dagger(0) \rangle \approx e^{-i\epsilon(k_p)t} \int_{-\Lambda}^\Lambda \frac{dk}{2\pi} e^{ik(x-ut)} \approx e^{-i\epsilon(k_p)t} \delta(x - ut). \]  

(2.71)

We can now turn to the question of how the momentum of the high energy particle, \( k_p \), should be chosen to study \( S^{-+}(q,\omega) \) near the threshold for arbitrary \( q \). From Eq. (2.67) we see that a high energy particle of momentum \( k_p \) gives terms in the transverse Green’s function oscillating at wave-vectors \( \pi + k_p - k_F \) and \( \pi + k_p + k_F \). Thus we see that there may actually be two choices for \( k_p \) which will give a contribution to the transverse Green’s function oscillating at a specified wave-vector \( q \):

\[
k^\pm_p \equiv q + \pi \mp k_F .
\]  

(2.72)

In general, both must be considered in calculating the singularity behaviour of \( G^{-+}(q,\omega) \). However, the \( k_p \)'s are restricted by the requirement that they are allowed particle momenta,

\[
k_F < k_p < 2\pi - k_F , \quad \text{(mod } 2\pi\text{)}.
\]  

(2.73)

(Recall that \( k_F = \pi/2 + \pi m > \pi/2 \).) Thus we see that the high energy particle of momentum \( k^+_p \) contributes to \( S^{-+}(q,\omega) \) for \( q \) in the range \( [2k_F - \pi, \pi] \) and the
particle of momentum $k_p^-$ contributes for $q$ in the range $[-\pi, \pi - 2k_F]$. For a given $q$ there is at most one possible high energy particle momentum contributing to $S^{-+}(q, \omega)$. Having identified the appropriate high energy particle momentum we may now complete the calculation by Fourier transforming Eq. (2.66) using Eqs. (2.68)-(2.71). The result is:

$$ S^{-+}(q, \omega) \propto \int dx dt \frac{e^{i(\omega - \epsilon(k_p^+))t}}{(vt - x - i\epsilon)^{\nu_k^+} (vt + x + i\epsilon)^{\nu_k^-}} \delta(x - ut), \quad (2k_F - \pi < q < \pi) $$

$$ S^{-+}(q, \omega) \propto \int dx dt \frac{e^{i(\omega - \epsilon(k_p^-))t}}{(vt - x - i\epsilon)^{\nu_k^-} (vt + x + i\epsilon)^{\nu_k^+}} \delta(x - ut), \quad (-\pi < q < \pi - 2k_F). $$

(2.74)

The $x$-integrals may be done trivially using the $\delta$-functions.

$$ S^{-+}(q, \omega) \propto \int dt \frac{e^{i(\omega - \epsilon(k_p^+))t}}{[(v - u)t - i\epsilon]^\nu_k^+ [(v + u)t + i\epsilon]^\nu_k^-}, \quad (2k_F - \pi < q < \pi) $$

$$ S^{-+}(q, \omega) \propto \int dt \frac{e^{i(\omega - \epsilon(k_p^-))t}}{[(v - u)t - i\epsilon]^\nu_k^- [(v + u)t + i\epsilon]^\nu_k^+}, \quad (-\pi < q < \pi - 2k_F). $$

(2.75)

The $t$-integrals can now be done by contour methods. Note that, if $v > u$, they are only non-zero for $\omega > \epsilon(k_p^+)$ and $\omega > \epsilon(k_p^-)$ respectively, corresponding to a lower threshold. Using the free particle cosine dispersion relation $v > u$ is always satisfied for particle excitations. While this dispersion relation is known to be exact, apart from an overall factor, including interactions for $\hbar = 0$ it is in general modified. We might expect that $v > u$ remains true for particles, at least for small enough $\hbar$. However, see below. Assuming this, we obtain:

$$ S^{-+}(q, \omega) \propto \frac{\theta(\omega - \omega_L(q))}{|\omega - \omega_L(q)|^{\mu(q)}} $$

(2.76)

where the singular energies are given by:

$$ \omega_L(q) = \epsilon(k_p^+), \quad (2k_F - \pi < q < \pi) $$

$$ = \epsilon(k_p^-), \quad (-\pi < q < \pi - 2k_F). $$

(2.77)
The critical exponents are given by

\[ \mu(q) = 1 - v_R^+(k_p^+) - v_L^+(k_p^+), \quad (2k_F - \pi < q < \pi) \]

\[ = 1 - v_R^-(k_p^-) - v_L^-(k_p^-), \quad (-\pi < q < \pi - 2k_F) \tag{2.78} \]

with \(v_{R,L}^\pm(k)\) given by Eqs. (2.69) and (2.70). Note that the same phase shift parameters \(\gamma_{R,L}\) determine both longitudinal and transverse spectral functions; however we need to know them at the momentum of the high energy particle or hole which is not the same for longitudinal and transverse spectral functions, for given \(q\). In general, the phase shift parameters depend on momentum as well as field, becoming momentum independent at \(h = 0\). It follows from parity that \(\kappa_L(k) = \kappa_R(-k)\).

Since, for \(q > 0\), \(k_p^-(-q) = -k_p^+(q)\), (mod 2\(\pi\)) \(v_L^-(q) = v_R^+(q)\) and \(v_R^-(q) = v_L^+(q)\) and hence \(\mu(-q) = \mu(q)\).

It is interesting to compare both the singular energies and exponents to those predicted by standard bosonization as \(q\) approaches the zero energy points \(q \approx \pm H = \pm(2k_F - \pi)\) and \(q \approx \pi\). Near these zero energy points we may linearize the \(\epsilon(k)\) giving: \(\omega_L(q) \approx v|q + H|\) and \(v|q - \pi|\), precisely the singular energies predicted by standard bosonization. This X-ray edge calculation also confirms the conjecture made in Sec. 2.2.2 that the diverging singular energies at the different low energy momenta are smoothly connected. On the other hand, the exponents appear to disagree with the standard bosonization results for all \(\Delta\) and \(h\), a similar observation to the one in Ref. [25]. This can be seen, for example, by considering the limit \(\Delta \rightarrow 0\). In this case \(\gamma_{L,R}^\pm \rightarrow 0, K \rightarrow 1\) so \(v_{L,R}^\pm \rightarrow 1/4\) and \(\mu \rightarrow 1/2\), for all \(q\) and \(h\). On the other hand the standard bosonization result from Eq. (2.40) and (2.41) is \(\eta \rightarrow 1/8\) and hence \(\mu \rightarrow 3/4\). We can also compare the zero field predictions for general \(\Delta\). From Eq. (2.70)

\[ \mu = 2 - 1/(2K) - K, \quad (h = 0, \forall q). \tag{2.79} \]

On the other hand, standard bosonization predicts \(\mu = 1 - 2\eta = 2 - 1/(4K) - K\) for \(q \approx 0\) and \(\mu = 1 - 1/(4K)\) for \(q \approx \pi\). We expect that standard bosonization fails to predict critical exponents correctly for the transverse spectral function, as
discussed in sub-section 2.2.3. Given this situation, it is useful to check the SU(2) symmetric case, \( h = 0, \Delta = 1 \). In this case X-ray edge methods predict, from Eq. (2.79) \( v_R^- = v_L^+ = 0, v_R^+ = v_L^- = 1/2, \mu = 1/2 \) for the transverse spectral function independent of \( q \). The same exponents were found earlier[29] for the longitudinal spectral function [50] (In this case, they agree with standard bosonization near \( q = \pi \) but not near \( q = 0 \).)

By doing similar calculations we could find \( S^{+-} \), which is different than \( S^{-+} \) for \( h \neq 0 \). Following the same procedure, Eq. (2.66) is replaced by:

\[
S^{+-} \propto \langle d^\dagger(x,t) e^{i\pi H} \rangle e^{-i\sqrt{2\pi K} (\gamma \bar{\phi} + \bar{\phi} \gamma)} e^{-i\sqrt{2\pi K} (\gamma \bar{\phi} + \bar{\phi} \gamma)} e^{i(-k_h + \pi)x}
\]

where \( d \) now annihilates a particle in a filled state below the Fermi energy with momentum \( k_h \), i.e. creates a hole. This can again be factorized as:

\[
S^{+-}_j(t) = S^{(0)+-}(x,t) \langle d^\dagger(x,t) d(0) \rangle (2.80)
\]

where

\[
S^{(0)+-}(x,t) = e^{i(\pi - k_h + k_F)x} I^-(x,t) + e^{i(\pi - k_h - k_F)x} I^+(x,t) (2.81)
\]

and \( I^\pm(x,t) \) are the same functions defined in Eq. (2.68), except that \( k_h \) must lie in a different range, \( |k_h| < k_F \). Thus defining:

\[
k_h^\pm \equiv \pi - q \pm k_F (2.82)
\]

we see that the first term in Eq. (2.81) is non-zero for \( q \) in the range \([\pi - 2k_F, \pi]\) while the second is non-zero for \( q \) in the range \([-\pi, 2k_F - \pi]\). These are wider ranges than occur in \( S^{-+} \). (Recall that we assume \( H \geq 0 \) and hence \( k_F \geq \pi/2 \).) In particular, both terms can contribute for \( |q| < H \). Again, as \( q \) approaches the zero energy points, \( \pm H \) and \( \pi \) the singular energies approach those predicted by standard bosonization. Again as anticipated in sub-section 2.2, the singular energies at these zero energy points can be smoothly connected.

Another interesting feature is the shape of the singularity. For \( S^{-+} \) the singularity was one-sided, vanishing for \( \omega < \omega_L \). This was a consequence of the fact
that the velocity of the high energy particle always obeys $u < v$ assuming this feature of the non-interacting dispersion relation is unchanged by interactions. On the other hand for holes, again using the non-interacting dispersion relation, $u < v$ is only obeyed if $|k_h| < \pi - k_F$; there is a range of hole momentum near $k_F$ where the high energy hole has a higher velocity than the Fermi velocity. $|k_h^+| < \pi - k_F$ corresponding to $0 < q < 2\pi - 2k_F = \pi - H$. Thus, in this region the singularity is one-sided, $\propto \theta(\omega - \omega_L)$. On the other hand for $-H < q < 0$ and $\pi - H < q < \pi$, where $u > v$ the integral in Eq. (2.75) is also non-zero and gives the same critical exponent with a different amplitude for $\omega < \omega_L$. In this case we see that $\omega_L(q)$ is not a lower threshold. There is also spectral weight below this frequency. The qualitative shape of $S^{+-}(q, \omega)$ for $0 < q < H$ is sketched in Fig. [2.7].

We emphasize that a singularity is one-sided for $u < v$ and two-sided for $u > v$ where $v$ is the Fermi velocity and $u$ is the velocity of the high energy particle or hole. In general, these velocities depend on $\Delta$ and also $h$, being strongly renormalized by interactions. In [28], Fig. [15], it was illustrated that for $\Delta = 1$ and small non-zero field one of the cubic term in the bosonized Hamiltonian, due to band curvature effects, has a coupling constant $\eta_- < 0$. This may indicate a reversal of the sign of the effective mass due to (strong) interaction effects, implying a reversal of the sign of $u - v$ as the energy of the high energy particle or hole approaches the Fermi energy, corresponding to $|q| \rightarrow |2k_F - \pi|$ (or $q \rightarrow \pi$). Thus in this parameter range, the one-sided and two-sided nature of the 3 singularities in $S^{+-}$ and $S^{-+}$, discussed above, would be reversed.

Given that the singular energy, $\omega_L(q)$ is sitting inside a region of non-zero spectral weight, for certain ranges of $q$, we might ask whether it is reasonable to expect singular behaviour at this energy or whether the infinite peak might be broadened and made finite due to some sort of decay process for this high energy excitation. This important question also arises for the longitudinal structure function and for the fermion spectral function. It has been suggested [22, 26] that integrability might prevent this excitation from decaying, for some range of momentum, even though it is kinematically allowed, leaving the singularity intact. This is true because three-body scattering processes are required for it to decay and these are expected not to occur in this integrable model. This seemed to be consistent with Density Matrix Renormalization Group results for the fermionic spectral function.
Figure 2.7: The behaviour of $S^{+−}(\omega, q)$ correlation for $|q|<H$. There are two different hole excitations which contribute to the spectral function; the lower energy hole produces a cusp-like singularity.

In fact, we should also consider processes in which the heavy particle or hole decays by producing 3 other high energy quasi-particles, a 2-body process which is expected to be present even in this integrable model. Using the $-\cos k$ dispersion relation, this is kinematically allowed for high energy holes[51] in the region $u<v$, corresponding to $0<|q|<\pi−H$ (the upper branch for $0<|q|<H$) but not allowed for high energy particles for any $q$[22].

Putting these observations together, we expect the sharp one-sided singularity of $S^{−+}(q, \omega)$ to be present for $H<|q|<\pi$ and the 2-sided singularity of $S^{+−}(q, \omega)$ for $0<|q|<H$ and $\pi−H<|q|<\pi$ to be present. The one-sided singularity of $S^{++}$ for $H<|q|<\pi−H$ should be broadened by higher order interaction effects[22].
not taken into account in this treatment. See Fig. [2.8]. Again we emphasize
that the precise region of \( q \) over which singularities are broadened depends on the
dispersion relation, which is modified by interactions; here we have just stated it
using the \( -\cos k \) dispersion relation, valid at small \( \Delta \).

So far, we have set the rapidly oscillating operator \( m(x,t) \), defined in Eq. (2.66)
to zero. The effects of including it are discussed in the following section. It basic-
ally leads to additional terms in the transverse spectral function which have singu-
larities at different energies, including lower ones. However, these singularities are
of vanishing type, with exponent \( \mu < 0 \), dashed lines of Fig. [2.8]. The relatively
simple approach we have taken here is just sufficient to give the diverging singular
terms.

The situation is considerably simpler at zero field, \( h = 0 \). In this case, the free
dispersion relation is known to be exact, apart from an overall change of ampli-
tude, \( 2t \rightarrow v \). Thus the condition \( u < v \) is always satisfied so \( S^{++} = S^{+-} \) has only
one single-sided singularity at \( \omega_L = v \sin q \) with \( v \) given in Eq. (2.31) and critical
exponent given by Eq. (2.79). In this case, no decay processes are kinematically
allowed and no additional singularities occur, since the single hole or particle has
the lowest possible energy for given wave-vector.

### 2.4 Sub-dominant singularities

In Sec. 2.4 and 2.3 we ignored rapidly oscillating terms, \( m(x) \) of Eq. (2.65) in
the Jordan-Wigner string operator in calculating the transverse structure function
and also the effects of Umk depletion term which oscillates as \( e^{i4k_F x} \). We consider the
effect of including these terms here. Let us begin with the term:

\[
m(x) = \frac{1}{2ik_F} \psi_L^\dagger(x',t) \psi_R(x',t) e^{2ik_F x} + h.c.
\]  

Actually, this term represents a correction to standard bosonization, even without
using X-ray edge methods, so we consider its effects there. To make things as
simple as possible we also consider zero field, \( k_F = \pi/2 \). Then, after bosonizing
Figure 2.8: Singular points of zero temperature transverse spectral functions of the XXZ model, predicted by X-ray edge method. The solid lines indicate diverging singularities and dashed line the vanishing singularities. The grey thick line indicates the range of momentum over which interactions should broaden the diverging singularity. In Fig. [2.8a] and [2.8b] the lower dashed line is given by particle excitations and upper one is given by hole excitation.
The standard bosonized expression for $S^-$ in Eq. (2.38) is modified to:

$$S_j^- \propto e^{-i\sqrt{\pi/\theta(x)}} \left[ C(-1)^j + C^- \cos(\sqrt{4\pi K} \phi(x)) \right] \times \exp[i(-1)^j C' \sin(\sqrt{4\pi K} \phi(x))] \times \exp[i C e^{2i k_F j + i\sqrt{4\pi K} \phi(x)} + h.c.] \right]. \quad (2.84)$$

for a non-universal constant $C'$. We now Taylor expand the exponential and use double angle formulas. We see that the staggered and uniform parts of $S_j^-$ have a series in increasingly irrelevant operators:

$$S_s^- = e^{-i\sqrt{\pi/\theta(x)}} \sum_{n \in \mathbb{Z}} a_{2n} e^{i 2n \sqrt{4\pi K} \phi}$$

$$S_u^- = e^{-i\sqrt{\pi/\theta(x)}} \sum_{n \in \mathbb{Z}} a_{2n+1} e^{i(2n+1) \sqrt{4\pi K} \phi}. \quad (2.85)$$

The effect of including the $e^{im}$ factor is simply to renormalize the coefficient of the leading operator in $S_u^-$ and $S_s^-$ together with producing the irrelevant corrections. Now consider non-zero field. Eq. (2.84) get replaced by:

$$S_j^- \propto e^{-i\sqrt{\pi/\theta(x)}} \left[ C(-1)^j - C^- \cos((2k_F - \pi) j + \sqrt{4\pi K} \phi(x)) \right] \times \exp[i C' e^{2i k_F j + i\sqrt{4\pi K} \phi(x)} + h.c.]. \quad (2.86)$$

We again get a series of irrelevant operators but now all at different wave-vectors:

$$S_j^- = e^{-i\sqrt{\pi/\theta(x)}} \sum_{n \in \mathbb{Z}} a_n e^{i(2nk_F + \pi) j + in \sqrt{4\pi K} \phi}. \quad (2.87)$$

It is interesting to note that this expansion contains precisely the same terms as the one derived by Haldane[15] for a boson annihilation operator in a Luttinger liquid. We also see why the replacement of the exponential Jordan-Wigner string operator by a cosine form, its Hermitian part, is not really necessary. Keeping the complete expansion in Eq. (2.87), we get the same set of operators either way.

Now consider the effect of the term in Eq. (2.83) in the X-ray edge approach. After the unitary transformation of Eq. (2.62) the term in $S_j^-$ linear in the $\vec{d}$ opera-
tor, with momentum $k$, is:

$$S_j \propto d e^{\frac{i}{\sqrt{2\pi}}(\gamma_R \phi_R + \gamma_L \phi_L)} \sum_{n \in \mathbb{Z}} a_n e^{i[(2n+1)k_F + \pi + k]j + i(2n+1)\sqrt{2\pi}k_R}. \tag{2.88}$$

This expansion is similar to the one derived by Haldane\cite{15} for a fermion annihilation operator. The momentum $q$ at which the $n^{th}$ term contributes to the spectral function is:

$$q = (2n+1)k_F + \pi + k \tag{2.89}$$

where the momentum $k$ must correspond to that of a high energy hole, $|k| < k_F$ in calculating $S^+$ or to that of a high energy particle, $k_F < |k| < \pi$, in calculating $S^-$. Note that by ignoring $m(x)$ in Sec. 2.2.2 we only considered the $n = 0$ and $n = -1$ terms in the sum of Eq. (2.88). The $n^{th}$ term in the expansion of $S_j^-$ in Eq. (2.88) leads to a singular term in the transverse spectral function,

$$S(q, \omega) \propto \frac{1}{|\omega - \omega(q)|^\mu} \tag{2.90}$$

at the energy $\omega(q)$ given by the energy of the corresponding particle or hole:

$$\omega_n(q) = \pm \varepsilon [q - (2n+1)k_F - \pi]. \tag{2.91}$$

We see that, for general $k_F$, these thresholds can occur at arbitrarily low energy. (For rational $k_F$ there is a finite number of them and there a lowest one at a non-zero energy.) The corresponding critical exponent is given by:

$$\mu^{(n)} = 1 - \nu^{(n)} + \nu^{(n)} \tag{2.92}$$

where $\nu^{(n)}_{L,R}$ are the left and right scaling dimension of the $n^{th}$ operator in Eq. (2.88). These obey:

$$\nu^{(n)}_{L,R} \quad = \quad \frac{1}{4} \left[ \left( \frac{\gamma_R}{\pi \sqrt{K}} + (2n+1)\sqrt{K} \right)^2 + \left( \frac{\gamma_L}{\pi \sqrt{K}} - (2n+1)\sqrt{K} \right)^2 \right]$$

$$= \frac{1}{2} \left[ (2n+1)\sqrt{K} + \frac{\gamma_R - \gamma_L}{2\pi \sqrt{K}} \right]^2 + \frac{1}{2} \left( \frac{\gamma_L + \gamma_R}{2\pi \sqrt{K}} \right)^2. \tag{2.93}$$
Thus the two largest values of $\mu$ occur for $n = 0$ and $-1$ for $|\gamma_R - \gamma_L|/(2\pi K) < 1$. At zero field, $\gamma_L = \gamma_R$ so this condition is satisfied. Also at small $\Delta$, $\gamma_{L,R}$ are $O(\Delta)$ so the condition is again satisfied. It should remain satisfied for a large range of field and $\Delta$ quite possibly including the entire Luttinger liquid regime, but without determining the $\gamma_{L,R}$ explicitly we can’t determine this range. It certainly includes weak fields $h \ll J$ relevant to most ESR experiments. For zero field we have explicitly:

$$v_R^{(n)} + v_L^{(n)} = \frac{K}{2} (2n + 1)^2 + \frac{(1 - K)^2}{2K}$$ (2.94)

so we see that the exponents for sub-dominant singularities ($n \neq 0, -1$) obey $\mu < -3/2$ for all $K$ in the Luttinger liquid regime $K > 1/2$. At $\Delta = 0$,

$$v_R^{(n)} + v_L^{(n)} = \frac{1}{2} (2n + 1)^2$$ (2.95)

and $\mu < -7/2$ for all sub-dominant singularities. We expect that $\mu < 0$ for all sub-dominant singularities a wide range of field and $\Delta$ including the weak field regime. So the approximation of dropping $m(x)$ made in sub-section 2.2.2 appears quite generally valid.

However, we must also consider the other terms in $m \propto \psi_R^\dagger d$, $\psi_L^\dagger d$. These give contributions to the transverse spectral functions proportional to matrix elements in the $\tilde{d}$ space containing more operators. Consider, for example, the case of a high energy particle. Then, to first order in these operators we either obtain $\tilde{d}(-\epsilon)\tilde{d}^\dagger(0)|0> = 0$ or else a matrix element:

$$\langle 0|\tilde{d}(x,t)\tilde{d}(x-\epsilon,t)\tilde{d}^\dagger(-\epsilon)\tilde{d}^\dagger(0)|0\rangle.$$ (2.96)

In fact, this is also zero as $\epsilon \to 0$ as follows from Wick’s theorem and translation invariance:

$$\langle 0|\tilde{d}(x,t)\tilde{d}(x-\epsilon,t)\tilde{d}^\dagger(-\epsilon)\tilde{d}^\dagger(0)|0\rangle =$$

$$\{ \langle 0|\tilde{d}(x,t)\tilde{d}^\dagger(0,0)|0\rangle^2 - \langle 0|\tilde{d}(x-\epsilon,t)\tilde{d}^\dagger(0,0)|0\rangle^2 \} \xrightarrow{\epsilon \to 0} 0.$$ (2.97)

Now consider the higher order expansion in the terms in $m$ proportional to $\tilde{d}$ and
\( \bar{d} \). Even orders in the expansion give

\[
[\bar{d}(-\epsilon)\bar{d}(-\epsilon)]^{n}\bar{d}^{\dagger}(0)|0\rangle \propto \bar{d}^{\dagger}(0)|0\rangle. \tag{2.98}
\]

The factor in the Green’s function involving Fermi surface excitations has \( S^- \) dressed by \( n \psi_{L,R} \) operators and \( n \psi_{L,R}^{\dagger} \) operators, all at the same point. The \((\psi_{L}^{\dagger}\psi_{R})^{n}\) and \((\psi_{R}^{\dagger}\psi_{L})^{n}\) terms just give contributions the same as Eq. (2.88), modifying the \( a'_n \) coefficients. Other products give higher dimension operators using:

\[
\psi_{L}^{\dagger}\psi_{L} \propto A + B\partial_{x}\phi_{R} + C\partial_{x}\phi_{L} \tag{2.99}
\]
et cetera. Odd terms in the expansion in the terms in \( m \), which are proportional to \( \bar{d} \) and \( \bar{d}^{\dagger} \), give zero as \( \epsilon \to 0 \), since they are proportional to the same matrix element, Eq. (2.96).

Till now we have considered the effect of particle excitation on \( S^{--} \). In general high-energy hole excitations, also could contribute to \( S^{--} \) as well as particle excitations to \( S^{+-} \). Now we will find the effect of hole excitations on \( S^{--} \). Hole excitations only give us higher order corrections to \( S^{+-} \), which have sub-dominant singularities, but to complete our discussion we find the vanishing singularity exponent of hole excitation to \( S^{+-} \); similar argument holds for particle excitation effects on \( S^{+-} \). In addition to the Eq. (2.65), there is another term which contributes to \( S^{+-} \) of the following form

\[
S^{+-}_{j}(t) = e^{i\pi j}e^{ik_{j}}\langle\psi_{R}(j,t)\cos[\pi N_{j}(t)]\cos[\pi N_{0}(0)]\psi_{R}^{\dagger}(0,0)\rangle. \tag{2.100}
\]

by similar argument as discussed in section [2.3] we could do the canonical and unitary transformations to decouple bosonic fields from high-energy excitations. Now the zero order term gives us the naive bosonization results; the interesting contribution comes from the first order expansion of \( m \propto \psi_{R}^{\dagger}d_{h}, \psi_{L}^{\dagger}d_{h} \), where \( d_{h} \) is hole creation operator. The first order correction of expansion has the following
form

\[ S^{-+} \approx \langle \bar{\psi}_R(x,t) \bar{\psi}_R(x,\xi,t) d_R^{\dagger}(x,\xi,t) \cos[k_F x + \sqrt{\pi K} \phi(x,t)] \times \]

\[ e^{i\sqrt{2\pi K} [\bar{\psi}_R(0,0) + \gamma_R \phi_0(x,t)]} e^{i\sqrt{2\pi K} [\bar{\psi}_R(0,0) + \gamma_L \phi_L(x,t)]} \times \]

\[ \cos[\sqrt{\pi K} \phi(0,0)] d_R(\xi,0) \bar{\psi}_R(\xi,0) \bar{\psi}_R(0,0) e^{i[2k_F - k_h + \pi]x} \]

Similar to Eq. (2.67) we could decompose \( S^{-+} \) to two terms as follow

\[ S^{-+}(x,t) = e^{i(\pi - k_h + k_F)x} I_h^-(x,t) + e^{i(\pi - k_h + 3k_F)x} I_h^+(x,t) \]  \hspace{1cm} (2.101)

where the expression for \( I_h^\pm \) is similar to Eq. (2.68) with exponents given by

\[ \nu_R^\pm = \frac{1}{4} \left( \frac{\gamma_R}{\pi \sqrt{K}} + \frac{2}{\sqrt{K}} + (2 \pm 1) \sqrt{K} \right)^2 \]

\[ \nu_L^\pm = \frac{1}{4} \left( \frac{\gamma_L}{\pi \sqrt{K}} + \frac{2}{\sqrt{K}} - (2 \pm 1) \sqrt{K} \right)^2 \]  \hspace{1cm} (2.102)

In general, the higher order correction will include more powers of \( \psi_R \psi_L \) and general expression would be

\[ \nu_R^{(n)\pm} = \frac{1}{4} \left( \frac{\gamma_R}{\pi \sqrt{K}} + \frac{2}{\sqrt{K}} + (2n \pm 1) \sqrt{K} \right)^2 \]

\[ \nu_L^{(n)\pm} = \frac{1}{4} \left( \frac{\gamma_L}{\pi \sqrt{K}} + \frac{2}{\sqrt{K}} - (2n \pm 1) \sqrt{K} \right)^2 \]  \hspace{1cm} (2.103)

with momentum given by

\[ k^{(n)} = \pi - k_h + (2n + 1)k_F \]  \hspace{1cm} (2.104)

and the energy of the excitation for given momentum \( q \) is

\[ \omega_n(q) = \pm \varepsilon [-q + (2n + 1)k_F + \pi] \].  \hspace{1cm} (2.105)

\( \omega_n \) and \( \bar{\omega}_n \) for \( n = 1 \), are depicted by dashed lines in Fig(2.8), which represents
vanishing singularities of spectral function. The sum of exponents is

\[ \tilde{\nu}^{(n)} + \tilde{\nu}^{(n)} = \frac{1}{2} \left[ (2n + 1) \sqrt{K} + \frac{\gamma_R - \gamma_L}{2\pi \sqrt{K}} \right]^2 + \frac{1}{2} \left( \frac{\gamma_L + \gamma_R}{2\pi \sqrt{K}} + \frac{2}{\sqrt{K}} \right)^2 \] (2.106)

We see that our results Eq. (2.93) and (2.106) are the same as Eq. (17) of Ref [27], which is the singularity exponent for boson creation operator, upon identifying \( \delta_{\pm} \rightarrow \gamma_{R/L}/\sqrt{K} \). The actual values of these phase shift parameters are in general different in the two models however, being determined by Galilean invariance in the Bose gas model. This correspondence might have been anticipated since a boson creation operator is related to the corresponding fermion one by a Jordan-Wigner string operator[15] just as is the \( S^+_j \) operator. Furthermore, the XXZ model is equivalent to a lattice boson model with an infinite on-site repulsion which restricts the occupancy to 0 or 1.

Now we look at the effect of Umklapp scattering term at zero magnetic field. The Umklapp scattering term is in the following form

\[ H_U = -g \left[ e^{-4ik_Fx} \psi_R^\dagger(x) \psi_R(x) \psi_L(x) \psi_L(x) + h.c \right] \] (2.107)

At non-zero magnetic field we could ignore this term as it is highly oscillatory, due to \( e^{i4k_Fx} \) prefactor. At zero field we have \( 4k_F = 2\pi \); thus this term does not oscillate and we need a more careful treatment. In the bosonized form of the XXZ model, it can be seen that the Umklapp term is irrelevant for \( 0 < \Delta < 1 \), and is marginal for \( \Delta = 1 \), thus in this regime we could look at the effect of this term perturbatively.

We focus on the effect of this term on \( S^{-+} \). In general the higher order Umklapp term could be written as follow

\[ U_{2\tilde{m} + m} = \prod_{i=1}^{m+\tilde{m}} (\psi_R^\dagger(z_i))^2 (\psi_L(z_i))^2 \prod_{j=1}^{\tilde{m}} (\psi_L^\dagger(z_j'))^2 (\psi_R(z_j'))^2 \] (2.108)

Where \( m \) and \( \tilde{m} \) are arbitrary integers, and this term is actually \( 2\tilde{m} + m \) order in the Umklapp perturbation. These operators gives us zero corrections unless we keep higher powers of the \( m(x) \) term, Eq. [2.83], at least to power \( 2m \). Thus the
most general non-zero term of both Umklapp and oscillatory term \( m(x) \) is in the following form

\[
P_{n,m,\tilde{m}} = U_{2\tilde{m}+m}(\psi_L^\dagger(x)\psi_R(x))^m(\psi_L^\dagger(0)\psi_R(0))^m
\]  

(2.109)

Now by bosonizing the above expression and plugging it into the definition of \( S^{-+} \) we have

\[
S^{-+} \propto \int \langle \bar{d}(x) \cos(k_F + \sqrt{\pi K}\phi(x))e^{\frac{1}{\sqrt{2\pi K}}} (\gamma_R\phi_L(x) + \gamma_L\phi_R(x)) e^{i\sqrt{4\pi K}m-\tilde{m})\phi(x)} \cos(\sqrt{\pi K}\phi(0)) \rangle
\]

\[
e^{-\frac{i}{2\sqrt{4\pi K}}\Sigma^m+\tilde{m}\phi(z_j)} e^{i\sqrt{4\pi K}\Sigma^\tilde{m}\phi(y_j)} e^{i\sqrt{4\pi K}(n+m)\phi(0)} d^\dagger(0) \prod d^2 y_j \prod d^2 z_j
\]

The effect of this term on the singularity exponents of \( S^{-+} \) could be evaluated by power counting and the result is given by the following expression

\[
v_R = \left( \frac{\gamma_R}{2\pi K} - n\sqrt{K} \pm \frac{\sqrt{K}}{2} \right)^2 + K(m^2 + 2m + 4\tilde{m}) - (m + 2\tilde{m})
\]

\[
v_L = \left( \frac{\gamma_L}{2\pi K} + n\sqrt{K} \pm \frac{\sqrt{K}}{2} \right)^2 + K(m^2 + 2m + 4\tilde{m}) - (m + 2\tilde{m})
\]

(2.110)

The \(-(m + 2\tilde{m})\) term in above equations comes from the integration variables \( z_j, y_i \). The overall exponent is given by the summation of these two exponents, thus we have

\[
v_R + v_L = \frac{1}{2} \left( \frac{\gamma_R + \gamma_L}{2\pi \sqrt{K}} \right)^2 + \frac{1}{2} \left( \frac{\gamma_L - \gamma_R}{2\pi \sqrt{K}} + (2n \mp 1)\sqrt{K} \right)^2
\]

\[
+ 2Km^2 + 2(2\tilde{m} + m)(2K - 1)
\]

(2.111)

As we are considering the effect of Umklapp term at zero field, \( 4k_F = 2\pi \); these are singularity exponents of the spectral function at threshold frequencies given by Eq. [2.91]. Compared to Eq. [2.93], we see that for fixed \( n \) higher order Umklapp terms give larger and larger exponents, and are more irrelevant. Therefore, at each
threshold energy, we get a set of singularities with progressively weaker exponents. In this case, these corrections seem truly unimportant. That is, we don’t get any new singular energies, just sub-dominant corrections to the singularities at the energies we already have.

One important point is that if we take \( n, m = 0 \) but arbitrary \( \bar{m} \), at half filling and for \( \Delta = 1 \) we have \( 2K - 1 = 0 \); thus higher order non-chiral Umklapp corrections do not change the singularity exponents, based on power counting. But we should be careful at that limit, because our result was based on power counting; in general upon evaluating the integrals more carefully, there could be some logarithmic corrections to the correlations functions which could change the behaviour of spectral functions near singular frequencies.

Till now we only considered the effect of Umklapp terms only at zero magnetic field. At finite magnetic field the Umklapp interaction has the following form

\[
\mathcal{H}_U = g_U \cos 4(\sqrt{\pi K} \phi(x) + (k_F - \pi/2a)x)
\]  

(2.112)

Where \( a \) is the lattice spacing. In general this term is oscillatory and could be dropped out at low energies. But for weak enough magnetic field, the wavelength of the oscillation is very long, therefore in that limit this term should be treated carefully. We claim that at low enough temperatures and weak magnetic field the Umklapp term affects neither the threshold frequency nor the singularity exponents, but it will change the overall behaviour of the spectral function; the reason is as follow. If we include the effect of Umklapp term perturbativley, it could be easily shown that such higher order terms can not change the oscillation wave-vector of the spectral functions. It only modifies the non-oscillatory part of the spectral function without changing the oscillatory part. Therefore, if the oscillations wave-vector remains intact the threshold frequency does so.

The singularity exponents does not change because, to find the singularity exponents of spectral functions, we need to study the behaviour of spectral functions at frequencies, \( \omega_L \), around the threshold frequencies, \( \omega_L \). In principle the probe
frequency could be chosen as close as possible to the singular frequency such that the Umklapp term effects would be irrelevant at those energy difference scales, \(|\omega - \omega_L| \ll |(k_F - 2\pi/a)v|\). Thus the Umklapp term would not change the singular exponent at \(\omega_L\); we expect a cross over regime where the effect of Umklapp will be important at energies near to \(|\omega - \omega_L| \approx (k_F - 2\pi/a)v|\).

### 2.5 Electron spin resonance with Uniform Dzyaloshinskii-Moriya Interactions

Electron spin resonance provides a sensitive probe of spin dynamics. A microwave field is weakly Zeeman coupled to the \(q = 0\) components of the spin operators. In the standard (Faraday) configuration, the microwave field is polarized perpendicular to a static magnetic field. For simplicity we restrict ourselves to the relatively simple situation of Eq. (2.1), with DM vector and magnetic field in the \(z\)-direction. Then, as discussed in Sec. 2.1, a uniform DM interaction added to the XXZ model of Eq. (2.1) simply shifts the parameters \(J\) and \(\Delta\) and the momentum, \(q\) in the transverse spectral function. Therefore the ESR adsorption intensity is proportional to the transverse spectral function at \(q = \alpha = \arctan(D/J)\). Low temperature ESR measurements on quasi-1D antiferromagnets with uniform DM interactions could therefore probe the edge singularities predicted by X-ray edge methods that disagree with standard bosonization results due to the effects of band curvature. Such ESR results would be especially useful if they were done with circularly polarized microwave radiation since then \(S_-^+\) and \(S_+^-\) could be measured separately.

A further major challenge for such ESR experiments would be that the theoretical predictions give \(S^{\omega \omega_h}(\alpha, \omega, h)\) for fixed \(h\) as a function of \(\omega\). However, in an ESR experiment, \(\omega\) is normally fixed at the resonant frequency of a microwave cavity and \(h\) is varied. \(\omega\) can only be varied by using a sequence of microwave cavities with different resonant frequencies. Alternatively, theoretical line-shapes could be produced for fixed \(\omega\) and varying \(h\) but these would be complicated since the critical exponent \(\alpha\) varies with \(h\). For simplicity, we just discuss the line shape versus frequency at fixed \(h\) here.

We begin by discussing the \(T = 0\) limit. The ESR adsorption intensity can be
simply read off from the results of Sec. 2.2.2, 2.3. We first consider the case of zero static field with the microwave field in the xy plane. Then the adsorption intensity has a lower threshold near which:

$$I(\omega) \propto \frac{\theta(\omega - v \sin \alpha)}{(\omega - v \sin \alpha)^\mu}$$ (2.113)

with $\mu = 2 - 1/(2K) - K$. Here $v$ and $K$ are determined in terms of $\Delta_{eff} = \Delta \cos(\alpha)$ by Eq. (2.31). For small $\alpha$ we expect the results of standard bosonization to apply at somewhat higher energies, $\omega - v \alpha \gg \alpha^3 J$. In this region we obtain:

$$I(\omega) \propto \frac{(\omega + v \alpha)^{1+2\eta}}{(\omega - v \alpha)^{1-2\eta}}$$ (2.114)

with $\eta = (1 - 2\eta)/(8K)$. Note that $1 - 2\eta = 2 - 1/(4K) - K \neq \mu$, a different exponent than occurs at the threshold. As discussed in sub-section 2.2.2, $I(\omega)$ in Eq. (2.114) is non-monotonic, eventually passing through a minimum and starting to increase again as $\omega$ increases. However, since the formula is only valid in the low energy regime, $\omega \ll J$, whether or not this minimum occurs in the frequency region where the formula is valid depends on $\alpha$ and $\Delta_{eff}$.

If $\Delta_{eff} \geq \cos \alpha$, the value resulting from $\Delta = 1$, then the minimum predicted by standard bosonization is not in the region where the approximation is valid. In this case the intensity is monotone decreasing up to high frequencies where our techniques break down. $\Delta_{eff}$ is typically close to 1. In fact, with some assumptions about the higher energy levels of the magnetic ion, it is exactly one [52]. In this case, the transverse spectral function becomes the same as the longitudinal one discussed extensively in [28, 29, 31, 53]. The edge exponent has the value $\mu = 1/2$, first obtained from the 2-spinon approximation [53] in this case and the standard bosonization prediction of Eq. (2.114), with $\eta = 0$, reduces to a $\delta$-function which fails to capture many features of the actual spectral function for non-zero $\alpha$. In particular there is a narrow peak of width $\propto \alpha^3$ followed by a slowly decaying tail at higher $\omega$.

At non-zero field, $h$, we may again use the results of Sec. 2.2.2, 2.3, which are less complete in this case. The X-ray edge results of Sec. 2.3 imply a quantum phase transition as the magnetic field is increased, occurring when the field-induced
magnetization, \( m(h) \), obeys \( \alpha = H \equiv 2\pi m \approx K h/(\pi/v) \) as can be seen from Fig. [2.8]. \( S^- \) has a threshold singularity at a frequency \( \omega_L \approx v(\alpha + H) \) for \( H < \alpha \ll 1 \). A threshold singularity was also predicted in III for \( S^+ \) in this field range, at a higher frequency, of approximately \( v(\alpha + H) \). However, as discussed at the end of that sub-section, we expect this to be broadened. On the other hand, for \( H > \alpha \), we expect \( S^+ \) to have a sharp 2-sided singularity at a frequency of approximately \( v(H - \alpha) \). The other threshold singularity predicted for \( S^+ \) at \( v(H + \alpha) \) in 2.2.2 is likely to be broadened. (The presence of two peaks at these energies was first predicted in [54] and was observed experimentally in [43].) The precise energies and critical exponents for these singularities could be predicted by numerical Bethe ansatz calculations but analytic expressions are not available. Assuming \( \alpha, H \ll 1 \), we expect the spectral functions to cross over to the form predicted by standard bosonization at energies somewhat higher than the singularities, \( (H - \alpha)^2 a J \ll v |H - \alpha| \ll J \):

\[
S^- \propto \frac{[\omega + v(H - \alpha)]^{1+2\eta}}{[\omega + v(\alpha - H)]^{1-2\eta}} \quad (H < \alpha) \\
S^+ \propto \frac{[\omega + v(\alpha - H)]^{1+2\eta}}{[\omega + v(H - \alpha)]^{1-2\eta}} \quad (H > \alpha). \quad (2.115)
\]

As discussed above and sketched in Fig. [2.2], these functions are non-monotonic but the minimum only occurs in the energy region \( \omega \ll J \), where the approximation holds, for a certain parameter range of \( \alpha, \Delta \) and \( h \). In addition to these dominant singularities, as discussed in 2.4, we expect many additional weaker vanishing singularities extending down to low energies.

**Finite Temperature Broadening**

At finite temperature the sharp peaks are broadened. This can be calculated using standard bosonization for \( (H - \alpha)^2 a J \ll T \ll J \). At finite \( T \) the spectral function of Eq. (2.114) becomes:

\[
I \propto \text{Im}\{(\sin(2\pi \eta))(2\pi T)^\eta B(1 + \eta - i(\omega + v \alpha)/(4\pi T), \omega + v \alpha)/(4\pi T), 0, -1 - 2\eta) \times B(\eta - i(\omega - v \alpha)/(4\pi T), 1 - 2\eta)\}. \quad (2.116)
\]
where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Euler beta function. For weak anisotropy, small $\alpha$ and $1 - \Delta_{\text{eff}}$, and hence $\eta \ll 1$, a Lorentzian line-shape occurs:

$$I \propto \frac{1}{(\omega - v\alpha)^2 + (4\pi T \eta)^2}$$  \hspace{1cm} (2.117)

with a similar broadening at finite $H$. The width of the peak is $4\pi T \eta \approx 2T (1 - \Delta_{\text{eff}})/\pi$ for $\Delta_{\text{eff}}$ close to 1. This is essentially the same result derived in [40] for the ESR width due to exchange anisotropy parallel to the magnetic field.

In section 2.3, we found the singularity exponent and behaviour of the transverse spectral function near the thresholds at zero temperature using X-ray edge methods. Now we look at the finite temperature effects on the spectral functions, and we find that finite temperature results in a non-Lorentzian broadening of the transverse spectral functions near the thresholds for $|\omega - \epsilon(q)|, T \ll q^2/2m$. Non-zero temperature has two effects on the spectral function Eq. (2.80). First, the Green’s function for excitations near the fermi surface, $S^{(0)}$ is modified to the usual finite $T$ form by a conformal transformation. Secondly, the Green’s function for the $\bar{d}$ operators would be modified to finite $T$ form, with step functions $\theta(\epsilon)$ replaced by Fermi functions $n_F(\epsilon)$. This would allow a hole contribution to $S^{-+}$ and a particle contribution to $S^{+-}$. However, at low $T \ll \epsilon(k_F)$ these would be negligible. So the only important effect may be in $S^{(0)}$. Thus in this regime and for $(2k_F - \pi < q < \pi)$ we have

$$S^{-+}(q, \omega) \propto \int dx dt e^{i(\omega - \epsilon(q))t} \delta(x - ut) \frac{(2\pi T)^{\nu_+^L}}{(\sin(2\pi T(\epsilon + i(t - x/v))))^{\nu_+^L}} \frac{(2\pi T)^{\nu_+^R}}{(\sin(2\pi T(\epsilon + i(t + x/v))))^{\nu_+^R}}.$$

By doing the integration over $x$ we have

$$S^{-+}(q, \omega) \propto \int_{-\infty}^{\infty} dt e^{i(\omega - \epsilon(k_F^\pm))t} \frac{(2\pi T)^{\nu_+^L}}{(\sin(2\pi T(\epsilon + i(1 - u/v)t)))^{\nu_+^L}} \frac{(2\pi T)^{\nu_+^R}}{(\sin(2\pi T(\epsilon + i(1 + u/v)t)))^{\nu_+^R}}$$

(2.118)

By evaluating the above integral we can get the finite $T$ behaviour of the spectral
Figure 2.9: The behaviour of $S^{+ -} (\omega, q)$ spectral function at finite temperature for the case $\nu_R = 1/2, \nu_L = 0$, corresponding to $\Delta = 1, h = 0$. We see that for small enough $T$ the broadening is asymmetric.

In Fig. [2.9] we have depicted the spectral function for different values of temperature. As temperature gets higher the broadening increases; as can be seen, for small $T$ the broadening is asymmetric and so is non-Lorentzian. Furthermore, the width is $O(T)$, not suppressed by a factor of $1 - \Delta_{eff}$ as predicted by standard bosonization. Since the effects predicted by the new theoretical methods occur at
very low energy scales, a highly one-dimensional spin compound would probably
be needed to observe them, in order that three dimensional exchange processes
would be negligible. Furthermore, materials like KCuGaF$_6$ with both uniform and
staggered intra-chain DM interactions may not be suitable since the staggered DM
interactions tend to have a larger effect than the uniform ones[40]. Thus identifying
the right material to test these predictions remains an open challenge. An alterna-
tive approach might be to study metallic quantum wires with spin-orbit couplings.
It was shown in [54] that analogous phenomena occur in that system.

2.6 Conclusions

By applying X-ray edge techniques, we have obtained results on the transverse
spectral function of the XXZ spin chain in a magnetic field. We illustrated why
standard bosonization techniques fail near threshold energies, even when these oc-
cur at low energy. In the zero field case we have exactly determined a critical ex-
ponent governing the lower edge singularity, for all $|\Delta| < 1$ and all wave-vectors.
For the finite field case, we have shown how this exponent can be determined from
parameters which can be obtained from solving Bethe ansatz equations and which
also determine the behaviour of the longitudinal structure function, fermion spec-
tral function and the finite size spectrum. We have argued that, for general magne-
tization, a large number of increasingly weaker singularities occur in the spectral
function, extending all the way down to zero energy. We derived results for the fi-
nite temperature spectral function using X-ray edge methods, obtaining strikingly
different behaviour than that given by standard bosonization at $0 < 1 - \Delta_{\text{eff}} \ll 1$.
The line-shape is non-Lorentzian and the line width is $O(T)$, unsuppressed by $1 - \Delta_{\text{eff}}$.
We pointed out that electron spin resonance measurements on spin chain
compounds with uniform Dzyaloshinskii-Moriya interactions would provide a way
of experimentally confirming, for the first time, the new bosonization results being
obtained on spin chains, using X-ray edge techniques.

In the case of staggered DM interactions, the most interesting ESR signal oc-
curs when the magnetic field is transverse to the DM vector. This may also be the
case for uniform DM interactions, but we leave this for future work.
Chapter 3

Toward rigorous proof of edge magnetism in graphene nano-ribbons

3.1 Introduction

Graphene is a two dimensional allotrope of Carbon which has many interesting electronic properties. In graphene the Carbon atoms are arranged in honeycomb lattice. The $sp^2$ hybridization of the atomic $s$ orbital with two $p$ orbitals lead to trigonal planar structure, leads to the formation of so called $\sigma$ bond between the neighboring carbon atoms, with distance equal to 1.42Å. This $\sigma$ band is responsible for holding the carbon atoms in two dimensions and the robustness of graphene. The remaining $p$ orbital is perpendicular to plane of this planar structure and the resulting covalent bond between $p$ orbitals of the neighboring atoms lead to the formation of $\pi$ band, which is responsible for many low-energy electronic and transport properties of graphene.

The first theoretical study of the band structure of graphene was done by P. R. Wallace in 1946 [32]; he showed the unusual semimetallic behavior of it. The more systematic study of the low-energy excitations of graphene leads to its most interesting properties. Semenoff [33] showed that the low energy excitations are
massless chiral, Dirac fermions. Quite interestingly these excitations were propagating like massless fermions but with fermi velocity which is about 1/300 of velocity of light.

In addition to interesting properties of excitations of bulk graphene, it turns out that graphene with some specific boundary conditions has very interesting properties too. It could be shown that a semi-infinite graphene sheet with zigzag boundary or edge, supports localized zero energy states at the boundary. Mean field theoretical study of these edge states for graphene with electron-electron interactions, Hubbard interaction [34, 35], revealed that the edge states are spin polarized. In this work we rigorously study this problem and show that the ground state of the effective edge Hamiltonian is spin polarized.

In the following section we look at the band structure of the bulk graphene and its low energy excitations, in section 3.3 we derive the low-energy effective Hamiltonian which describes the excitations and effect of interactions on low energy behavior of it. In section 3.4 we look at the edge states of graphene and will give a hand-waving argument based on Lieb's theorem about the magnetism of edge states.

In section 3.5 we derive effective Hamiltonian description of edge states and prove the ferromagnetism of its ground state. Then we take into account the effect of next-nearest-neighbor hopping terms and stability of ferromagnetic ground state in 3.6. Finally in section 3.7 by taking into account the effect of bulk excitations in proper field theoretical method, we find the effective higher order corrections to edge Hamiltonian by integrating out these excitations.

3.2 Band structure of single layer graphene

Graphene is two-dimensional layer of carbon atoms arranged in honeycomb lattice. Honeycomb lattice is a bipartite lattice of two triangular sub-lattices, which in this work we distinguish as sub-lattice A and B. The basis vectors of triangular Bravais Lattice are given by

\[
\vec{a}_1 = \frac{a}{2} \left( 3, \sqrt{3} \right) \quad \vec{a}_2 = \frac{a}{2} \left( 3, -\sqrt{3} \right) \quad (3.1)
\]
where \( a \approx 1.42 \text{Å} \) is the distance between two neighbor carbon atoms. Graphene is made of two copies of triangular lattice generated with \( \vec{a}_1, \vec{a}_2 \), which are displaced by \( \vec{\delta}_1 \). Each carbon atom has three nearest-neighbours, where their positions are given by

\[
\vec{\delta}_1 = \frac{a}{2} \left( 1, \sqrt{3} \right) \quad \vec{\delta}_2 = \frac{a}{2} \left( 1, -\sqrt{3} \right) \quad \vec{\delta}_3 = -a (1, 0) \quad (3.2)
\]

The tight-binding Hamiltonian of \( \pi \) band of graphene is derived from the overlapping of the wavefunction of \( p_z \) orbital of each Carbon atom with its neighboring atoms, which gives the hopping parameter of this orbital. In general there could be hopping between any two carbon atom but as the distance between the atoms increases the hopping amplitude decreases and the only important terms are the nearest-neighbor hopping \( t \approx 2.8 eV \) and the next-nearest-neighbor hopping \( t' \approx 0.1 eV \).

The tight-binding Hamiltonian for graphene is given by

\[
H = -t \sum_{\langle i, j \rangle, \sigma} \left( a^\dagger_{i, \sigma} b_{j, \sigma} + h.c. \right) - t' \sum_{\langle\langle i, j \rangle\rangle, \sigma} \left( a^\dagger_{i, \sigma} a_{j, \sigma} + b^\dagger_{i, \sigma} b_{j, \sigma} + h.c. \right) \quad (3.3)
\]

where \( a_i \) and \( b_j \) are electron annihilation operators on sub-lattice \( A \) and \( B \), respectively, and \( \langle \cdots \rangle \) means summation only over nearest neighbors and \( \langle \langle \cdots \rangle \rangle \) represents summation over next-nearest-neighbors. Location of the \( NNN \) neighbors of each Carbon is given by \( \pm a_1, \pm a_2 \) and \( \pm (a_2 - a_1) \).

The spectrum of Eq. (3.3) can be easily derived by using Fourier representation of annihilation operators

\[
a_{\vec{r}} = \frac{1}{\sqrt{N_A}} \sum_{\vec{k}} e^{i \vec{k} \cdot \vec{r}} a_{\vec{k}} \quad b_{\vec{r}} = \frac{1}{\sqrt{N_B}} \sum_{\vec{l}} e^{i \vec{l} \cdot \vec{r}} a_{\vec{l}} \quad (3.4)
\]

In this representation we have

\[
H = -t \sum_{\vec{k}, \sigma} \left( \phi(\vec{k}) a^\dagger_{\vec{k}, \sigma} b_{\vec{k}, \sigma} + h.c. \right) - 2t' \sum_{\vec{k}, \sigma} \psi(\vec{k}) \left( a^\dagger_{\vec{k}, \sigma} a_{\vec{k}, \sigma} + b^\dagger_{\vec{k}, \sigma} b_{\vec{k}, \sigma} \right) \quad (3.5)
\]

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The diagonalization of the Hamiltonian Eq. (3.5), gives us the spectrum of the excitations

$$E_{\pm} (\vec{k}) = \pm t |\phi(\vec{k})| - 2t' \psi(\vec{k})$$  

(3.7)

By looking at Fig. 3.1, there are two special points in the Brillouin Zone (BZ), where two energy bands touch each other, $\vec{K}$ and $\vec{K}'$.

$$\vec{K} = \frac{2\pi}{3a} \left(1, \frac{1}{\sqrt{3}} \right) \quad \vec{K}' = \frac{2\pi}{3a} \left(1, -\frac{1}{\sqrt{3}} \right)$$  

(3.8)

As we see the band structure is gapless, and excitations near these points have linear dispersion. These points are named Dirac points which leads to many interesting properties of graphene.

From Eq. (3.7) it is clear that when $t' = 0$, the energy spectrum is symmetric around zero energy and we have particle-hole symmetry. This could also be seen in the lattice representation of Hamiltonian (3.3), particle-hole transformation for bi-partite lattice is given by

$$a_{i, \sigma} \rightarrow a_{i, \sigma}^\dagger \quad b_{i, \sigma} \rightarrow -b_{i, \sigma}^\dagger$$  

(3.9)

We see that the first term in Eq. (3.3) is invariant under this transformation while the second term is not. It is also instructive to look at the dispersion near the Dirac points; to do so, we need to expand the dispersion (3.7) near $\vec{K}$ or $\vec{K}'$. Letting $\vec{k} = \vec{K} + \vec{q}$, for small momentum $q \ll |\vec{K}|$

$$E_{\pm} (q) \approx \pm v_F |q| + O((q/K)^2),$$  

(3.10)

where $v_F \approx 10^6 m/s$ is the Fermi velocity. This is exactly similar to the dispersion of relativistic massless particles, with the only difference that speed of excitations
Figure 3.1: Honeycomb lattice and its Brillouin zone. Left: lattice structure which is used. Right: the Brillouin zone and Dirac points

is two orders of magnitude smaller than the velocity of light. This very important and interesting property of graphene, enables the study of properties of relativistic particles in graphene.

In addition to nearest neighbor hopping term, there is also small amount of next-nearest-neighbor hopping term. But the only effect of including the next-nearest-neighbor term is that it shifts the energy of Dirac points and changes higher order terms of the dispersion of the excitations:

$$E_{\pm}(q) \simeq 3t' \pm v_F |q| - \frac{3q^2a^2}{4} \left(3t' \pm \frac{t}{2} \sin(3\theta_q)\right)$$

$$\theta_q = \arctan \left(\frac{q_x}{q_y}\right)$$

(3.11)
As we see, to leading order the dispersion has rotational symmetry around \( \mathbf{q} = 0 \), while higher order terms break that symmetry and in general the energy depends both on magnitude and the direction of momentum.

### 3.3 Dirac fermions and low-energy effective hamiltonian

We saw in the previous section that the graphene band structure is gapless and the excitations near the Dirac points have linear dispersion. Following [33, 55] in this section we explicitly show that these excitations could be described by a Hamiltonian which has the same form as the Hamiltonian describing relativistic fermions, so called Dirac Hamiltonian.

As the only effect of \( t' \) is to shift the Dirac points energy without changing the leading order low-energy dispersion, we could safely assume that \( t' = 0 \). To find the effective Hamiltonian for excitations near the Dirac points, we write our fermion operators as follow

\[
\begin{align*}
a_n, \sigma & \simeq e^{-i\mathbf{K} \cdot \mathbf{R}_n} \psi_{A,n,\sigma} + e^{-i\mathbf{K}' \cdot \mathbf{R}_n} \psi_{A,n,\sigma}' \\
b_n, \sigma & \simeq e^{-i\mathbf{K} \cdot \mathbf{R}_n} \psi_{B,n,\sigma} + e^{-i\mathbf{K}' \cdot \mathbf{R}_n} \psi_{B,n,\sigma}'
\end{align*}
\]

(3.12)

where \( \mathbf{K}, \mathbf{K}' \) are the two Dirac points, \( \psi_{A/B,n,\sigma} \) and \( \psi_{A/B,n,\sigma}' \) represent excitations near \( \mathbf{K}, \mathbf{K}' \) respectively, and are slowly varying operators in position space. From Eq. (3.3) we need to evaluate terms like \( a_n^\dagger b_n' \) where \( n, n' \) are two neighboring sites

\[
\sum_{\delta} a_n^\dagger b_{n+\delta} = \sum_{\delta} e^{-i\mathbf{K} \cdot \mathbf{R}_n} \psi_{A,\delta}^\dagger (\mathbf{R}_n) \psi_{B,\delta} (\mathbf{R}_n + \mathbf{\delta}) + e^{-i\mathbf{K}' \cdot \mathbf{R}_n} \psi_{A,\delta}^\dagger (\mathbf{R}_n) \psi_{B,\delta} (\mathbf{R}_n + \mathbf{\delta})
\]

(3.13)

where we have ignored terms proportional to \( e^{i(\mathbf{K} - \mathbf{K}')} \cdot \mathbf{R}_n \), as they are varying very fast and can be neglected in study of low-energy Hamiltonian. By expanding the slowly varying field \( \psi_{B}(\mathbf{R}_n + \mathbf{\delta}) \) around \( \mathbf{R}_n \) we have

\[
\psi_{B}(\mathbf{R}_n + \mathbf{\delta}) \approx \psi_{B}(\mathbf{R}_n) + \mathbf{\delta} \nabla \psi_{B}(\mathbf{R}_n) + O(\nabla^2)
\]

(3.14)
where higher order terms are irrelevant in RG sense. By using above equation and Eq. (3.13) we get

\[
\sum_{\delta} \langle \delta \rangle a_n b_{n+\delta} = \sum_{\delta} e^{-i\vec{K} \cdot \vec{\delta}} \psi_A^\dagger (\vec{R}_n) \psi_B (\vec{R}_n) + e^{-i\vec{K}' \cdot \vec{\delta}} \psi_A'^\dagger (\vec{R}_n) \psi_B' (\vec{R}_n)
\]
\[
+ \sum_{\delta} e^{-i\vec{K} \cdot \vec{\delta}} \psi_A (\vec{R}_n) \vec{\partial} \cdot \nabla \psi_B (\vec{R}_n) + e^{-i\vec{K}' \cdot \vec{\delta}} \psi_A' (\vec{R}_n) \vec{\partial} \cdot \nabla \psi_B' (\vec{R}_n)
\]

By using the following identities we could simplify previous equation

\[
\sum_{\delta} e^{i\vec{K} \cdot \vec{\delta}} = \sum_{\delta} e^{i\vec{K}' \cdot \vec{\delta}} = 0
\]
\[
\sum_{\delta} e^{i\vec{K} \cdot \vec{\delta}} \vec{\delta} = -\frac{3a}{2} e^{i\pi / 3} (1, i)
\]
\[
\sum_{\delta} e^{i\vec{K}' \cdot \vec{\delta}} \vec{\delta} = -\frac{3a}{2} e^{i\pi / 3} (1, -i)
\]

(3.15)

we get

\[
\sum_{\delta} a_n b_{n+\delta} = -\frac{3ae^{i\pi / 3}}{2} \left( \psi_A^\dagger (\vec{R}_n) (\partial_x + i\partial_y) \psi_B (\vec{R}_n) + \psi_A'^\dagger (\vec{R}_n) (\partial_x - i\partial_y) \psi_B' (\vec{R}_n) \right)
\]

(3.16)

The low-energy Hamiltonian will be

\[
H \simeq -\frac{3tae^{i\pi / 3}}{2} \times \int dxdy \left( \psi_A^\dagger (\vec{r})(\partial_x + i\partial_y) \psi_B (\vec{r}) + \psi_A'^\dagger (\vec{r})(\partial_x - i\partial_y) \psi_B' (\vec{r}) \right) + h.c.
\]

(3.17)

By defining \( v_F = 3ta/2 \) and

\[
\Psi_1(x) = \begin{pmatrix} e^{-i\pi x / 2} \psi_A \\ e^{i\pi x / 2} \psi_B \end{pmatrix} \quad \Psi_2(x) = \begin{pmatrix} e^{-i\pi x / 2} \psi_A' \\ e^{i\pi x / 2} \psi_B' \end{pmatrix}
\]

(3.18)
we get

\[ H = -i v_F \int dx \, dy \left[ \Psi_1^\dagger(\vec{r}) \sigma \cdot \nabla \Psi_1(\vec{r}) + \Psi_2^\dagger(\vec{r}) \tilde{\sigma} \cdot \nabla \Psi_2(\vec{r}) \right] \quad (3.19) \]

where \( \sigma = (\sigma_x, \sigma_y), \tilde{\sigma} = (\sigma_x, -\sigma_y), \) are Pauli matrices. This Hamiltonian is Dirac Hamiltonian for massless two dimensional Dirac fermions. We have two copies of Dirac Hamiltonian for each \( \vec{K}, \vec{K}' \) which are known as two “valleys”. This representation of theory is more convenient to study the effect of interactions perturbatively.

For this work we are interested to study the effect of Hubbard interaction on edges of graphene. Let’s first look at the effect of this interaction on bulk graphene. The hubbard interaction, which is screened on-site Coulomb repulsion, is given by

\[ H_U = U \sum_i c_i^\dagger \sigma_i c_i^\dagger c_i \quad (3.20) \]

where \( U \) is so called Hubbard interaction strength. One important point to mention is that, in graphene density of states vanishes linearly and thus the Coulomb interaction is not fully screened. But effectively longer range Hubbard interactions are weaker and as a first step we could ignore them. Also as we will show shortly even on-site Hubbard repulsion is irrelevant in renormalization group sense and with more involved argument it could be shown that long range Coulomb repulsion is marginally irrelevant [56] in renormalization group (RG) sense.

In low-energy picture the Hubbard interaction term is

\[ H_U = U \int dx dy \Psi_1^\dagger(\vec{r}) \Pi_{A/B} \Psi_1(\vec{r}) \Psi_2^\dagger(\vec{r}) \Pi_{A/B} \Psi_2(\vec{r}) \quad (3.21) \]

where \( \Pi_{A/B} \) is projection matrix to sub-lattice \( A/B \). To study the RG flow of this interaction for weak interactions \( U \ll t \), we need to find the scaling dimension of the fields \( \Psi \). To find the dimension of \( \Psi \) we look at the kinetic term in Lagrangian picture, and the term will be

\[ \mathcal{L} \propto \int dx \, dy \, dt \, \Psi^\dagger \sigma \cdot \nabla \Psi \quad (3.22) \]
from this equation we see that dimension of fermionic field is \( D[\Psi] = L^{-1} \), where
\( L \) means dimension of length, as length and energy are inversely related, \( D[\Psi] = E \).
The interaction term in Lagangian picture is
\[
\mathcal{L}_U = \int dx dy dt \Psi_{\uparrow}^\dagger(\vec{r}) \Pi_{A/B} \Psi_{\downarrow}(\vec{r}) \Psi_{\uparrow}^\dagger(\vec{r}) \Pi_{A/B} \Psi_{\downarrow}(\vec{r})
\]
This term has scaling dimension of length, \( D[\mathcal{L}_U] = L^{-1} \equiv E \). As the dimension of this term is proportional \( E \), in renormalization flow picture this means that this term re-normalizes to zero as we integrate out high-energy terms, and terms like this are called irrelevant in study of low-energy properties of the system. If the scaling dimension of some terms became \( E^{-n} \), those terms are called relevant, in RG sense, and term with no scaling dimension are called marginal.

As a result the Hubbard interaction term is irrelevant for weak interactions; this means for small \( U/t \) the low energy picture is semimetal with fermionic excitations governed by Eq. (3.19). Many numerical studies of phase diagram of tight-binding honeycomb lattice with Hubbard interaction confirm this picture for finite range of interaction strength \( U < U_c, U_c \approx 3.8t \), where for \( U > U_c \) the ground state is Anti-Ferromagnetic Mott Insulator \[57\] . In this work we are interested to study the effect of weak Hubbard interaction on magnetic properties of edges of graphene.

### 3.4 Edge states of graphene

In previous section we studied the band structure of bulk, infinite size, graphene. We showed that low-energy excitations of graphene are massless Dirac like fermions and also weak Hubbard interaction is irrelevant and does not change the qualitative picture of low-energy physics. One of the many fascinating properties predicted for graphene \[55\] is that a non-interacting nanoribbon with zigzag edges has bands of states with energy exponentially small in the ribbon width, localized at the edges \[34, 58-62\]. Unzipping of carbon nanotubes has recently provided a technique for producing nano-ribbons with clean edges and Scanning Tunnelling Microscopy (STM) on such ribbons \[63\] has shown evidence for interacting edge states.
Figure 3.2: A nanoribbon with an upper zigzag edge and lower bearded edge and armchair edges on sides. In this example, $L = 5$ and $W = 6$.

Among the infinite possibilities for edges of a graphene sample, there are three possible edge configurations which support translational invariance over short distance, so called *Zigzag*, *Armchair* and *Bearded* edges, Fig 3.2. Among these three, the zigzag and bearded edges lead to zero-energy bands.

To show the existence of zero-mode states, we look at a semi-infinite graphene sheet with zigzag edge, by taking limit of $L, W \to \infty$ in Fig 3.2. In this geometry the tight-binding Hamiltonian is given by

$$
\mathcal{H} = -t \sum_{m=-\infty}^{\infty} \sum_{n=0}^{\infty} a_{\sigma}^{\dagger}(m,n) b_{\sigma}(m,n) + a_{\sigma}^{\dagger}(m,n) b_{\sigma}(m-1,n) + a_{\sigma}^{\dagger}(m,n) b_{\sigma}(m,n-1) + h.c
$$

(3.24)
again $a$ and $b$ are electron annihilation operators for $A$ sites and $B$ sites, and $m, n$ are position indices along $x$-direction and $y$-direction, respectively. By using translational invariance along the $x$-direction and Fourier transforming the operators in that direction we have

$$H = -t \sum_{n,k} a^\dagger_\sigma(k,n) b_\sigma(k,n) (1 + e^{ika'}) + a^\dagger_\sigma(k,n) b_\sigma(k,n - 1) + h.c.$$  

(3.25)

where $a' = \sqrt{3} a$. By using the fact that $k$ is a conserved quantum number, in general any eigenstate of above Hamiltonian could be written as follow

$$|E, k, \sigma \rangle = \sum_{n=0}^{\infty} \left( \alpha_n^E a^\dagger_\sigma(k,n) + \beta_n^E b^\dagger_\sigma(k,n) \right) |0\rangle.$$  

(3.26)

To find the coefficients $\alpha_n^E$ and $\beta_n^E$ of zero-energy mode we should solve $H|0, k, \sigma \rangle = 0$. It is easy to show that the following state is the solution to this equation

$$|0, k, \sigma \rangle = \sum_n \alpha_n^E a^\dagger_\sigma(k,n) |0\rangle$$

$$\alpha_n^E = N_k (-2\cos \frac{kd'}{2})^n e^{i\kappa a' / 2}$$  

(3.27)

where $N_k$ is the renormalization factor for wave function, and is given by

$$N_k^2 = \frac{1}{\sum_{n=0}^{\infty} |2\cos \frac{kd'}{2}|^{2n}}.$$  

(3.28)

This equation tells us that for semi-infinite zigzag sheet, normalizable zero-energy states exist if and only if $|2\cos kd'| < 1$, which restricts the values of $k$ to $k \in \left[ \frac{2\pi}{3a'}, \frac{4\pi}{3a'} \right]$. We should notice the fact that the weight of the wavefunction of edge states is non-zero only on $A$-sub-lattices.

This result is only valid for semi-infinite graphene sheet with zigzag edge; if we have a finite ribbon with zigzag edges on both sides the result is different. Then we have two edges and if we try to solve eigenvalue problem for Eq. (3.26) we see that it is coupled equation and there is no exact result for $\alpha^E$ and $\beta^E$ for $E = 0$. Actually numerical solution of those equation does not give a band of zero-
modes in contrast to semi-infinite sheet [64, 65]. The intuitive picture is that the overlapping of the wave-functions of each edge lifts the degeneracy of zero-modes and leads to exponentially small energies for the same range of momentum. The band structure for finite ribbon with Zigzag-Zigzag (ZZ) edges are depicted in Fig. 3.3a.
The other possible and interesting boundary condition is the case that we have a finite ribbon with zigzag edge on, let’s say, upper edge and bearded edge on lower edge similar to Fig. 3.2. For this geometry as we see the number of atoms in A-sublattice and B-sublattice are different, \( N_A - N_B \propto L \). The tight-binding Hamiltonian with only nearest-neighbor terms is a matrix which transforms an \( N_A \)-dimensional space on \( N_B \)-dimensional space; from linear algebra we know that this Hamiltonian should have \( |N_A - N_B| \) zero eigenvalues. This can be shown explicitly and the exact form of the wave function is exactly the same as Eq. (3.27)

\[
|0,k,\sigma\rangle = \sum_n \alpha_{k,n} \alpha^\dagger_{\sigma}(k,n)|0\rangle
\]

\[
\alpha_{k,n} = \mathcal{N}_k (-2\cos \frac{k\alpha'}{2})^n e^{jkn'/2}
\]  \hspace{1cm} (3.29)

where \( \mathcal{N}_k \) is the renormalization factor for wave function, and is given by

\[
\mathcal{N}_k^2 = \frac{1 - |2\cos \frac{k\alpha'}{2}|^{2N_y}}{1 - |2\cos \frac{k\alpha'}{2}|^2}.
\]  \hspace{1cm} (3.30)

As \( N_y \) is finite, which is the number of unit cells along the width of the ribbon, there is no normalization restriction on \( k \). One interesting and important point to notice, is that for \( k \in [\frac{2\pi}{La'}, \frac{4\pi}{La'}] \) we have \( |2\cos \frac{k\alpha'}{2}| < 1 \) and from second line of Eq. (3.29) we see that for this range of \( k \) the weight of wave-function decreases exponentially as \( n \) increases, which means the wave function is localized around \( n = 0 \), or the zigzag edge. But for \( k \in [-\frac{2\pi}{La'}, \frac{2\pi}{La'}] \) we get \( |2\cos \frac{k\alpha'}{2}| > 1 \) and this leads to wave-functions which are localized around \( n = N_y \), or Bearded edge. The numerical result of band structure of this configuration is depicted in Fig. 3.3b.

If we impose periodic boundary condition along the \( x \)-direction and assuming there are \( L \) unit cells along that direction, then we have \( L \) zero-energy states with momenta given by

\[
k = \frac{2\pi j}{La'} \quad j = 0, 1 \cdots, L - 1
\]  \hspace{1cm} (3.31)

To summarize the results, we showed that the tight-binding model of graphene nano-ribbons with ZB edge has exact zero energy modes, one-third of these modes
are localized around the zigzag edge and two-third are localized around the Bearded edge.

3.4.1 Lieb’s theorem and edge magnetism

In condensed matter physics there aren’t many exact statements about the properties of the ground states of many-body systems. Lieb’s theorem is one of those few which convinces us about the magnetism of edges states of graphene with Hubbard interaction. Lieb’s theorem is an exact statement about the magnetic properties of the ground state of the Hubbard model at half-filling:

\textit{Lieb’s Theorem:} Consider a tight-binding repulsive Hubbard model \( U > 0 \) on bipartite lattice and hopping term only between \( A \) and \( B \) sites and half-filled band. Then the ground state is unique, up to spin degeneracy, and has spin \( S = \lfloor N_A - N_B \rfloor / 2 \).

We saw that for graphene ribbon with ZB boundary, numbers of atoms are different in two sub-lattices and \( N_A - N_B = L \). Then Lieb’s theorem tells us that if we turn on on-site Hubbard repulsion, no matter how small \( U \) is, the ground state of this system has to have spin \( S = L/2 \).

We showed in section [3.3] that weak Hubbard interactions are irrelevant in low-energy effective picture of bulk graphene and the ground state of bulk graphene remains paramagnetic semi-metal. So if the bulk is not magnetized then where does this spin \( L/2 \) live?

The only physical explanation of the Lieb’s theorem result seems to be that the fully polarized edge state multiplet persists as the (unique) ground state as we turn on \( U \), also the spin of the ground state predicted from Lieb’s theorem is in agreement with the number of edge modes. This picture can be further substantiated by calculating the weak interaction between the upper and lower edges, of order \( U^2 / (tW^2) \). This interaction is found to be ferromagnetic, as we show below. Thus there must be a spin \( \approx L/6 \) on the zigzag edge and \( \approx L/3 \) on the bearded edge, with these two spins coupled ferromagnetically.
Now consider replacing the bearded edge by a second zigzag edge. Lieb’s theorem [66] now implies a zero spin ground state since we have equal numbers of $A$ and $B$ sites. Now, at $U = 0$, we have approximately $L/3$ edge states on both lower and upper edges. These mix to form two bands, with $2\pi/3 \leq k \leq 4\pi/3$, with energies exponentially small in $W$ and symmetric around $E = 0$. Ignoring inter-edge interactions, we expect spin $\approx L/6$ on both upper and lower edges. In this case, the intra-edge interaction of order $U^2/(tW^2)$ is antiferromagnetic, implying a zero spin ground state consistent with the result from Lieb’s theorem. A further consistency check can be obtained by going smoothly between zigzag and bearded lower edges by turning on the hopping term, $t'$ on the hairs. Lieb’s theorem implies spin $L/2$ for all $t$, $t'$ and $U > 0$. For $t' = 0$ we have a ZZ ribbon together with $L$ decoupled sites sitting below the lower edge. The ZZ ribbon has spin 0 but we can obtain a state with total spin $L/2$ by polarizing the electron spins at the decoupled sites. Although the zigzag ribbon has total spin 0, for large $W$ we expect that the upper and lower edges have spin $\approx L/6$ with antiferromagnetic inter-edge coupling. Turning on $t'$ produces an effectively antiferromagnetic coupling between the spin $\approx L/6$ on the lower zigzag edge and $L/2$ on the nearly decoupled sites. This gives a moment $\approx L/3$ which is now ferromagnetically coupled to the upper edge, giving a total spin of $L/2$ as required by Lieb’s theorem.

Assuming that the ground state remains an unpolarized Dirac liquid up to $U = U_c$, the magnetism of the edges seems to follow from Lieb’s theorem for large $W$. If the transition at $U_c$ is into a bulk antiferromagnetic state (with, for example, spin up on $A$ sites and spin down on $B$ sites) then the edge magnetism should persist, since it is of this type, and may be regarded as a sort of precursor of the bulk antiferromagnetic order. The simplest possibility is that the system goes from Dirac liquid into Mott-Hubbard insulator at $U_c$ but numerical evidence [67] has been presented for a spin liquid phase at intermediate $U$, of unknown edge magnetic properties.

We note that the above arguments also apply to carbon nanotubes [59, 68, 69]. Indeed, since we have been considering periodic boundary conditions in the $x$-direction, we have actually been discussing tubes, of circumference $L$ and length $W$. The magnetic moments exist on the upper and lower caps (i.e. rings) of the nan-
otubes with ferromagnetic or antiferromagnetic inter-ring coupling for a bearded or zigzag lower ring respectively. (The half-filled bulk of the nanotube might be in a 1D version of a Mott-Hubbard insulating state but this only serves to weaken the effects of bulk states on edge states.)

This is an intuitive argument and need to be examined carefully, in the following section we will find an effective Hamiltonian which describes the edge modes in presence of Hubbard interaction and will prove that the ground state of that Hamiltonian is ferromagnetic state.

3.5 Projected Hubbard Model of the edge states

In this section we find the effective Hamiltonian which describes the dynamics of edge states. As we showed the exact form of edge states is only known for either semi-infinite graphene sheet with zigzag edge or finite ribbon with zigzag-bearded edges. In this section we focus on the case of semi-infinite sheet with zigzag edge, similar result holds for ZB case.

To find the effective low-energy model describing the edge states, we keep all the edge states and only bulk states near the Dirac points, within cut-off given by $\Lambda$. To write the fermion operator in term of low-energy excitations, edge states and near the Dirac point excitations, we need to consider that for semi-infinite sheet the edges are only on the sub-lattice $A$. Thus we have

$$a_\sigma(k,y) = \alpha_{k,y} e_\sigma(k) + \Theta(k) \phi_{A,\sigma}(k,y) + \Theta'(k) \phi'_{A,\sigma}(k,y)$$
$$b_\sigma(k,y) = \Theta(k) \phi_{B,\sigma}(k,y) + \Theta'(k) \phi'_{B,\sigma}(k,y)$$

(3.32)

Where $a(k,y)$ and $b(k,y)$ are original electron operator on each sub-lattice, which are Fourier transformed along the $x$ direction. $\Theta(k) = \theta(\Lambda - |k - 2\pi/3a|)$ and $\Theta'(k) = \theta(\Lambda - |k - 4\pi/3a|)$ are sharp cut-off for the excitations near the Dirac points and $\phi_{A/B,\sigma}(k,y)$ are slowly varying operators as function of $y$, also $\alpha_{k,y}$ is given by Eq. (3.27)

$$\alpha_{k,n} = (-2\cos \frac{ka}{2})^n e^{ikna/2} \alpha_{k,0}$$

(3.33)
The equation \(3.32\) could be written in a compact form as

\[
\Psi_{\sigma}(k,y) = \alpha_{k,y} e_{\sigma}(k) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \Theta(k) \Psi_{1,\sigma}(k,y) + \Theta'(k) \Psi_{2,\sigma}(k,y) \tag{3.34}
\]

By Fourier transforming the operators along the \(x\) direction the Hubbard interaction Eq. \(3.20\) becomes

\[
\mathcal{H}_U = U N_x \sum_{k,k',q} A_{\uparrow}(m,k+q) A_{\uparrow}(m,k') A_{\downarrow}(m,k'-q) A_{\downarrow}(m,k') + a \leftrightarrow b \tag{3.35}
\]

Now by plugging in the Eq. \(3.38\) into the Hubbard Hamiltonian Eq. \(3.35\), we will have different kinds of interacting terms as follow: a) \(4 - \text{edge} \) interaction, which describes the first order induced interaction on the edges. b) \(2 - \text{edge} 2 - \text{bulk} \) term, which describes the interaction between two edge operator with two bulk operator, c) \(3 - \text{edge} 1 - \text{bulk} \) term and finally d) \(1 - \text{edge} 3 - \text{bulk} \) term. We describe each term in detail as follow:

\textit{4-edge interaction:}

By only keeping the edge operators, the first order effective interaction of edge excitations is given by

\[
\mathcal{H}_{U} = \frac{U}{N_x} \sum_{k,k',q} \Gamma(k,k',q) e_{\uparrow}(k+q) e_{\downarrow}(k) e_{\uparrow}(k'-q) e_{\uparrow}(k') \\
\Gamma(k,k',q) = \sum_{m} \alpha_{k+q,m} \alpha_{k,m} \alpha_{k',q,m} \alpha_{k',m} \tag{3.36}
\]

The summation over \(m\) can be done exactly and the result is

\[
\Gamma(k,k',q) = \frac{|(1 - (2\cos \frac{k}{2})^2)(1 - (2\cos \frac{k+q}{2})^2)(1 - (2\cos \frac{k'-q}{2})^2)(1 - (2\cos \frac{k'}{2})^2)|^{\frac{1}{2}}}{1 - 16\cos \frac{k}{2} \cos \frac{k+q}{2} \cos \frac{k'-q}{2} \cos \frac{k'}{2}} \tag{3.37}
\]

where all the momenta, \(k,k',k+q,k'-q\) are restricted to the interval \([2\pi/3, 4\pi/3]\), as there is no edge mode outside this interval.
2-edge, 2-bulk interaction:

For 2−edge 2−bulk interactions we have 6 different terms which we need to study. To simplify the terms we write the electron operators on A sites as follow

\[ a_\sigma(k,y) = \alpha_{k,y}e_\sigma(k) + \Phi_{A,\sigma}(k,y) \]

\[ \Phi_{A,\sigma}(k,y) = \Theta(k)\phi_{A,\sigma}(k,y) + \Theta'(k)\phi^\dagger_{A,\sigma}(k,y) \]  

(3.38)

by using this notation we have all six term as follow

\[ H_1 = \frac{U}{N_x} \sum \lambda(k+q,k,y)e^\dagger_\uparrow(k+q)e_\downarrow(k)\Phi^\dagger_{A,\downarrow}(k'-q,y)\Phi_{A,\downarrow}(k',y) + \uparrow\leftrightarrow\downarrow \]

\[ H_2 = -\frac{U}{N_x} \sum \lambda(k+q,k',y)e^\dagger_\downarrow(k+q)e_\uparrow(k')\Phi^\dagger_{A,\uparrow}(k'-q,y)\Phi_{A,\uparrow}(k,y) + \uparrow\leftrightarrow\downarrow \]

\[ H_3 = -\frac{U}{N_x} \sum \bar{\lambda}(k+q,k'-q,y)e^\dagger_\uparrow(k+q)e_\uparrow(k')\Phi^\dagger_{A,\uparrow}(k',y)\Phi_{A,\downarrow}(k,y) + \uparrow\leftrightarrow\downarrow \]  

(3.39)

Where

\[ \lambda(k+q,k,y) = \alpha^\ast(k+q,y)\alpha(k,y) \]

\[ \bar{\lambda}(k+q,k,y) = \alpha^\ast(k+q,y)\alpha^\ast(k,y) \]  

(3.40)

To first order, mean-field level, we could replace the bulk operators in Eq. (3.39) by their expectation values, where at half-filling \( \langle a_\sigma^\dagger(k+q,y)a_\sigma k,y \rangle = \delta_{\sigma,\sigma'}\delta_{q,0}/2 \) and by using Eq. (3.38) we have

\[ \langle \Phi^\dagger_{A,\sigma}(k'-q,y)\Phi_{A,\sigma'}(k',y) \rangle = \frac{1}{2}\delta_{\sigma,\sigma'}\delta_{q,0} (1-|\alpha_{k,y}|^2) \]

\[ \langle \Phi_{A,\sigma}(k,y)\Phi_{A,\sigma'}(k',y) \rangle = 0 \]  

(3.41)

From first line and knowing the fact that \( \alpha_{k,y} \) exponentially goes to zero as function of \( y \), we see that the bulk states remain at half filling. By using this result and also
Eq. (3.36) the final form of the projected edge Hamiltonian is

\[
\mathcal{H} = -\frac{U}{2N_x} \sum_{k,k',q} \Gamma(k,k',0) e_\sigma^\dagger(k) e_\sigma(k) + \frac{U}{N_x} \sum_{k,k',q} \Gamma(k,k',q) e_\uparrow^\dagger(k+q) e_\uparrow(k) e_\downarrow^\dagger(k' - q) e_\downarrow(k')
\]  
(3.42)

In section 3.7 we come back and consider in more details the effect of fluctuations of bulk excitations. They lead to higher order interaction terms between and on the edges, and also interesting results about the correlation between the two edges for finite ribbon. Let’s first study the ground state properties of Hamiltonian 3.42.

### 3.5.1 Ferromagnetic ground state

As we see the Hamiltonian 3.42 has very complicated form but we will see that it could be written in a special form, such that we could rigorously prove the ferromagnetism of its ground state at half-filling.

Hamiltonian 3.42 could be written in more symmetric form, which is manifestly SU(2) symmetric and particle-hole symmetric.

\[
\begin{align*}
\mathcal{H} &= \frac{1}{2} \sum_{k,k',q} \Gamma(k,k',q) \left[ \sum_\sigma e_\sigma^\dagger(k+q) e_\sigma(k) - \delta_{q,0} \right] \times \\
&\quad \left[ \sum_\sigma e_\sigma^\dagger(k'-q) e_\sigma'(k') - \delta_{q,0} \right] + E_0 \\
E_0 &= -\frac{1}{2} \sum_{k,k'} \Gamma(k,k',0)
\end{align*}
\]  
(3.43)

Here \(e_\alpha(k)\) annihilates an electron in an edge state with momentum \(k\) and spin \(\alpha = \uparrow\) or \(\downarrow\). The interaction function is given by Eq. (3.37), and the sum over \(k, k'\) and \(q\) is restricted to the band in which \(2\pi/3 < k, k', k+q, k'-q < 4\pi/3\) and \(\Gamma(k,k',q)\) is strictly positive [70]. Periodic boundary conditions in the \(x\)-direction imply \(k = 2\pi n/L\) so the number of wave-vectors \(N \approx L/3\). Note that we are considering the case of half-filling in the entire lattice and that the edge Hamiltonian is therefore
invariant under the particle-hole symmetry transformation:

$$e_\alpha(k) \leftrightarrow e_\alpha^+(k).$$ \hspace{1cm} (3.44)

This is highly unusual since normally a particle-hole symmetry transformation relates a particle and hole at different wave-vectors. Here with an exactly flat band, the particle and hole operators occur at the same wave-vectors. It is important to note that $\Gamma(k,k',q)$ arose from summing the wave-function of the edge states over sites at arbitrary distance $n$ from the zigzag edge and can be written:

$$\Gamma(l,k,q) = \sum_{n=0}^{\infty} g_n(k) g_n(l) g_n(l+q) g_n(k-q)$$ \hspace{1cm} (3.45)

where

$$g_n(k) = \theta(1 - |2\cos k/2|) \sqrt{1 - \left(2\cos k/2\right)^2} \left(2\cos k/2\right)^n.$$ \hspace{1cm} (3.46)

Thus, dropping the constant $E_0$, we may write:

$$\mathcal{H} = \frac{1}{2} \sum_{n,q} O_n^+(q) O_n(q)$$ \hspace{1cm} (3.47)

with

$$O_n(q) = \sum_k g_n(k) g_n(k+q) \left[ \sum_\sigma e_\sigma^+(k+q) e_\sigma(k) - \delta_{q,0} \right]$$ \hspace{1cm} (3.48)

It follows that all eigenstates of $H$ are non-negative. It is easy to show that fully spin-polarized state is a zero energy eigenstate and therefore a ground state. To check this consider, for example, the representative fully polarized state where all electron spins are in the up direction. Then clearly $O_n(q)$ annihilates this state for all non-zero $q$ since the spin up terms in $O_n(q)$ try to produce a spin up electron in an occupied state with wave-vector $k+q$ while the spin down terms try to annihilate a spin down electron in a vacant state of wave-vector $k$. $O_n(0)$ also annihilates this state since the occupancy of each single particle state is precisely 1.

It is also possible, though more difficult, to argue that the fully polarized multiplet, of spin $S = L/6$, are the unique groundstates of the projected 1D Hamiltonian. To prove that fully polarized states are the unique ground states of $H$ we need to
prove that the only states annihilated by \( O_n(q)^\dagger O_n(q) \) for all \( n \) and \( q \) are fully polarized (that is, have maximal total spin). For convenience, in this paragraph, we take all momenta to be in the region of \([-\pi/3, \pi/3]\), which can be obtained by shifting all of them by \( \pi \). Suppose \( |\psi\rangle \) is such that for any \( n, q \), \( O_n(q)|\psi\rangle = 0 \). Then we have

\[
\sum_k g_n(k) g_n(k + q) [\sigma^+(k + q) \sigma(k) - \delta_{q,0}] |\psi\rangle = 0 \tag{3.49}
\]

and by knowing that \( g_n \) is even function and \( g_n(k) g_n(k + q) = g_n(-k) g_n(-k - q) \), we rewrite above equation as

\[
\sum_{k > 0} g_n(k) g_n(k + q) \left[ \sigma^+(k + q) \sigma(k) + \sigma^+(k) \sigma(-k - q) - 2\delta_{q,0} \right] |\psi\rangle = 0 \tag{3.50}
\]

(Repeated spin indices are summed in this section.) For fixed \( q \) and using the definition of \( g_n \) we have, for any \( n \) that

\[
\sum_{k > 0} \left( 4\sin\left(\frac{k}{2}\right) \sin\left(\frac{k + q}{2}\right) \right)^n |\psi_k^{(q)}\rangle = 0 \tag{3.51}
\]

\[
|\psi_k^{(q)}\rangle = \sqrt{1 - (2\sin k/2)^2} \sqrt{1 - (2\sin (k + q)/2)^2} \times \left[ \sigma^+(k + q) \sigma(k) + \sigma^+(k) \sigma(-k - q) - 2\delta_{q,0} \right] |\psi\rangle \tag{3.52}
\]

Since \( n \) runs from 0 to \( \infty \), the number of independent momenta is \( L/3 \) and all the \( \left( 4\sin(\frac{k}{2}) \sin(\frac{k + q}{2}) \right) \) are different, the determinant of the Vandermonde matrix is non-zero so Eq. (3.51) is satisfied if and only if for any \( k, q \) we have

\[
\left[ \sigma^+(k + q) \sigma(k) + \sigma^+(k) \sigma(-k - q) - 2\delta_{q,0} \right] |\psi\rangle = 0 \tag{3.53}
\]

First, using Eq. (3.53) for \( q = 0 \), we get \( n(k) + n(-k) = 2 \), thus the only possible terms have \( n(k) = n(-k) = 1 \) or \( n(k) = 0 \) and \( n(-k) = 2 \) or vice versa. In general
\(|\psi\rangle\) could be written as a linear combination of Fock states \(\prod c_\sigma^\dagger(k)|0\rangle\). We first will show that in the expansion of \(|\psi\rangle\) in terms of such states there is no Fock state which for any momentum \(k\) we have a vacancy or double occupancy in that momentum state. In other words, in the expansion of \(|\psi\rangle\), with condition 3.53 and \(n(k) + n(-k) = 2\), only Fock states with singly occupied momentum states are allowed.

Suppose that there is a state which has the property \(n(k) + n(-k) = 2\) for any \(k\) and has double occupancy at momentum \(l\) (vacancy at momentum \(-l\)); call this state \(\phi\):

\[|\phi\rangle = |\cdots, 0, \downarrow, \uparrow, \cdots\rangle\]  \hspace{1cm} (3.54)

and we suppose \(\langle\phi|\psi\rangle \neq 0\). We impose the condition 3.53 on \(|\psi\rangle\) for \(q = -2l\) and \(k = l\). Thus we should have \(e_\sigma^\dagger(-l)e_\sigma(l)|\psi\rangle = 0\). Let us first look at the action of \(e_\sigma^\dagger(-l)e_\sigma(l)\) on \(\phi\),

\[e_\sigma^\dagger(-l)e_\sigma(l)|\phi\rangle = e_\sigma^\dagger(-l)e_\sigma(l)|\cdots, 0, \downarrow, \uparrow, \cdots\rangle\]

\[= |\cdots, \uparrow, \cdots, \downarrow, \cdots\rangle - |\cdots, \downarrow, \cdots, \uparrow, \cdots\rangle\]  \hspace{1cm} (3.55)

Now, in order to satisfy the condition \(e_\sigma^\dagger(-l)e_\sigma(l)|\psi\rangle = 0\), we should have some other Fock states in the expansion of \(|\psi\rangle\) such that the action of \(e_\sigma^\dagger(-l)e_\sigma(l)\) on them could cancel the terms created in the second line of Eq. (3.55). \(e_\sigma^\dagger(-l)e_\sigma(l)\) only acts on states with momentum \(l\) and \(-l\), as a result does not change the spin configurations of the other (singly occupied) states. There are only three possible Fock states which have the same configurations of the singly occupied states are:

\[|1\rangle = |\cdots, \downarrow, \cdots, 0, \cdots\rangle\]

\[|2\rangle = |\cdots, \uparrow, \cdots, \downarrow, \cdots\rangle\]

\[|3\rangle = |\cdots, \downarrow, \cdots, \uparrow, \cdots\rangle\]  \hspace{1cm} (3.56)
if we operate $e^\dagger_\alpha(-l)e_\alpha(l)$ on these states, we get

\[
e^\dagger_\alpha(-l)e_\alpha(l)|1\rangle = 0
\]
\[
e^\dagger_\alpha(-l)e_\alpha(l)|2\rangle = \cdots, \downarrow \uparrow, \cdots, 0, \cdots
\]
\[
e^\dagger_\alpha(-l)e_\alpha(l)|3\rangle = -|\cdots, \downarrow \uparrow, \cdots, 0, \cdots\rangle
\]

(3.57)

None of these states are able to cancel the terms created on (3.55). Then the assumption is wrong and we have to have $\langle \phi | \psi \rangle = 0$. Having proven this, we show that in the expansion of $|\psi\rangle$ in terms of singly occupied Fock states, only symmetric combinations like the following are acceptable

\[
|\cdots, \uparrow, \cdots, \downarrow \rangle + |\cdots, \downarrow, \cdots, \uparrow \rangle
\]

(3.58)

Suppose that, the Fock expansion of $|\psi\rangle$ has a term like

\[
|\cdots, \uparrow, \cdots, \downarrow \rangle
\]

Now by choosing $k = k_1$ and $q = k_2 - k_1$ we should have

\[
(e^\dagger_\alpha(k_2)e_\alpha(k_1) + e^\dagger_\alpha(-k_1)e_\alpha(-k_2)|\psi\rangle = 0
\]

We also have

\[
e^\dagger_\alpha(k_2)e_\alpha(k_1)|\cdots, \uparrow, \cdots, \downarrow \rangle = |\cdots, 0, \cdots, \downarrow \uparrow \rangle
\]
\[
e^\dagger_\alpha(k_2)e_\alpha(k_1)|\cdots, \downarrow, \cdots, \uparrow \rangle = -|\cdots, 0, \cdots, \downarrow \uparrow \rangle
\]

(3.59)

Thus we see that the symmetric combinations leads to zero, while the anti-symmetric ones give us a non-zero result. Thus $|\psi\rangle$ must be fully symmetric under exchanging all spins and is therefore of maximal spin.
Figure 3.4: Energy to add a spin down electron of momentum $k$ for various values of $\eta \equiv \Delta / U \equiv (t^2 - V_e) / U$.

3.6 Effects of the Excitations in presence of NNN-hopping and single site potential

In this section we investigate the effects of NNN hopping and single site potential on the stability of the ferromagnetic ground state. One interesting quantity that follows from the Hamiltonian is the energy to add a spin down electron of momentum $k$, which is the same as the energy to remove a spin up electron of momentum $k$:

$$\varepsilon_k = \frac{U}{2L} \sum_{k'} \Gamma(k, k', 0). \quad (3.60)$$

This quantity is plotted (at $L \to \infty$) in Fig. 3.4. It vanishes linearly at the Dirac points, $k = 2\pi / 3, 4\pi / 3$. In principle, $\varepsilon_k$ could be measured in Angle-Resolved Photoemission Spectroscopy (ARPES) experiments. The corresponding electron addition or removal energy is given by $\varepsilon_k$. The corresponding density of states $\propto 1/|d\varepsilon_k / dk|$ could be measured by Scanning Tunneling Microscope (STM). With a spin-polarized STM tip and an edge fully polarized in the $z$-direction, it would only be possible to tunnel in a spin-down electron or tunnel out a spin-up electron.

We have calculated numerically the lowest energy particle-hole state of total
Figure 3.5: Lowest energy particle-hole state (circles) and bottom of the particle-hole continuum (lines) for various values of $\eta \equiv \Delta/U \equiv (t_2 - V_e)/U$.

momentum $q$, for $L$ up to 602 ($N = 200$). This is plotted in Fig. 3.5 along with the bottom of the particle-hole continuum. We see that a strongly bound exciton exists for most values of $q$, as might be expected in this strongly interacting system. However, the binding energy vanishing at $q = \pm 2\pi/3$. This vanishing can be understood from the fact that $\Gamma(k, k', q)$ vanishes when $k$ or $k'$ is at a band edge $2\pi/3$ or $4\pi/3$ so the zero energy particle and hole become non-interacting at wave-vector $2\pi/3$ and $-2\pi/3$ or vice versa.

While Lieb’s theorem continues to imply a fully polarized ground state at sufficiently small $U$ for any hopping terms between opposite sub-lattices ($A$ to $B$), adding a small $[O(U)]$ second neighbor hopping term, $t_2$, may destroy the fully polarized state. Likewise, a single site potential, $V_e$, acting at the edge of the ribbon only, could destroy the fully polarized state. Temporarily ignoring interactions, the zigzag edge states survive at finite $t_2$ and $V$ but develop a non-zero dispersion given, to first order in $\Delta \equiv t_2 - V_e$, by [71]: $E_2(k) - \varepsilon_F = \Delta(2\cos k + 1)$. breaking the particle-hole symmetry. Here we are assuming, for simplicity, that the bulk chemical potential is at the energy of the bulk Dirac points, which becomes
\[ \varepsilon_F = 3t_2. \] (Shifting \( \varepsilon_F \) away from the Dirac points, the Hubbard interactions have a larger effect in the bulk rendering the edge model approach more questionable.) Including a small \( U \), the energy to add a spin down electron or remove a spin up electron at momentum \( k \) now becomes

\[ E_{p/h}(k) = \varepsilon_k \pm \Delta(2\cos k + 1). \] (3.61)

respectively, where \( \varepsilon_k \) is given in Eq. (3.60). \( E_p(k) \) is plotted in Fig. 3.4 for several values of \( \Delta \). We see that for \(|\Delta| < \Delta_c \approx 0.109U\), the energy to add an electron or hole remains positive, so the edge states remain undoped. A local minimum at \( k = \pi \) develops in \( E_p(k) \) for \( \Delta > .087U \), and \( E_p(k) \) becomes negative in the vicinity of \( k = \pi \) for \( \Delta > \Delta_c \). The lowest energy of a particle-hole state, and the bottom of the particle-hole continuum for various values of \( \Delta \) are shown in Fig. 3.5. We see that the exciton becomes unbound except for wave-vectors near zero, as \(|\Delta| \) increases. For \(|\Delta| > \Delta_c \) the edge states become doped, adsorbing electrons or holes from the bulk. The simplest assumption for \(|\Delta| > \Delta_c \) is that a Fermi sea of spin-down electrons or spin up holes forms near \( k = \pi \), for \( \Delta > \Delta_c \) or \( \Delta < -\Delta_c \) respectively. This assumption is reasonable since there appear to be no bound excitons for \( \Delta > \Delta_c \). We also calculated for \( \Delta \) near \( \Delta_c \) and \( L \leq 74 \), the lowest energy state with \( M = N/2 - 2 \), finding no states below the 2-particle, 2-hole continuum, consistent with this assumption. These are exact eigenstates of the Hamiltonian of Eq. (3.43), (3.61) with the added holes or particles non-interacting. The corresponding exact result for magnetization versus \( \Delta \) is plotted in Fig. 3.6, given this assumption. The non-interacting nature is a simple consequence of the fact that the on-site Hubbard model only gives interaction between electrons of opposite spin. On the other hand, we cannot rule out the possibility that the ground state for \( \Delta > \Delta_c \) contains a finite density of spin-up holes as well as the spin-down electrons (and similarly for \( \Delta < -\Delta_c \)). In that case, Hubbard interactions have a non-trivial effect. In any event, adding a nearest neighbour Coulomb repulsion term to the bulk Hamiltonian has no effect on the projected edge Hamiltonian, since such a term acts between \( A \) and \( B \) sites whereas the zigzag edge states live entirely on one sublattice. On the other hand, a second neighbour Coulomb repulsion, \( U_2 \), produces interactions between electrons with parallel spins in the projected
edge Hamiltonian. While this doesn’t change our conclusions qualitatively in the undoped phase, it will produce interaction effects in the ground state for the doped case even if contains only particles or only holes. However, we might expect $U_2 \ll U$, in which case these effects could be quite small. Thus in general we expect a one or two component Luttinger liquid for $|\Delta| > \Delta_c$. On the other hand the edge phase occurring for $|\Delta| < \Delta_c$ is definitely not a Luttinger liquid. Instead, it might be described as a fully spin-polarized semi-metal since all levels are filled with spin-up electrons and there is a non-zero electron and hole addition energy for all wave-vectors accept the band-edges, $2\pi/3$ and $4\pi/3$.

### 3.7 Effective inter-edge and intra-edge interactions

There are also important effects of $O(U^2/t)$ which arise from the interactions between bulk and edge states. We can consider integrating out the bulk states to obtain a low energy effective action for the edge states. Due to the gapless nature of the bulk Dirac spectrum, this produces long range retarded interactions among the edge excitations. Decay processes of edge into bulk electrons are forbidden by energy-momentum conservation but the Feynman diagrams of Fig. 3.7 induce quartic interaction terms. For large $W$ and low energies we may calculate these
interactions keeping only the low energy bulk states near the Dirac points, using the corresponding Dirac propagators. Note that we ignore interaction effects in the bulk, as discussed above. This is rather similar to an RKKY interaction. The interaction involving the dynamical spin operators \[ \vec{S}_{U/L}(\omega, q) \] on the upper and lower edge, respectively is:

\[
S_{\text{inter}} = \int \frac{dq d\omega}{(2\pi)^2} \vec{S}_U(\omega, q) \cdot \vec{S}_L(-\omega, -q) J_{\text{inter}}(\omega, q, W) \quad (3.62)
\]

where

\[
J_{\text{inter}}(\omega, q, W) = 2 U^2 \int \frac{d\omega' dk}{(2\pi)^2} G(\omega', k, 0, W) G(\omega - \omega', -k, 0, W). \quad (3.63)
\]

Here \( G(\omega, k, 0, W) \) is the bulk free electron Green’s function with momentum \( k \) in the \( x \)-direction at \( y = 0 \) and \( y = L_y \) with appropriate zigzag or bearded boundary conditions and projected onto the sublattices corresponding to the upper and lower edge (\( A - A \) for zigzag-bearded or \( A - B \) for zigzag-zigzag (ZZ)). Using the linearized, Dirac dispersion relation, which is valid at small \( 1/W, \omega/t \), and \( q \),

\[
G_{\text{ZZ}}(\omega, k, y = 0, y' = W) = \frac{2iv_F^2}{W} \sum_n (-1)^n \frac{k_n^2 \omega}{ \epsilon^2(k_x, k_n)(\omega^2 + \epsilon^2(k_x, k_n))} \quad (3.64)
\]

where \( \epsilon(\vec{k}) = v_F|\vec{k}| \) is the Dirac dispersion relation. \( G_{\text{ZZ}} \) is given by the same expression with \( \omega \) replaced by \( i\epsilon(k_x, k_n) \) in the numerator inside the sum. The sum over \( n \) can be taken up to an arbitrary ultra-violet cut-off whose value doesn’t affect the behavior at small \( 1/W, \omega/t \) and \( q \). \( k_n = \pi n/W \) for the ZB case. Although the wave-vectors of edge modes are phase-shifted from these values in the ZZ case, this can be ignored at leading order in \( 1/W \), allowing us to again use \( k_n = \pi n/W \).

It is straightforward to evaluate \( J_{\text{inter}}(\omega, q, W) \) numerically with the two types of edges. The characteristic scales for the \( \omega \) and \( q \) dependence of \( J_{\text{inter}} \) are set by \( t/W \) and \( 1/W \), respectively. Since the energy scale of the inter-edge interaction in Eq. (3.64) is \( U^2/(tW^2) \), it should be permissible to ignore the retardation, and evaluate \( S_{\text{inter}} \) at \( \omega = q = 0 \) to calculate the properties of low energy states. This
Figure 3.7: Feynman diagrams inducing edge interactions from integrating out bulk states.
gives:

\[ J_{ZB/ZZ}(W) = \mp c \frac{U^2}{t} \frac{1}{W^2} \]  

(3.65)

where the positive constant \( c \) is given by the convergent sums and integral:

\[
c \equiv \frac{\sqrt{3}}{\pi} \times \sum_{n,m=1}^{\infty} (-1)^{n+m} \times \int_{-\infty}^{\infty} d\kappa \frac{n^2 m^2}{(\kappa^2 + m^2)(\kappa^2 + n^2)} \frac{1}{\sqrt{\kappa^2 + m^2 + \sqrt{\kappa^2 + n^2}}} \approx 0.20
\]

(3.66)

(A similar result was obtained in [73, 74] for the ZZ case.) We see that the ground state for the zigzag-bearded ribbon has spin \( L/2 \) while that for the zigzag-zigzag case has spin 0, as shown above rigorously using Lieb’s theorem. The remarkable fact that the change in sign of this tiny coupling drastically changes the spin of the ground state provides evidence for the polarized nature of the edge spins. There is also a large manifold of low energy states, which are simply the eigenstates of \( J_{ZZ} \vec{S}_T \cdot \vec{S}_B \) with \( S_T = S_B = L/6 \) (in the ZZ case).

Another important effect of \( O(U^2/t) \) is the intra-edge interaction, independent of \( W \). For a zigzag edge by integrating out the low-energy bulk excitations, the spin part is:

\[
S_{\text{intra}} = \int \frac{dq d\omega}{(2\pi)^2} \vec{S}(\omega, q) \cdot \vec{S}(\omega, q) J_{\text{intra}}(\omega, q)
\]

(3.67)

with

\[
J_{\text{intra}}(\omega, q) = 2 U^2 \int_{k,\omega'/v_f < \Lambda} \frac{d\omega' dk}{(2\pi)^2} G(\omega', k, y = y' = 0) G(\omega - \omega', q - k, y = y' = 0)
\]

(3.68)

Now the free bulk Green’s function, with zigzag edge boundary conditions, may be evaluated for a semi-infinite system, giving, at small \( k_x \) (measured from a Dirac
point) and small $\omega$:

$$G(\omega, k_x, y = y' = 0) \approx 2i\nu_F^2 \int \frac{dk_y}{2\pi} \frac{k_y^2}{(v_F k)^2} \frac{\omega}{\omega^2 + (v_F k)^2}$$  \hspace{1cm} (3.69)$$

By using this green function, the $J_{\text{intra}}$ of Eq. (3.68) is ultraviolet divergence and the integral should be cut off at some point $\Lambda$. Although the resulting $J_{\text{intra}}(\omega, q)$ is cut off dependent, by ignoring the weak retardation, the corrections to the energy of the excitons is proportional to $J_{\text{intra}}(0, q) - J_{\text{intra}}(0, 0)$, which is cut off independent. For small $\omega$ and $q$ these $O(U^2)$ intra-edge interactions become more singular than the $O(U)$ terms by logarithmic factors of $q^2 \ln q$.

$$\varepsilon_{\text{ex}}(q) \approx 0.36 U q^2 - \frac{\sqrt{3}(4 - \pi)}{(2\pi)^2}(U^2 / t)q^2 \ln q^2$$  \hspace{1cm} (3.70)$$

As mentioned above, Eq. (3.68) only includes the effect of low energy bulk excitations; it is still possible that the high energy bulk excitations could wipe out this singularity of the exciton dispersion relation. By using the exact form of the bulk wavefunctions one can determine the exact intra-edge interaction of $O(U^2)$. This has a more complicated form than Eq. (3.68). Nonetheless, it can be shown that the only part of this interaction which contributes to this $\ln q$ singular correction to the exciton dispersion relation is the contribution from low energy bulk excitations of the form of Eq. (3.68).

We leave a more detailed study of these effects of $O(U^2)$ and higher for the future. A reasonable approach might be to ignore the bulk interactions, since they are irrelevant, but analyze the bulk-edge Hubbard interactions using the renormalization group. This corresponds to a novel type of boundary critical phenomena in which the bulk is a massless (2+1) dimensional Dirac liquid and the edge is a one-dimensional spin-polarized semi-metal. The arguments based on Lieb’s theorem imply that the edge magnetic moment remains stable against weak interactions.

### 3.8 Details of field theory calculations

In previous section we gave the result of integrating out bulk excitations and the effective induced higher order inter– and intra– edge interactions. In this section
we give the more detailed procedure of finding those higher-order interactions. We will consider two cases of graphene ribbon with zigzag-bearded and zigzag-zigzag edges.

As we discussed in section 3.3 the effective Hamiltonian describing bulk excitations is Dirac Hamiltonian

\[
H = -iv_F \int dx \, dy \left[ \Psi_1^\dagger(\vec{r}) \sigma \nabla \Psi_1(\vec{r}) + \Psi_2^\dagger(\vec{r}) \bar{\sigma} \nabla \Psi_2(\vec{r}) \right] \quad (3.71)
\]

For infinite graphene sheet, we could simply work in momentum space and fermion propagators are simply given by

\[
\langle \Psi_1(\vec{q}, \omega) \Psi_1^\dagger(\vec{q}, \omega) \rangle = \frac{1}{\vec{q} \cdot \sigma + i\omega} \quad \langle \Psi_2(\vec{q}, \omega) \Psi_2^\dagger(\vec{q}, \omega) \rangle = \frac{1}{\vec{q} \cdot \bar{\sigma} + i\omega} \quad (3.72)
\]

But for graphene ribbons, we do not have translational invariance along the width of the ribbon. What we have is a field theory with boundaries, and boundary conditions will change the form of single particle Green functions, which are needed to evaluate Feynman diagrams of Fig. 3.7. Let's find the effect of boundary conditions on low-energy field operators and also the green functions.

To find the impact of boundary conditions on low-energy field operators representation we follow the same approach as [75]. We start by Hamiltonian 3.71, and by using translational invariance along the \(x\)-direction we have

\[
\Psi_1(\vec{r}) = e^{ik_x x} \begin{pmatrix} \phi_A(y) \\ \phi_B(y) \end{pmatrix}, \quad \Psi_2(\vec{r}) = e^{ik_x x} \begin{pmatrix} \phi_A'(y) \\ \phi_B'(y) \end{pmatrix} \quad (3.73)
\]

The eigenfunction equation around \(K\) is given by

\[
\begin{pmatrix} 0 & k_x - \partial_y \\ k_x - \partial_y & 0 \end{pmatrix} \begin{pmatrix} \phi_A(y) \\ \phi_B(y) \end{pmatrix} = \tilde{\varepsilon} \begin{pmatrix} \phi_A(y) \\ \phi_B(y) \end{pmatrix} \quad (3.74)
\]

By solving the above equations we will find that

\[
\phi_B = Ce^{\gamma y} + De^{-\gamma y} \\
\tilde{\varepsilon} \phi_A = (k_x - \partial_y) \phi_B \quad (3.75)
\]
where the eigenvalue equation is $\tilde{\varepsilon}^2 = k_x^2 - z^2$, and $z$ could be found by imposing the correct boundary conditions (bc). The boundary conditions for $ZB$ and $ZZ$ ribbons are

$$\begin{align*}
\phi_B(0) = \phi_B'(0) = \phi_B(L_y) = \phi_B'(L_y) &= 0 \\
\phi_A(0) = \phi_A'(0) = \phi_A(L_y) = \phi_A'(L_y) &= 0
\end{align*}$$

(3.76)

where $L_y$ is the width of the ribbon, first line is $bc$ for $ZB$ ribbon and the second line is for $ZZ$ ribbon. The reason for this choice of boundary condition is more vivid if we look at Fig. 3.2. From that figure we see that the first row is zigzag edge which starts with atoms only on $A$ sub-lattice. We could imagine that some fictitious atoms are connected to these atoms from some fictitious previous row, if it exists, but the weight of wave-function is zero on those atoms. Similar argument holds for other edge.

For both $ZB$ and $ZZ$ edges, which zigzag edge starts at first row and is only on $A$ sub-lattice we have, $\phi_B(0) = 0$; this impose the condition that $C + D = 0$ for both cases. By using this condition and also Eq. (3.75) we get

$$\begin{align*}
\phi_B &= \sin(z y) \\
\tilde{\varepsilon} \phi_A &= (k_x \sin(z y) - z \cos(z y))
\end{align*}$$

(3.77)

For $ZB$ ribbon, boundary condition for lower edge is $\phi_B(L_y) = 0$ resulting in $\sin(z L_y) = 0$ which restricts the values of $z$ to $z_n = \frac{n\pi}{L_y}$. This is very interesting result, which confirms the existence of zero mode edge states. By using $\tilde{\varepsilon}^2 = k_x^2 - z^2$, for any value of $n$ if we choose $k_x = z_n$ then we get zero energy state.

For $ZZ$ ribbon the boundary condition is $\phi_A(L_y) = 0$, gives us the following transcendental equation to solve for $z$:

$$\tan(z L_y) = \frac{z}{k_x}$$

(3.78)

As we see, in contrast to $ZB$ ribbon where $z_n$ was independent of $k_x$, for $ZZ$ ribbon first of all there is no simple expression for $z_n$, and also the values of $z_n$ depends on $k_x$; for each $k_x$ by solving Eq. (3.78) we get a set of solutions for $z_n$. This implies
$z_n$ should be a function of $k_x$, but its dependence on $k_x$ is very weak and in general we could write $z_n(k_x) = [n\pi + \delta_n(k_x)]/L_y$, where $\delta_n(k_x) \in [0, \pi/2]$ and is slowly varying function of $k_x$.

Having found the effect of boundary conditions on the low-energy wave-functions and taking number of the unit cells along the width of the ribbon is $N_y$, which leads to $L_y = 3aN_y/2$, we have

$$
\Phi_B(k_x, y) = \frac{1}{\sqrt{N_y}} \sum_{k_y} \sin(k_y y) c_k
$$

$$
\Phi_A(k_x, y) = \frac{v_f}{\sqrt{N_y}} \sum_{k_y} \frac{1}{E_k} [k_x \sin(k_y y) - k_y \cos(k_y y)] c_k
$$

(3.79)

where $E_k = \pm v_f \sqrt{k_x^2 + k_y^2}$, and we changed the notation from $z$ to $k_y$, and values of $k_y$ depends on the boundary conditions.

We will see shortly that, to integrate out bulk excitations, we need these two single particle Green functions $\mathcal{T} \langle \Phi_A(k_x, \tau, y = 0) \Phi_A^\dagger(k_x, 0, y = L_y) \rangle$ and $\mathcal{T} \langle \Phi_A(k_x, \tau, y = 0) \Phi_B^\dagger(k_x, 0, y = L_y) \rangle$, for ZB ribbon and ZZ ribbon, respectively, so let’s evaluate them here.

For the case of zigzag-bearded we need

$$
G_{\text{ZB}} \equiv \mathcal{T} \langle \Phi_A(k_x, \tau, y = 0) \Phi_A^\dagger(k_x, 0, y = L_y) \rangle
$$

$$
= \frac{v_f^2}{N_y} \sum_{k_y} \frac{k_y^2 \cos(k_y L_y)}{E_k^2} \mathcal{T} \langle c_k(\tau) c_k^\dagger(0) \rangle
$$

(3.80)
In imaginary time representation we have $c_k(\tau) = e^{-E_k\tau}c_k$, thus we get

$$G_{ZB}(k_x, \tau, y = 0, y = L_y) = \frac{v_f^2}{N_y} \sum_{k_y} k_y^2 \cos(k_y L_y) \frac{1}{iE^2_k} \Theta(\tau)e^{-E_k\tau}c_k^\dagger - \frac{1}{E^2_k} \Theta(-\tau)e^{-E_k\tau}c_k^\dagger$$

$$= \frac{v_f^2}{N_y} \sum_{k_y} k_y^2 \cos(k_y L_y) \frac{1}{E^2_k} \Theta(\tau)\Theta(E_k)e^{-E_k\tau} - \Theta(-\tau)\Theta(-E_k)e^{-E_k\tau}$$

$$= \frac{v_f^2}{N_y} \sum_{k_y} k_y^2 \cos(k_y L_y) \frac{1}{\varepsilon_k} \Theta(\tau)e^{-\varepsilon_k\tau} - \Theta(-\tau)e^{\varepsilon_k\tau} \tag{3.81}$$

Where $\varepsilon_k = v_f \sqrt{k_x^2 + k_y^2}$. Now by taking the Fourier transform, we need

$$G_{ZB}(k_x, \omega, y = 0, y = L_y) = \frac{-v_f^2}{N_y} \sum_{k_y} \frac{k_y^2 \cos(k_y L_y)}{\varepsilon_k^2} \left[ \frac{1}{i\omega - \varepsilon_k} + \frac{1}{i\omega + \varepsilon_k} \right]$$

$$= \frac{2iv_f^2}{N_y} \sum_{k_y} \frac{k_y^2 \cos(k_y L_y)}{\varepsilon_k^2} \frac{\omega}{\omega^2 + \varepsilon_k^2} \tag{3.82}$$

For the case of zigzag-zigzag ribbon we have

$$G_{ZZ} \equiv \mathcal{T} \langle \Phi_A(k_x, \tau, y = 0)\Phi_B^\dagger(k_x, 0, y = L_y) \rangle$$

$$= \frac{-v_f}{N_y} \sum_{k_y} \frac{k_y \sin(k_y L_y)}{E_k} \mathcal{T} \langle c_k(\tau)c_k^\dagger(0) \rangle \tag{3.83}$$

In imaginary time representation we have $c_k(\tau) = e^{-E_k\tau}c_k$ thus we get

$$G_{ZZ}(k_x, \tau, y = 0, y = L_y) = \frac{-v_f}{N_y} \sum_{k_y} k_y \sin(k_y L_y) \frac{1}{E_k} \Theta(\tau)e^{-E_k\tau}c_k^\dagger - \frac{1}{E_k} \Theta(-\tau)e^{-E_k\tau}c_k^\dagger$$

$$= \frac{-v_f}{N_y} \sum_{k_y} k_y \sin(k_y L_y) \frac{1}{E_k} \Theta(\tau)\Theta(E_k)e^{-E_k\tau} - \Theta(-\tau)\Theta(-E_k)e^{-E_k\tau}$$

$$= \frac{-v_f}{N_y} \sum_{k_y} k_y \sin(k_y L_y) \frac{1}{E_k} \Theta(\tau)e^{-\varepsilon_k\tau} + \Theta(-\tau)e^{\varepsilon_k\tau} \tag{3.84}$$
by doing the Fourier transformation we get
\[ G_{ZZ}(k_x, \omega, y = 0, y = L_y) = \frac{v_f}{N_y} \sum_{k_y} \frac{k_y \sin(k_y L_y)}{\epsilon_k} \left[ \frac{1}{i \omega - \epsilon_k} - \frac{1}{i \omega + \epsilon_k} \right] \]
\[ = \frac{-2v_f}{N_y} \sum_{k_y} \frac{k_y \sin(k_y L_y)}{\omega^2 + \epsilon_k^2} \] (3.85)

The boundary conditions for \( ZB \) case \( \Phi_B(y = 0) = \Phi_B(y = L_y) = 0 \), restricts the values of \( k_y \) to \( k_y = \frac{n\pi}{L_y} \) where \( n \) is an integer between 0, \( \cdots, N_y \), thus for \( ZB \) case we have \( \cos(k_y L_y) = (-1)^n \). But for \( ZZ \) case the boundary conditions, \( \Phi_B(y = 0) = \Phi_A(y = L_y) = 0 \), gives us \( \tan(k_y L_y) = k_y/k_x \).

For the case of \( ZZ \) case we could write
\[ k_y^{(n)} L_y = n\pi + \delta(n, k_x) \]
where now \( \delta(n, k_x) \in [0, \pi/2] \), and is given by \( \tan(\delta(n, k_x)) = k_y^{(n)}/k_x \). By this representation we have
\[ \sin(k_y^{(n)} L_y) = \sin(n\pi + \delta(n, k_x)) = (-1)^n \sin(\delta(n, k_x)) \]
\[ = (-1)^n \frac{\tan(\delta(n, k_x))}{\sqrt{1 + \tan^2(\delta(n, k_x))}} = (-1)^n \frac{k_y^{(n)}}{\sqrt{k_x^2 + (k_y^{(n)})^2}} \] (3.86)

Thus the green functions are
\[ G_{ZB}(k_x, \omega, y = 0, y = L_y) = \frac{2iv_f^2}{N_y} \sum_n \frac{k_y^{(n)}(-1)^n \omega}{\epsilon^2(k_n, k_x) \omega^2 + \epsilon^2(k_n, k_x)} \]
\[ G_{ZZ}(k_x, \omega, y = 0, y = L_y) = \frac{-2v_f^2}{N_y} \sum_n \frac{(k_y^{(n)})^2(-1)^n \epsilon(k_y^{(n)}, k_x)}{\epsilon^2(k_y^{(n)}, k_x) \omega^2 + \epsilon^2(k_y^{(n)}, k_x)} \] (3.87)

Where \( k_n = \frac{n\pi}{L_y} \) and \( k_y^{(n)} = \frac{n\pi}{L_y} + \frac{\delta(n, k_x)}{L_y} \). By knowing that \( \delta(n, k_x) \in [0, \pi/2] \), to leading order in \( L_y \), we could approximate \( k_y^{(n)} = \frac{n\pi}{L_y} \) and green functions formula
simplifies to

\[ G_{ZB}(k_x, \omega, y = 0, y = L_y) = \frac{2v_f^2i}{N_y} \sum_{n} \frac{k_n^2(-1)^n \omega}{\epsilon^2(k_n, k_x) \omega^2 + \epsilon^2(k_n, k_x)} \]

\[ G_{ZZ}(k_x, \omega, y = 0, y = L_y) = \frac{-2v_f^2}{N_y} \sum_{n} \frac{k_n^2(-1)^n \epsilon(k_n, k_x)}{\epsilon^2(k_n, k_x) \omega^2 + \epsilon^2(k_n, k_x)} \]  (3.88)

### 3.8.1 Integrating out bulk excitations

In this section we focus on the case of graphene ribbon with ZB boundary condition; similar calculation with slightly minor changes applies for ZZ ribbon. From section 3.5 we saw that by representing electron operators in terms of edge-modes and bulk excitations, to first order in $U$ we get the following edge-bulk interactions

\[ \mathcal{H}_1 = \frac{U}{N_x} \sum \lambda(k+q,k,y)e_\uparrow^\dagger(k+q)e_\uparrow(k)\Phi_{A,\uparrow}(k',y)+\uparrow\leftrightarrow\downarrow \]

\[ \mathcal{H}_2 = -\frac{U}{N_x} \sum \lambda(k+q,k',y)e_\downarrow^\dagger(k+q)e_\downarrow(k')\Phi_{A,\downarrow}(k'-q,y)\Phi_{A,\uparrow}(k,y)+\uparrow\leftrightarrow\downarrow \]

\[ \mathcal{H}_3 = -\frac{U}{N_x} \sum \lambda(k+q,k'-q,k,x)e_\uparrow^\dagger(k+q)e_\downarrow^\dagger(k'-q)\Phi_{A,\uparrow}(k,y)\Phi_{A,\downarrow}(k',y) + h.c. \]  (3.89)

Where

\[ \lambda(k+q,k,y) = \alpha^\dagger(k+q,y)\alpha(k,y) \]

\[ \tilde{\lambda}(k+q,k,y) = \alpha^\dagger(k+q,y)\alpha^*(k,y) \]  (3.90)

where $\alpha(k,y)$ is exponentially localized at the zigzag edge for $k \in I_1 \equiv \left[ \frac{2\pi}{3}, \frac{4\pi}{3} \right]$, and localized at bearded edge for $k \in I_2 \equiv \left[ -\frac{2\pi}{3}, \frac{4\pi}{3} \right]$. $\Phi_{A,\sigma}(k,y)$ is representing low-energy bulk excitations, as a result of this, values of $k$ should be near the two Dirac points $\pm 2\pi/3$.

As we mentioned before $\Phi_{A/B,\sigma}(k,y)$ is slowly varying function of $y$. Thus in equation (3.89) we could assume that $\Phi_{A/B,\sigma}(k,y)$ is more or less independent of $y$.
and keeps its values at either zigzag edge, \( y = 0 \), or the bearded edge \( y = L_y \). Then we need to evaluate sum of \( \lambda(k + q, k, y) \) and \( \tilde{\lambda}(k + q, k, y) \) over \( y \). Let us define

\[
\lambda(k + q, k) = \sum_y \alpha^*(k + q, y) \alpha(k, y)
\]

\[
\tilde{\lambda}(k + q, k) = \sum_y \alpha^*(k + q, y) \tilde{\alpha}(k, y)
\] (3.91)

It is easy to check that for large \( N \) both \( \lambda(k + q, k) \) and \( \tilde{\lambda}(k + q, k) \) are exponentially small if \( k, k + q \) belong to different edges. Now let us look at the effect of momentum restrictions from \( \Phi_A \). From Eq. 3.89 we could see that for \( H_1 \) and \( H_2 \), \( q \) is either near 0 or \( \pm 2\pi/3a \). For \( q \approx 0 \) we have \( \lambda(k + q, k) = 1 \) up to first order in \( q \), thus

\[
\mathcal{H}^{(0)}_1 = \frac{U}{N_x} \sum_{k \in I_1} e_g^\dagger(k + q) e^\dagger(k) \Phi^\dagger_{A,\uparrow}(k' - q, y \approx 0) \Phi_{A,\downarrow}(k', y \approx 0) + \uparrow\leftrightarrow\downarrow
\]

\[
+ \frac{U}{N_x} \sum_{k \in I_2} e_g^\dagger(k + q) e^\dagger(k) \Phi^\dagger_{A,\uparrow}(k' - q, y \approx L_y) \Phi_{A,\downarrow}(k', y \approx L_y) + \uparrow\leftrightarrow\downarrow
\]

\[
\mathcal{H}^{(0)}_2 = -\frac{U}{N_x} \sum_{k \in I_1} e_g^\dagger(k + q) e^\dagger(k) \Phi^\dagger_{A,\downarrow}(k' - q, y \approx 0) \Phi_{A,\uparrow}(k', y \approx 0) + \uparrow\leftrightarrow\downarrow
\]

\[
+ \frac{U}{N_x} \sum_{k \in I_2} e_g^\dagger(k + q) e^\dagger(k) \Phi^\dagger_{A,\downarrow}(k' - q, y \approx L_y) \Phi_{A,\uparrow}(k', y \approx L_y) + \uparrow\leftrightarrow\downarrow
\] (3.92)

For \( q \approx 0 \), it could be shown that it leads to terms which are less relevant and could be ignored. Now that we have the expression for edge-bulk interaction Eq. 3.92 and also the bulk propagators Eq. (3.88), we could integrate out the bulk excitations.

**Inter-edge interaction:**

To find the inter-edge effective interactions we only need to consider the loop integrals which connect zero-mode excitations of different edges. An example of
these kind of terms to second order in $\mathcal{H}_1^{(0)}$ is given by

$$\delta \mathcal{H} = \left( \frac{-iU}{N_x} \right)^2 \sum e_\uparrow^\dagger(k + q, \tau)e_\uparrow(k, \tau)e_\uparrow^\dagger(l + q', 0)e_\uparrow(l, 0) \times$$

$$\langle \Phi_{A,\uparrow}^\dagger(k' - q, y \approx 0, \tau)\Phi_{A,\downarrow}(k', y \approx 0, \tau) \times$$

$$\Phi_{A,\uparrow}^\dagger(l' - q', y \approx L_y, 0)\Phi_{A,\downarrow}(l', y \approx L_y, 0) \rangle$$

(3.93)

Where operators are at time $\tau$ and 0. This is not the only possible term, to find the full inter-edge interaction we need to find four more terms, which could be found with the same approach.

The correlation function in the second line of Eq. (3.93) could be written as

$$G = \frac{1}{N_x} \langle \Phi_{A,\uparrow}^\dagger(k' - q, y \approx 0, \tau)\Phi_{A,\downarrow}(k', y \approx 0, \tau) \times$$

$$\Phi_{A,\uparrow}^\dagger(l' - q', y \approx L_y, 0)\Phi_{A,\downarrow}(l', y \approx L_y, 0) \rangle$$

$$= \frac{1}{N_x} \langle \Phi_{A,\uparrow}^\dagger(k' - q, y \approx 0, \tau)\Phi_{A,\downarrow}(l', y \approx L_y, 0) \rangle \times$$

$$\langle \Phi_{A,\uparrow}^\dagger(l', y \approx 0, \tau)\Phi_{A,\downarrow}^\dagger(l' - q', y \approx L_y, 0) \rangle$$

$$= \frac{-\delta_{k''-q',q}^\prime\delta_{k''-q} G_{ZB}(k' - q, -L_y, \tau)G_{ZB}(k', L_y, -\tau)}{N_x}$$

(3.94)

The Kronecker delta function leads to $q = -q'$ and the minus sign in the fifth line comes from the anti-commuting nature of fermionic operators, which lead to the minus sign for fermion loops. The Green function $G_{ZB}(k, L_y, \tau)$ was derived in previous sub-section and is given by Eq. (3.88). For the rest of this section we drop the $L_y$ dependence to simplify the notation.

By taking the time Fourier transform of above equation we see that we need to evaluate the following integral

$$f(\omega, q) = \int \frac{dq' d\omega'}{(2\pi)^2} G_{ZB}(\omega', q')G_{ZB}(\omega' - \omega, q')$$

(3.95)

And if we do the same calculation for the rest of the terms and carefully add them together we find that the effective intra-edge interaction induced by integrating out
bulk excitation has the form

\[
\delta \mathcal{H}_{z-b} = -\frac{U^2 a}{N_s v_f} \sum_{\omega, q} f(\omega, q) [2S_U(\omega, q)S_L(-\omega, -q) + \frac{1}{2}N_U(\omega, q)N_L(-\omega, -q)]
\]

(3.96)

where \( S_{U/L} \) and \( N_{U/L} \) are the total spin and total number of electrons for upper(zigzag) and lower(bearded) edges, respectively. Before going forward to evaluate the function \( f(\omega, q) \) there are few important points that we need to consider.

First, we see that the induced interaction has "retardation", meaning that it couples operators at different times and its Fourier transform contain a function of \( f(\omega, q) \). This retardation was expected from the beginning because the bulk excitations were gapless. Second, in addition to spin-spin exchange interaction between the edges, as we see in Eq. (3.96) there is also a long range Coulomb-like interaction proportional to \( N_U \ast N_L \), which is also retarded.

In general retardation and long-range interactions complicate the study of ground state properties, but in this case we could ignore the retardation and ignore the frequency dependency of these interactions. The reason for such assumption is that, the characteristic scale for \( \omega \) and \( q \) is \( t/L_x \) and \( 1/L_y \) (where \( t \) is the hopping amplitude). But if we calculate \( f(\omega, q) \), we see that the strength of induced interactions is proportional to \( U^2 / t^2 L_y^2 \). In our perturbative study, we assumed that \( U/t \ll 1 \); this means that for ribbons with large width, \( L_y \gg a \), the strength of induced interaction is weakened by factors of \( U/t \) and \( (a/L_y)^2 \). This justifies the assumption that we could take \( \omega = 0 \) and \( q = 0 \), and only evaluate \( f(0,0) \).

\[
f_{\text{ZB}}(0,0) = \frac{-4v_f^4}{N_x^2} \sum_{n,m} (-1)^{n+m} \int \frac{dl \ d\omega }{(2\pi)^2} \frac{k_n^2 k_m^2}{\epsilon_n^2 \epsilon_m^2} \frac{\omega^2}{(\omega^2 + \epsilon_n^2)(\omega^2 + \epsilon_m^2)}
\]

(3.97)

\[
f_{\text{ZB}}(0,0) = \frac{-2v_f^4}{N_x^2} \sum_{n,m} (-1)^{n+m} \int \frac{dl }{(2\pi)} \frac{k_n^2 k_m^2}{\epsilon_n^2 \epsilon_m^2} \frac{1}{(\epsilon_n + \epsilon_m)}
\]

Where \( \epsilon_n = v_f \sqrt{k_n^2 + l^2} \) and \( k_n = n\pi/L_x \), going from the first line to second line is simple contour integration. This integral could be done analytically but the sum-
mation is only possible numerically, and the result was discussed in section 3.7, Eq. (3.65).

For ZZ ribbon we only should replace the $G_{ZZ}$ from Eq. (3.88) into Eq. (3.95), from which we could find $f_{ZZ}(0, 0)$ which has exactly the same result as Eq. (3.97) but with important different sign. This difference in the sign of induced exchange interaction leads to Ferromagnetism and Anti-Ferromagnetism of two edges for ZB and ZZ, respectively.

Integrating out bulk excitations, in addition to giving inter-edge interactions which gives makes the total spin of ground consistent with Lieb’s theorem, also gives us induced intra-edge interactions, which we briefly discuss here.

**intra-edge**: Similar to the inter-edge case, we look at second order perturbation of Eq. (3.92), and only keep loop diagrams which connects edge modes which are localized on same edge, e.g zigzag edge at $y = 0$ this gives terms like:

\[
\delta \mathcal{H} = \left( -\frac{iU}{N_y} \right)^2 \sum_c \langle \Phi_{A,\downarrow}^+(k + q, \tau) \Phi_{A,\uparrow}^+(l + q', 0) \Phi_{A,\downarrow}^+(l, 0) \rangle \times \\
\langle \Phi_{A,\uparrow}^+(k', y \approx 0, \tau) \Phi_{A,\downarrow}^+(k, y \approx 0, \tau) \rangle
\]

By using similar calculations, of section 3.8, we find the needed green function

\[
G_{\text{intra}}(\omega, k_x) = \frac{2v_f i}{N_y} \sum_n \frac{k_n^2}{\varepsilon^2(k_n, k_x)} \frac{\omega}{\omega^2 + \varepsilon^2(k_n, k_x)}
\]

Because we are only interested to find effective interaction terms on single edge, we could simply work with semi-infinite graphene sheet and replace the sum with the integral in above equation. The rest of calculations is exactly similar to inter-edge case we find similar interaction as Eq. (3.96), with the following function for $f(\omega, q)$

\[
f(\omega, q) = \int \frac{dq' d\omega'}{(2\pi)^2} G_{\text{intra}}(\omega', q') G_{\text{intra}}(\omega' - \omega, q' - q)
\]
The effect of this term on excitation’s spectrum was discussed in section 3.7. And they make the ferromagnetic state more robust while changing the dispersion of the excitations.

3.9 Conclusion

In this chapter by using the projection method [35] we study the effective Hamiltonian of the edge modes of graphene. We expect this method to become valid in the weakly interacting limit of the Hubbard model. We show rigorously that the ground state of the projected Hamiltonian is ferromagnetic and as a result the edges are spin polarized. Then we include the effect of nearest neighbor hopping terms and study the stability of ferromagnetic state of the edge as function of next nearest neighbor hopping strength, and we show that the fully polarized state remains intact for some range of NNN hopping term and having passed some critical value the polarization gradually decreases.

Then in final section we take into account the effect of bulk excitations. Integrating out the bulk excitations leads to higher order interactions. The important result of doing so is that it leads to long range anti-ferromagnetic exchange interaction between two edges of a graphene ribbon. This means that for a graphene ribbon with both edges in zigzag shape each edge is spin polarized and the total spins of the edges are coupled anti-ferromagnetically.

Another effect of integrating out the bulk excitation is to have higher order interaction correction to the projected Hamiltonian. By studying these correction we see that they even make the magnetism of the edges more robust.
Chapter 4

Conclusion

In this thesis we study two different one-dimensional interacting systems. In chapter 2 we try to understand the transverse dynamical structure factors of XXZ spin chain which could teach us about the excitations of the system. In chapter 3 we look at another interesting one dimensional system, which is the edge states of graphene with zigzag boundaries, and the problem of the fully polarized magnetic ground state of this system.

In chapter 1 we showed that using standard bosonization method and Luttinger Liquid theory is no reliable way to study the nontrivial line shape of dynamical structure factors. We showed in section 2.2.3 that for the study of DSFs the band curvature terms, which are irrelevant in standard method, give rise to divergent terms, in higher orders of perturbative approach, near some threshold frequencies and make the standard method unreliable. If someone persists to use standard method to study the line shapes the only way could be to sum up all these divergent terms, which appear at all orders of perturbation. Keeping track of and summing all these terms if not impossible, is very difficult and cumbersome approach.

The more practical approach is beyond bosonization methods, X-ray edge method. In this approach the band dispersion is kept intact, while the perturbation is made in terms of interaction strength. In this approach the parameters of the new effective Hamiltonian could be derived perturbatively in terms of the interaction strength, but for exactly solvable models like XXZ spin chain, by using Bethe
ansatz solutions the parameters could be derived for any interaction strength. But the resulting theory could work as a phenomenological ground for the study of more diverse systems.

By using this method we obtained results on the transverse spectral function of XXZ spin chain in a magnetic field. In the zero field case we have exactly determined a critical exponent governing the lower edge singularity, for all $|\Delta| < 1$ and all wave-vector. For the finite field case, we have shown how this exponent can be determined from parameters which can be obtained from solving Bethe ansatz equations and which also determine the behavior of the longitudinal structure function, fermion spectral function and the finite size spectrum. We have argued that, for general magnetization, a large number of increasingly weaker singularities occur in the spectral function, extending all the way down to zero energy. We derived results for the finite temperature spectral function using X-ray edge methods, obtaining strikingly different behaviour than that given by standard bosonization at $0 < 1 - \Delta_{\text{eff}} \ll 1$. The line-shape is non-Lorentzian and the line width is $O(T)$, unsuppressed by $1 - \Delta_{\text{eff}}$. We pointed out that electron spin resonance measurements on spin chain compounds with uniform Dzyaloshinskii-Moriya interactions would provide a way of experimentally confirming, for the first time, the new bosonization results being obtained on spin chains, using X-ray edge techniques.

In the case of staggered DM interactions, the most interesting ESR signal occurs when the magnetic field is transverse to the DM vector. This may also be the case for uniform DM interactions, but we leave this for future work.

In chapter 3 we look at different 1D system. The tight binding honeycomb lattice with zigzag boundaries has been known to have states localized near the edges and so effectively are one dimensional, and interestingly they have zero-energy flat bands. Thus they are highly susceptible to the effect of interactions. A hand-waving argument based on Lieb’s theorem gives some intuition that including Hubbard interactions could make the edges magnetized. In section 3.5 we found the effective projected Hamiltonian of the edge states, this Hamiltonian is non-local and has very complicated form, in that section we proved that the ground state of the effective edge Hamiltonian at half filling is fully polarized ferromagnetic state, which confirms the Lieb’s theorem prediction.
The study of the particle addition or removal energy $\varepsilon_k$ could be probed experimentally. In principle $\varepsilon_k$ could be measured by using ARPES experiments. The density of states of the edge modes could be measured by using STM experiment, and as the ground state is predicted to be fully polarized state (suppose in $z$-direction), it would be only possible to tunnel in a spin-down electron or tunnel out a spin-up electron.

Then we studied the effects of unavoidable NNN hopping terms and showed that those terms would not change the ground state up to some critical value $\Delta_c$ and having passed that value the magnetization decreases monotonically to zero. For longer range Coulomb repulsion, we see that the next neighbor repulsion could not change our results but second and higher order terms in principle could affect our prediction, however we expect $U_2 \ll U_0$ and their effects are quite small.

As the excitations of bulk graphene are gapless, simply projected Hamiltonian is not enough. In section 3.7 by integrating out the bulk excitations we found induced interactions between the edges of graphene ribbons and also some higher order interactions on a single edge too.

The inter-edge interaction depends on the boundary conditions for the ribbon. For a ribbon with two zigzag edges the resulting interaction is spin exchange interaction with antiferromagnetic coupling, while for a ribbon with one zigzag edge and other bearded edge the interaction term is ferromagnetic exchange. Again both results are in complete agreement with Lieb’s theorem prediction. The intra-edge makes the ferromagnetic ground state more robust but it contributes some singular corrections of like $q^2 \ln q$ to the energy of the excitons. We leave a more detailed study of these effects of $O(U^2)$ and higher for the future. A reasonable approach might be to ignore the bulk interactions, since they are irrelevant, but analyze the bulk-edge Hubbard interactions using the renormalization group. This corresponds to a novel type of boundary critical phenomena in which the bulk is a massless (2+1) dimensional Dirac liquid and the edge is a one-dimensional spin-polarized semi-metal. The arguments based on Lieb’s theorem imply that the edge magnetic moment remains stable against weak interactions.
Bibliography


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[50] In Ref. ([27]) it was stated that the transverse spectral function exponent had been derived by X-ray edge methods for $h = 0, \Delta = 1$ and that it agreed with the result of Ref. ([29]) for the longitudinal spectral function. However, no details of the derivation were given nor was the exponent given for any other values of $\Delta$ or $h$. → pages 44

[51] In [22] the case $k_F < \pi/2$ was considered. To apply those results to the case $k_F > \pi/2$, that we are considering here, we must make a particle-hole transformation. → pages 46


[60] Hélène Feldner, Zi Yang Meng, Andreas Honecker, Daniel Cabra, Stefan Wessel, and Fakher F. Assaad. Magnetism of finite graphene samples: Mean-


[68] Closely related observations were made in M.J. Schmidt, Phys. Rev. B 84, 241403(R) (2011). → pages


[70] In the case where $L$ is a multiple of 3 there are states exactly at the band edges $\pm 2\pi/3$. We choose not to include them in the edge Hamiltonian since they are delocalized over the entire ribbon. → pages

[71] For the case of $t_2$ this is shown in K. Sasaki, S. Murukami and R. Saito, Appl. Phys. Lett. 88, 113110 (2006). For the case of the edge potential, it is shown in [35]. → pages

[72] There are additional inter-edge interactions involving the number operators and pair creation operators on upper and lower edges which will be discussed
in a later article, however these have little effect at large $w$. the spin term dominates because the edges are spin polarized. → pages[90]


Appendix A

Derivation of X-Ray edge Hamiltonian

The bosonization method which discussed in 2.2 is a powerful method to find the correlation and spectral functions of particular model at low-energies in the limit of $q \to 0$. But as we discussed in 2.2.3 it has its limitation to find the singularity exponents of spectral functions near their singular points. The band curvature terms which were irrelevant by power counting, became divergent near those singular points. Thus the result of bosonization for the singularity exponents of SF for finite momentum $q$, are no longer trustworthy and we need look for new models or extension of existing models to deal with it.

During the derivation of effective model in 2.2, we defined a sub-band cutoff $\Lambda_F \ll J$ near the two Fermi points and only kept the excitations within those sub-bands. When we are dealing with correlations at finite momentum $q$, it is natural to think that particle or hole excitations with momentum close to $q$ should have significant effect on the correlations and in the naive bosonization method as we are looking at the limit $\Lambda_F \to 0$, we implicitly ignore the effect of these important excitations.

The natural extension results of 2.2 would be to define three sub-bands for fermionic excitations, two sub-bands for excitations near the Fermi points $\Lambda_F$ and third sub-band $\Lambda_d$ for high-energy particle or a deep hole, see Fig 2.6. By including
these sub-bands the fermion annihilation operator is

\[ c_j \equiv \Psi(x) \approx \psi_R(x)e^{ik_{F}x} + \psi_L(x)e^{-ik_{F}x} + d e^{ikx} \] \hspace{1cm} (A.1)

Where \( \psi_{R/L} \) are excitations near the Fermi points and \( d \) is either a high-energy particle or a deep hole with momentum, \( k = k_{F} + q \) for particle and \( k = k_{F} - q \) for hole. We focus for particle excitation for the rest of this section, similar results holds for a hole excitations.

The procedure is similar to what we did in 2.2, first we derive the low-energy effective Hamiltonian in terms of \( \psi_{R/L} \) and \( d \), then by using bosonization we bosonize the \( \psi_{R/L} \) while keeping the high-energy excitations in Fermionic form.

By using equations Eq (3.71), the kinetic part of effective Hamiltonian is

\[ H_0 \approx \frac{v_{F}}{2} \left[ (\partial_{x}\phi_R)^2 + (\partial_{x}\phi_L)^2 \right] + d^\dagger \left( -\epsilon - i u \frac{\partial^2}{2m} \right) d \] \hspace{1cm} (A.2)

where \( v_{F} = J \sin k_{F} \) is the fermi velocity, \( \epsilon = J \cos(k_{F} + q) \) is the energy of high-energy particle with velocity \( u = J \sin(k_{F} + q) \) and effective mass \( m = \left[ J \cos(k_{F} + q) \right]^{-1} \). Using Eq (??) the density operator could be written as

\[ n(x) = \Psi^\dagger(x)\Psi(x) \approx \rho_R + \rho_L + \left( e^{2ik_{F}x}\psi_L^\dagger\psi_R + h.c. \right) + d^\dagger d \] \hspace{1cm} (A.3)

By writing the density operator in bosonized form, the interaction term becomes

\[ H_{int} = \frac{g_4}{4\pi} \left[ (\partial_x \phi_R)^2 + (\partial_x \phi_L)^2 \right] - \frac{g_2}{2\pi} \partial_x \phi_R \partial_x \phi_L \\
+ \frac{2\Delta}{\sqrt{2\pi}} d^\dagger d [1 - \cos(k_{F} - k)] \partial_x \phi_R \\
+ \frac{2\Delta}{\sqrt{2\pi}} d^\dagger d [1 - \cos(k_{F} + k)] \partial_x \phi_L \] \hspace{1cm} (A.4)

where \( g_2 = g_4 = 2\Delta[1 - \cos(2k_{F})] \). Now by using Eq. (2.23) and writing \( \phi_{R,L} \) in
terms of bosonic field $\phi$ and its dual field $\bar{\theta}$ we have

\[
H = \frac{v}{2} \left[ K (\partial_x \bar{\theta})^2 + \frac{1}{K} (\partial_x \phi)^2 \right] + d^\dagger \left( -\epsilon - iud_x - \frac{\partial_x^2}{2m} \right) d \\
+ \frac{1}{2\sqrt{\pi}} \left( (\tilde{\kappa}_L - \tilde{\kappa}_R) \partial_x \bar{\theta} + (\tilde{\kappa}_L + \tilde{\kappa}_R) \partial_x \phi \right) d^\dagger d
\]  

(A.5)

where $\tilde{\kappa}_{R,L} = 2\Delta \left[ 1 - \cos(k_F \mp k) \right]$. By doing a canonical transformation that rescales the field $\phi \to \sqrt{K} \phi$ and $\bar{\theta} \to \theta / \sqrt{K}$ we have

\[
H = \frac{v}{2} \left[ (\partial_x \phi^R)^2 + (\partial_x \phi^L)^2 \right] + d^\dagger \left( -\epsilon - iud_x - \frac{\partial_x^2}{2m} \right) d \\
+ \frac{1}{\sqrt{2\pi K}} (\kappa_L \partial_x \phi^L + \kappa_R \partial_x \phi^R) d^\dagger d
\]  

(A.6)

with

\[
\kappa_{R,L} = \left( \frac{1+K}{2} \right) \tilde{\kappa}_{R,L} - \left( \frac{1-K}{2} \right) \tilde{\kappa}_{L,R}
\]  

(A.7)

This describes the Luttinger Liquid coupled to an impurity and have been discussed in [47-49].
Appendix B

Positivity of spectral function

In this appendix we will prove that spectral function Eq. (2.118) is positive. We have

\[ S^{-+}(q, \omega) \propto \int_{-\infty}^{\infty} dt \frac{e^{i(\omega - \epsilon(k_p))t}}{(2\pi T)^{\nu_R + \nu_L}} \left( \sin(2\pi T(\epsilon + i(1-u/v)t)) \right)^{\nu_R} \left( \sin(2\pi T(\epsilon + i(1+u/v)t)) \right)^{\nu_L} \]

By defining the branch cut on \((-i\infty, -i\epsilon) \cup (i\epsilon, i\infty)\) and doing the change of variable \(t \to -t\) in second integral, we have

\[ S^{-+}(q, \omega) \propto \text{Re}\{\exp\left(-i\pi \sqrt{\nu_L + \nu_R - 1}\frac{\nu_L \nu_R}{\nu_R + \nu_L} \frac{1}{(2\pi T)^{\nu_R + \nu_L - 1} e^{i(\omega - \epsilon(k_p))t/2\pi T}} \right) \}

We will prove shortly that above integral is positive in general, but let us first look at the special cases of either \(\nu_R = 0\) or \(\nu_L = 0\), which is relevant for weak anisotropy at zero magnetic field, so \(u < v\).
Suppose that $\nu = 0$ thus we have

$$S^{-+}(q, \omega) \propto (2\pi T)^{\nu R-1} \Re \left[ \exp \left( -\frac{\pi}{2} \nu R \right) \int_0^\infty dt \frac{e^{i(\omega - \epsilon(k_p))t/(2\pi T)}}{\sinh((1 - u/v)t)^{\nu R}} \right]$$

$$\propto (2\pi T)^{\nu R-1} \Re \left[ \exp \left( -\frac{\pi}{2} \nu R \right) B \left( -i\omega - \epsilon(k_p) \frac{\nu R}{4\pi T(1 - u/v)} + \nu R/2, 1 - \nu R \right) \right]$$

Where $B[x, y]$ is Euler’s beta function. Let’s define $W \equiv \frac{\omega - \epsilon(k_p)}{4\pi T(1 - u/v)}$, and by using the definition of beta function in terms of gamma function we have

$$S^{-+}(q, \omega) \propto (2\pi T)^{\nu R-1} \Re \left[ \exp \left( -\frac{\pi}{2} \nu R \right) \frac{\Gamma[-iW + \nu R/2] \Gamma[1 - \nu R]}{\Gamma[1 - (iW + \nu R/2)]} \right]$$

(B.3)

Then by using the identity that $\Gamma[1 - z] \Gamma[z] = \pi / \sin(\pi z)$ we have

$$S^{-+}(q, \omega) \propto (2\pi T)^{\nu R-1} \Re \left[ \exp \left( -\frac{\pi}{2} \nu R \right) \sin \pi(iW + \nu R/2) \right]$$

(B.4)

by writing the sine function in exponential form, we finally get

$$S^{-+}(q, \omega) \propto (2\pi T)^{\nu R-1} |\Gamma[iW + \nu R/2]|^2 \Gamma[1 - \nu R] e^{\pi W} \sin(\pi \nu R)$$

(B.5)

so we see the spectral weight is positive, for all values of $\nu R$. This expression also holds for the case of $u > v$.

Actually what we have shown is that the Fourier transform of $1/\sin(2\pi T(\epsilon + i(1 - u/v)t))^\nu$ is given by a real positive function, in the following form

$$\text{F.T.} \left[ \frac{1}{\sin(2\pi T(\epsilon + i(1 - u/v)t))^\nu} \right] = (2\pi T)^{\nu - 1} \left| \Gamma \left[ \nu/2 + i \frac{\omega}{4\pi T(1 - u/v)} \right] \right|^2 \Gamma[1 - \nu] e^{\pi \omega/(4\pi T(1 - u/v))} \sin(\pi \nu)$$
Where $F.T$ stands for Fourier Transform. Now by using above equation and taking the convolution of Eq. (2.119), we have

$$S - (q, \omega) \propto (2\pi T)^{v_R + v_L} \Gamma[1 - v_R] \sin(\pi v_R) \Gamma[1 - v_L] \sin(\pi v_L)$$

$$\int_{-\infty}^{\infty} d\omega_R d\omega_L \delta(\omega - \epsilon(k_p) - \omega_R - \omega_L) e^{\pi \omega_R / (4\pi T(1 - u/v))} e^{\pi \omega_L / (4\pi T(1 + u/v))} \times$$

$$\left| \Gamma \left[ v_R/2 + i \frac{\omega_R}{4\pi T(1 - u/v)} \right] \times \Gamma \left[ v_L/2 + i \frac{\omega_L}{4\pi T(1 + u/v)} \right] \right|^2 \quad \text{(B.6)}$$

We see that all the functions in above equation are positive; thus whole the integral is positive.