THEORETICAL STUDY OF INTERACTING ELECTRONS IN
ONE DIMENSION
GROUND STATES AND EXPERIMENTAL SIGNATURES

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# TABLE OF CONTENTS

| Section                                                                 | Page |
|------------------------------------------------------------------------|------|
| LIST OF FIGURES                                                        | 3v   |
| SYMBOLS                                                                | 3x   |
| ABSTRACT                                                               | xii  |
| 1 INTRODUCTION                                                         | 1    |
| 2 GROUND STATES AND EXPERIMENTAL SIGNATURES                           | 4    |
| 2.1 Novel electronic ground states in a quantum wire                   | 5    |
| 2.2 Experimental signature of spin-charge separation                   | 6    |
| 3 INTERACTING ONE DIMENSIONAL ELECTRON LIQUID                          | 8    |
| 3.1 Luttinger liquid paradigm and Bosonization                         | 8    |
| 3.2 Finite temperature spectral functions in Luttinger liquid          | 13   |
| 4 PHASE DIAGRAM OF THE ALUMINUM ARSENIDE QUANTUM WIRE                  | 15   |
| 4.1 Introduction                                                       | 15   |
| 4.2 Quantum wire bandstructure                                          | 18   |
| 4.3 The Fermionic Hamiltonian                                          | 22   |
| 4.4 Bosonizing the Hamiltonian                                         | 26   |
| 4.5 Analyzing the renormalization group equations                      | 31   |
| 4.6 Conclusion                                                         | 35   |
| 5 LUTTINGER LIQUID KINK                                                | 36   |
| 5.1 Introduction                                                       | 36   |
| 5.2 Theory                                                             | 38   |
| 5.3 Results and Discussion                                             | 39   |
| 5.4 Conclusion                                                         | 45   |
| LIST OF REFERENCES                                                     | 46   |
| APPENDICES                                                             | 54   |
| Appendix A: Luttinger parameters for the quantum wire                  | 54   |
| Appendix B: Renormalization group equations                            | 55   |
| Appendix C: Correlation functions for the quantum wire                 | 57   |
| C.1 Charge density wave (CDW) correlation functions                   | 58   |
| C.2 Spin density wave (SDW) correlation functions                     | 58   |
| C.3 Interband CDW                                                      | 59   |
| C.4 Interband SDW                                                      | 61   |
| Section                                                      | Page |
|--------------------------------------------------------------|------|
| C.5 Superconducting correlation functions                    | 64   |
| Appendix D: Variation of Luttinger liquid kink with interaction strength | 67   |
| VITA                                                        | 71   |
**LIST OF FIGURES**

| Figure | Page |
|--------|------|
| 3.1 In a 1D interacting system an individual electron cannot move without pushing all the neighboring electrons. As a result only collective excitations can exist [25]. | 8 |
| 3.2 Particle-hole spectrum. The momentum of the particle-hole excitations are denoted by $q$ and their energy by $\omega$. The Fermi velocity is given by $v_F$. (a) Due to the large volume of the available phase space in two and three dimensions, a particle-hole pair, for $q < 2k_F$, can have a continuum of energies extending from zero. Interactions cannot form coherently propagating particle-hole pairs. (b) Contrary to higher dimensions, in one dimension due to the reduced phase space the only allowed low-energy excitations are for the two Fermi points, $q = 0$ and $q = 2k_F$. Particle-hole excitations now have both a well defined energy and momentum for $\omega \rightarrow 0$ and $q \rightarrow 0$. A coherently propagating particle-hole pair can now form with a result that collective bosonic excitations are stable [25]. | 9 |
| 3.3 The original model of fermions with band curvature (a) is replaced by a model of fermions with a linear spectrum (b). This causes to introduce two species of fermions (right ($R$) and left ($L$) going fermions). Here $E_F$ is the Fermi energy and $k_F$ the Fermi wavevector [8, 25, 26]. | 10 |
| 3.4 The momentum shell renormalization group process involves decomposing the field into fast and slow moving fourier modes. All the fields with wavevector $q$ lying in the momentum shell $\Lambda/b < q < \Lambda$, with the scale factor $b$, are then integrated out leaving a reduced volume of radius $\lambda/b$. Next, the wavevectors are rescaled by $q' = bq$. As a result we recover the original volume in the momentum space [104–108]. | 12 |
| 4.1 Aluminum arsenide quantum wire fabricated using the cleaved edge overgrowth technique. The notation 2DEG refers to the two dimensional electron gas which couples to the quantum wire from either side. *Picture courtesy of Dr. M. Rother, Ph.D Thesis (2000), Technische Universität München, Germany.* | 15 |
4.2 Bandstructure of a quantum wire where there is only one band of lowest energy. When the first two bands are filled, interactions between the four Fermi points lead to gaps. The possibility of density reorganization is shown, in which it becomes energetically favorable for the first two subbands to match their Fermi momenta. This costs the kinetic energy of moving the densities away from the noninteracting values, but gains the CDW gap energy [110]. The notations $E$ and $k$ refer to energy and momentum respectively.

4.3 (a) The aluminum arsenide quantum wire bandstructure considered here has the four Fermi points indicated in the diagram. The two ellipses refer to the degenerate X and Y valleys [114] situated at the X-point (indicated by the open circle) of the Brillouin zone. Note the energy minimum for aluminum arsenide is not at the Γ-point. The distance between the two open circles is half an umklapp vector. (b) In our calculation the quantum wire bandstructure is modelled with the two degenerate bands labeled A and B referring to the degenerate X and Y valleys in an aluminum arsenide bandstructure. Even at the lowest densities, there are two degenerate subbands. In addition, the band minima are separated by half an umklapp vector, $k_U/2$, giving rise to new “umklapp” interactions which are present at all fillings. The Fermi points, represented by black dots on the figure, are at $k_{F,A}^{A\pm} = -k_U/4 \pm k^0_F$ and $k_{F,B}^{B\pm} = k_U/4 \pm k^0_F$ where $k_U$ is the umklapp vector, and $k^0_F$ is the magnitude of the Fermi wavevector measured from the bottom of each band. The notations $E$ and $k$ refer to energy and momentum respectively.

4.4 Representative low energy long wavelength intraband electron-electron scattering processes. In each figure $E$ and $k$ refer to energy and momentum respectively. The open and filled dots represent electrons which are taking part in the scattering processes with the arrows depicting the direction of scattering. The Fermi points are at $k_{F,A}^{A\pm} = -k_U/4 \pm k^0_F$ and $k_{F,B}^{B\pm} = k_U/4 \pm k^0_F$ (as described in Fig. 4.3(b)) where $k_U$ is the umklapp vector, and $k^0_F$ is the magnitude of the Fermi wavevector measured from the bottom of each band.
Figure 4.5 Representative low energy long wavelength interband electron-electron scattering processes. In each figure $E$ and $k$ refer to energy and momentum respectively. The open and filled dots represent electrons which are taking part in the scattering processes with the arrows depicting the direction of scattering. The Fermi points are at $k_F^A = \frac{-k_U}{4} \pm k_F^o$ and $k_F^B = \frac{k_U}{4} \pm k_F^o$ (as described in Fig. 4.3(b)) where $k_U$ is the umklapp vector, and $k_F^o$ is the magnitude of the Fermi wavevector measured from the bottom of each band. The inter-valley umklapp scattering (Fig. 4.5(e)) shown above is unique to this aluminum arsenide quantum wire bandstructure arrangement.

4.6 Phase diagram: Divergent correlation functions for the quantum wire in the presence of inter-valley umklapp scattering for the two regimes $K^p_\rho < 1$ (repulsive) and $K^p_\rho > 1$ (attractive). The notation CDW stands for charge density wave and SS for singlet superconductivity. In the diagram $k_\rho$ denotes the pairing momenta of the center-of-mass of the Cooper pairs. The finite pairing momentum is an indication of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state which is encouraged in this wire due to the presence of the umklapp interactions. Such a state is also known to lead to inhomogeneous superconductivity.

5.1 Schematic diagram of peak broadening due to interactions and finite temperature in the Luttinger liquid spectral function. The dashed lines denote the zero temperature dispersion tracking the charge part with velocity $v_\rho$ and the spin part with velocity $v_\sigma$. At $T \neq 0$, the peaks become thermally broadened as indicated by the shaded regions. In this case the effective dispersion now tracks the solid red line, so that the low energy part tracks the sum of the two broad spin and charge peaks, resulting in a low energy velocity $v_l$ which is between the spin and charge velocities. Note the high energy effective dispersion is parallel to the charge part but displaced, an effect due to finite temperature and interactions. This results in the high energy part extrapolating back to a value $k_{ex} \neq k_F$.

5.2 Intensity of the spectral function $A^\leq(k,\omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.15$. (a) The intensity of $A^\leq(k,\omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2, 0.3, \text{and } 0.4$. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2, 0.3, \text{and } 0.4$. In all cases the spin velocity $v_\sigma = 1eV\cdot\AA$ and the temperature $k_B T = 14meV$. 
5.3 MDC’s for $\gamma_\rho = 0.15$. The spin velocity $v_\sigma = 1$ eV-$\AA$ and the temperature $k_B T = 14$ meV. The ratio of spin to charge velocity is $r = 0.2$.

5.4 Temperature variation of the effective dispersion. The temperature varies from $k_B T = 4$ meV to $k_B T = 14$ meV, starting from the lower curve and moving to the upper curve. The interaction strength $\gamma_\rho = 0.15$, the spin velocity $v_\sigma = 1$ eV-$\AA$, and the ratio of spin to charge velocity $r = 0.3$.

5.5 Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions for $U = 16, 8, 4$ in units of the hopping integral $t$. The density $n = 0.3$. (a) The intensity of $A^<(k, \omega)$. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. (b) Comparison of the dispersions at different values of $U/t$. In all cases the spin velocity $v_\sigma = 1$ eV-$\AA$ and the temperature $k_B T = 14$ meV.

D.1 Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.20$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2, 0.3$, and $0.4$. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2, 0.3$, and $0.4$. In all cases the spin velocity $v_\sigma = 0.7$ eV-$\AA$ and the temperature $k_B T = 14$ meV.

D.2 Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.25$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2, 0.3$, and $0.4$. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2, 0.3$, and $0.4$. In all cases the spin velocity $v_\sigma = 0.7$ eV-$\AA$ and the temperature $k_B T = 14$ meV.

D.3 Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.30$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2, 0.3$, and $0.4$. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2, 0.3$, and $0.4$. In all cases the spin velocity $v_\sigma = 0.7$ eV-$\AA$ and the temperature $k_B T = 14$ meV.
D.4 Intensity of the spectral function $A^<(k,\omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.35$. (a) The intensity of $A^<(k,\omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2$, 0.3, and 0.4. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2$, 0.3, and 0.4. In all cases the spin velocity $v_\sigma = 0.7eV \cdot Å$ and the temperature $k_B T = 14meV$. . . . . .
| SYMBOLS       | Description                                                                 |
|--------------|-----------------------------------------------------------------------------|
| AlAs         | Aluminum Arsenide                                                          |
| GaAs         | Gallium Arsenide                                                            |
| Si           | Silicon                                                                     |
| Ge           | Germanium                                                                   |
| 1D           | One dimensional                                                            |
| QWR          | Quantum wire                                                                |
| $T$          | Temperature                                                                 |
| $L$          | Length of the quantum wire                                                  |
| $w$          | Width of the quantum wire                                                   |
| $d$          | Distance of the quantum wire from the back gate                             |
| $r$          | Ratio of spin to charge velocity                                            |
| $E_F$        | Fermi energy                                                               |
| $v_F$        | Fermi velocity                                                             |
| $k_F$        | Fermi wavevector                                                            |
| $k_{F}^{A \pm}$ | Fermi points of band $A$ in the aluminum arsenide bandstructure           |
| $k_{F}^{B \pm}$ | Fermi points of band $B$ in the aluminum arsenide bandstructure           |
| $k_{F}^{0}$  | Magnitude of the Fermi wavevector measured from the bottom of each band in the aluminum arsenide bandstructure |
| $m_e$        | Free electron mass                                                          |
| $m^*$        | Effective mass of electron                                                  |
| $n$          | Band index                                                                  |
| $s$          | Spin index                                                                  |
| $k_U$        | Umklapp vector                                                             |
| $v_\rho$     | Charge velocity                                                             |
| $v_\sigma$   | Spin velocity                                                               |
\(v^\pm_\rho\) Charge velocity in symmetric and anti-symmetric basis
\(v^\pm_\sigma\) Spin velocity in symmetric and anti-symmetric basis
\(K_\rho\) Charge Luttinger parameter
\(K_\sigma\) Spin Luttinger parameter
\(K^\pm_\rho\) Charge Luttinger parameter in symmetric and anti-symmetric basis
\(K^\pm_\sigma\) Spin Luttinger parameter in symmetric and anti-symmetric basis
\(\gamma_\rho\) Charge interaction strength
\(\phi_\rho\) Bosonic charge field
\(\partial_x \theta_\rho\) Conjugate momentum of \(\phi_\rho\)
\(\phi_\sigma\) Bosonic spin field
\(\partial_x \theta_\sigma\) Conjugate momentum of \(\phi_\sigma\)
\(\alpha\) Short distance cutoff in the bosonization theory
\(R^\dagger_{ns}\) Right moving fermion creation operator in band \(n\) with spin \(s\)
\(L^\dagger_{ns}\) Left moving fermion creation operator in band \(n\) with spin \(s\)
\(\eta_{Rns}\) Klein factor for the right moving fermion in band \(n\) with spin \(s\)
\(\eta_{Lns}\) Klein factor for the left moving fermion in band \(n\) with spin \(s\)
\(\Lambda\) Length scale in the renormalization group scheme
\(CDW\) Charge density wave
\(SDW\) Spin density wave
\(SS\) Singlet superconductivity
\(TS\) Triplet superconductivity
\(MDC\) Momentum distribution curve
\(EDC\) Energy distribution curve
\(A^<(k, \omega)\) Single hole spectral function at momentum \(k\) and energy \(\omega\)
\(E_{\text{kink}}\) Kink energy
\(FFLO\) Fulde-Ferrell-Larkin-Ovchinnikov
ABSTRACT

Datta, Trinanjan Ph.D., Purdue University, August, 2007. Theoretical study of interacting electrons in one dimension ground states and experimental signatures. Major Professor: Dr. Erica W. Carlson.

This dissertation focuses on a theoretical study of interacting electrons in one dimension. The research elucidates the ground state (zero temperature) electronic phase diagram of an aluminum arsenide quantum wire which is an example of an interacting one dimensional electron liquid. Using one dimensional field theoretic methods involving abelian bosonization and the renormalization group we show the existence of a spin gapped quantum wire with electronic ground states such as charge density wave and singlet superconductivity. The superconducting state arises due to the unique umklapp interaction present in the aluminum arsenide quantum wire bandstructure discussed in this dissertation. It is characterized by Cooper pairs carrying a finite pairing momentum. This is a realization of the Fulde-Ferrell-Larkin-Ovchinnikov state which is known to lead to inhomogeneous superconductivity. The dissertation also presents a theoretical analysis of the finite temperature single hole spectral function of the one dimensional electron liquid with gapless spin and charge modes (Luttinger liquid). The hole spectral function is measured in angle resolved photoemission spectroscopy experiments. The results predict a kink in the effective electronic dispersion of the Luttinger liquid. A systematic study of the temperature and interaction dependence of the kink provides an alternative way to detect spin-charge separation in one dimensional systems where the peak due to the spin part of the spectral function is suppressed.
1. INTRODUCTION

Electronic systems in which the kinetic energy is treated as the starting point with the Coulomb interaction as a perturbation can be described by a gas of weakly interacting quasiparticles. The quantum numbers of the quasiparticle are similar to the non-interacting particle they are derived from. The quasiparticle parameters, such as mass and charge, are redefined to their effective values due to interactions. The principal effects of the mutual electron-electron interaction are assumed to be adequately captured in these effective parameters. This is the Landau Fermi liquid paradigm [1–3]. Although it has been a cornerstone of solid state physics for over fifty years, there is increasing experimental [4–6] and theoretical evidence [7–10] for its inadequacy in systems where strong correlations dominate. The band structure limit of nearly free electrons [11] is not an appropriate starting point and one should approach the problem with the interactions considered on an equal footing with the kinetic energy of the system [8,12–15]. With this in mind we define strongly correlated systems as being those in which interactions have a profound effect on the ground state and the low-lying excitations. Examples include transition metal oxides [15], heavy fermion compounds [16–19], quantum Hall systems [5,20–23], high-temperature superconductors, [10,24] and one dimensional (1D) electronic systems [25–28] among others.

One dimensional electronic systems are inherently correlated. Due to the reduced phase space in 1D these systems behave in a way which is radically different from their higher dimensional counterparts, two and three dimensional electronic systems [1,11]. The usual concept of an electron-like elementary excitation gives away to a more exotic class of fractionalized excitations referred to as the spinon and the holon. These collective spin and charge modes, respectively, are the stable elementary excitations of the interacting 1D electron liquid and they propagate with different velocities,
a phenomenon referred to as spin-charge separation [25]. In a spirit similar to the Landau Fermi liquid theory, the paradigm for describing the 1D systems where the stable elementary spin and charge excitation fields have not acquired an expectation value (i.e. gapless) is called Luttinger liquid [7, 25, 26] - a terminology coined by Haldane [28].

Interacting 1D electrons in the Luttinger liquid phase are characterized by spin-charge separation [29–31], suppression of the density of states near the Fermi level, and a power law behavior in the correlation functions. Experimental evidence for Luttinger liquid behavior has been reported in many 1D systems, via, e.g., a suppression of the density of states near the Fermi level in ropes of carbon nanotubes [32] or power law behavior in the conductance vs. temperature in edge states of the fractional quantum Hall effect [33, 34] and carbon nanotubes [35]. Direct evidence of spin-charge separation is evident in the measured single hole spectral function of the Mott-Hubbard insulator SrCuO$_2$ [36].

A useful quantity to detect spin-charge separation is the finite temperature single hole spectral function [37] relevant in angle resolved photoemission spectroscopy (ARPES) experiments. In the literature, theoretical analyses of this effect have mostly been performed for the zero temperature spectral function [38, 39] of the Luttinger liquid. Since experiments are performed at nonzero temperatures a reliable comparison between theory and experiment can only be made with the finite temperature spectral functions, as described in chapter 5.

In nature there are materials which are quasi-1D [7, 40, 41]. Experimental data on their electronic structure and theoretical analysis of these compounds [10, 42–69] supports the idea that there may be a temperature regime where the electronic structure can be characterized as 1D. Luttinger liquid physics or other instabilities of the interacting 1D electron liquid are then usually assumed to provide a correct physical description of the ground state. However there are many assumptions behind this [5, 10]. Furthermore, being quasi-1D in nature these systems do not allow theoretical ideas [8, 26] and techniques which have been primarily developed for true
1D problems to be tested. Fortunately advances in semiconductor device fabrication technology have led experimentalists to create systems such as quantum wires (QWR’s) [70–73] and carbon nanotubes (CNTs) [74–76] which are more fitting as examples of a 1D system. The aluminum arsenide (AlAs) QWR studied in this dissertation is such an example.

This dissertation focuses on two projects. The first is concerned with characterizing the ground state electronic phase diagram of an AlAs QWR. Using 1D field theoretic methods involving abelian bosonization and the renormalization group this QWR is shown to have a spin gapped electronic phase of matter with a novel singlet superconducting ground state arising due to the unique umklapp interaction present in the AlAs bandstructure. The singlet state has Cooper pairs which carry a finite pairing momentum. This dissertation also presents a theoretical analysis of the finite temperature single hole Luttinger liquid spectral function measured in the ARPES experiments. The results predict a kink in the effective electronic dispersion of the finite temperature Luttinger liquid. Being a finite temperature effect all previous analyses which focused on the zero temperature spectral function had failed to capture this feature in the electronic dispersion. The kink analysis provides a way to detect spin-charge separation in 1D systems where the spin peak is muted due to repulsive interactions.

The dissertation is organized as follows. Chapter 1 provides a general introduction to 1D strongly correlated systems. Chapter 2 presents the reasons for studying the systems and the main motivation behind the projects. Chapter 3 introduces the interacting 1D electron liquid and, provides a brief overview of bosonization, the renormalization group, and the finite temperature spectral function of the Luttinger liquid. Chapter 4 focuses on the model Hamiltonian used to study the AlAs QWR, the interactions present, the RG approach applied to the system, and finally a discussion of the resulting phase diagram of the AlAs QWR. Chapter 5 presents the work on the finite temperature single hole spectral function of the Luttinger liquid. These chapters are followed by a list of references and appendices which detail the calculations.
2. GROUND STATES AND EXPERIMENTAL SIGNATURES

One of the challenging and motivating aspect of 1D strongly correlated physics is to determine, characterize, and explain the nature of electronic phases of matter arising from an interplay of strong electronic correlations and low dimensionality. Experimental signatures of these systems are equally intriguing [77].

In general, strongly correlated systems [8, 12] can support a rich variety of novel electronic phases of matter like high-temperature superconductivity in ceramic layered copper-oxide materials [10] and quantum Hall states [23] in the two-dimensional electron gas. Some of the exotic ground states also appear in magnetic systems where the electronic spins can order on long length-scales and give rise to low-energy magnetic excitations called spin-waves [8, 12, 78]. The spin degrees of freedom could also be correlated only on short length-scales and have gapped (confined) excitations. This is the “spin liquid” phase [79]. In most cases variation of the external parameters such as temperature, pressure or chemical doping can help tune transitions from one novel ground state to another [9]. Novel quantum phase transitions can also be realized in artificially engineered 1D nanostructures such as QWR’s where the electrons move along one direction but their transverse motions are quantum mechanically confined.

Experimental probes capable of detecting Luttinger liquid physics include ARPES [6], tunneling measurements [80], neutron scattering [81], and conductance measurements [70, 71]. ARPES and neutron scattering experiments are primarily used for the quasi-1D materials. The tunneling and conductance measurements are employed for the QWR and carbon nanotube systems.

Laboratory fabricated 1D systems, such as a QWR, present to us a unique challenge of studying a genre of correlated electron device in which there is a theoretically
controlled way of incorporating strong electron correlations. From a broader perspective because the device parameters in a QWR are experimentally tunable, they offer a genuine opportunity to study transitions between ground states in 1D, for example, charge-density-wave (CDW) to singlet superconductivity (SS). The AlAs QWR studied in this dissertation encourages the CDW and the SS electronic phases. In general, QWR systems allow to confirm 1D theories in a way that is not possible in bulk three dimensional materials or quasi-1D materials (since bulk materials are never really 1D) [7, 10]. There is a tremendous potential to control these physical systems we study as an aid to test theoretical predictions, and perhaps even paving the way towards designing new composite materials.

Spin-charge separation in quasi-1D systems can be probed using ARPES measurements which measure the single hole spectral function. The effect can be hard to detect experimentally due to interactions, finite temperature and experimental resolution. This dissertation presents a theoretical analysis of the finite temperature single hole Luttinger liquid spectral function [37] which predicts a kink in the effective electronic dispersion. This unique signature, a result of finite temperature and interactions had been overlooked previously.

2.1 Novel electronic ground states in a quantum wire

A QWR is an excellent realization of a 1D system [70–73,82,83] on which controlled experiments and theoretical calculations [84–88] can be performed. 1D combined with strong interactions cause the QWR’s to display markedly non-Fermi liquid behavior [70, 71, 84–87].

AlAs is a heavy mass system with degenerate valleys and anisotropic mass. By exploiting the valley degeneracy in AlAs, a single QWR has recently been fabricated with two degenerate nonoverlapping bands separated in momentum-space by half an umklapp vector \((k_U)\) [89,90], as illustrated in Fig. 4.3(b) using the cleaved edge overgrowth technique. The arrangement of the bands in momentum-space allows for
the possibility of multiple Fermi points (more than the usual case of two from a single band) at the Fermi energy (see Fig. 3.3(a)). The presence of multiple Fermi points implies multiple charge and spin channels, causing a rich phase diagram. Multiple Fermi points have been a recurring experimental and theoretical theme in recent years within the context of quasi-one dimensional systems [7, 40–54, 56–68, 91, 92]. In the context of these 1D AlAs QWR systems they are exciting because of the potential for experimentally accessible new ground states. The multiple Fermi points in this system are present even at the lowest densities. They have a new class of interactions, the everpresent umklapp interaction (see Fig. 4.5(e)), which has the possibility to favor exotic electronic phases of matter; as described in chapter 4. Specifically, a SS state with Cooper pairs carrying a finite pairing momentum is encouraged. Such a state is a realization of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, but in the present context for an interacting 1D system. This is known to lead to inhomogeneous superconductivity [93].

One dimension is characterized by strong quantum fluctuations. This prevents long-range order from developing in these system at finite temperatures. However, in order to realize a true long-range order and a phase transition at a finite temperature one can couple a set of 1D systems to dimensionally crossover to a two dimensional system [94]. For e.g., in the present context an array of QWR’s could be fabricated to investigate dimensional crossover from a 1D to a two dimensional system.

2.2 Experimental signature of spin-charge separation

The interacting 1D electron liquid is characterized by spin-charge separation where the stable elementary excitations, the holon and the spinon, propagate with different velocities. This is expected to give rise to separate spin and charge peaks in the single hole spectral function of the Luttinger liquid. Until recently a clear experimental detection of these two peaks has proven difficult, since the combined effects of interactions, thermal broadening, and finite experimental resolution can suppress the spin
peak for repulsive interactions. The measured peak in the effective electronic dispersion propagates with a combination of the spin and charge velocity at low energies but with only the charge velocity at high energies. This change in velocity gives rise to a kink in the effective electronic dispersion. A systematic study of the temperature and interaction dependence of this kink has been performed in this dissertation. This is an useful experimental signature especially when the two peaks are not directly visible in the Luttinger liquid spectral function to confirm the spin-charge separated nature of the material under investigation.

Angle resolved photoemission spectroscopy experiments on SrCuO$_2$ [36] have measured spin-charge separation by detecting the spin and charge dispersions separately in the single hole spectral function. Previous attempts to confirm spin-charge separation through detection of separately dispersing spin and charge peaks with ARPES [95,96] have been overturned [97,98], or lack independent verification of the spin and charge energy scales [99]. Indirect experimental evidence of spin-charge separation in 1D systems also exists. For example, the tunneling measurements via real-space imaging of Friedel oscillations using scanning tunneling microscopy on single-walled carbon nanotubes [100] and momentum- and energy- resolved tunneling between two coupled QWRs [80].

Theoretical analysis of the finite temperature single hole spectral function [77] indicates that within Luttinger liquid theory, the spinon branch is suppressed compared to the holon branch for repulsive interactions. This presents a difficulty in directly confirming spin and charge dispersions through measurements proportional to the single particle spectral function. Nevertheless spin-charge separation can be detected via the systematic temperature dependence of a kink in the electronic dispersion, even in cases where the spin peak is not directly resolvable, as described in chapter 5.
3. INTERACTING ONE DIMENSIONAL ELECTRON LIQUID

3.1 Luttinger liquid paradigm and Bosonization

Interactions have drastic effects in 1D compared to higher dimensions. As a consequence of strong electron-electron interactions the familiar concept of an electron-like quasiparticle has no meaning. Due to the reduced phase space individual motion of an electron is impossible (see Fig. 3.1), and all the stable elementary excitations are collective (see Fig. 3.2). A single fermionic excitation appears to split into a collective excitation carrying charge (holon) and another collective excitation carrying spin (spinon). The electron is said to have ‘fractionalized’. This is spin-charge separation where the collective charge and spin modes have in general different velocities. The minimal quantum numbers of the gapless modes are charge, spin, and (crystal) momentum. Here the “spin-modes” have spin 1/2 and charge 0 (spinon), and “charge modes” have spin 0 and charge e (holon). This is the interacting 1D electron gas where the bosonic quasiparticles are the key to solving our 1D problem. In this context it is important to note that the Luttinger liquid is a particular phase of the 1D electron gas where all the charge and spin modes are gapless [25]. The notion of a Luttinger liquid implies that all gapless 1D electronic systems share these properties at low energies [28].
Figure 3.2. Particle-hole spectrum. The momentum of the particle-hole excitations are denoted by $q$ and their energy by $\omega$. The Fermi velocity is given by $v_F$. (a) Due to the large volume of the available phase space in two and three dimensions, a particle-hole pair, for $q < 2k_F$, can have a continuum of energies extending from zero. Interactions cannot form coherently propagating particle-hole pairs. (b) Contrary to higher dimensions, in one dimension due to the reduced phase space the only allowed low-energy excitations are for the two Fermi points, $q = 0$ and $q = 2k_F$. Particle-hole excitations now have both a well defined energy and momentum for $\omega \to 0$ and $q \to 0$. A coherently propagating particle-hole pair can now form with a result that collective bosonic excitations are stable [25].

The particle-hole spectrum (see Fig. 3.2) holds the key to understanding the nature of the stable elementary excitations in 1D. In the low energy ($\omega \to 0$) and low momentum limit ($q \to 0$), particle-hole excitations in 1D form stable collective bosonic excitations which become the basis for solving the 1D models. As shown in Fig. 3.2 a particle-hole pair in two and three dimensions can have a continuum of energies extending from zero for $q < 2k_F$. Any electron-hole pair which tries to propagate coherently decays immediately into the electron-hole continuum. However in 1D, due to the Pauli exclusion principle there is a volume of excluded phase space (see Fig. 3.2). The only allowed low-energy excitations are for the two Fermi points, $q = 0$ and $q = 2k_F$. For low energy and low momentum the particle-hole excitations have
both a well defined energy and momentum. A coherently propagating particle-hole pair can now form with a result that collective bosonic excitations are stable [25].

The continuum model of a 1D interacting electron gas consists of approximating it by a pair of linearly dispersing branches of right- and left- moving, $R$ and $L$, respectively, spin-half fermions constructed around the right and left Fermi points respectively as shown in Fig. 3.3. This approximation captures the essential physics in the limit of low energy and long wavelength where the only important processes involve the fermionic excitations in the vicinity of the Fermi points. Now we use the basic idea of bosonization where we associate with the right- and left- moving fermionic fields a corresponding bosonic field. The crucial physical ingredient involves in recognizing that in 1D the stable elementary excitations in the limit of low energy and momentum are the collective charge and spin modes. The bosonization identity [8, 25, 27] is

$$\psi_{\xi,s} \equiv \frac{\eta_{\xi,s}}{\sqrt{2\pi\alpha}} \exp[-i\Phi_{\xi,s}(x)]$$  \hspace{1cm} (3.1)
which expresses the fermionic fields in terms of self-dual fields $\Phi_{\xi,s}(x)$ obeying

$$
\left[ \Phi_{\xi,s}(x), \Phi_{\xi,s'}(x') \right] = -i\pi \delta_{\xi,\xi'} \delta_{s,s'} \text{sign}(x' - x) \tag{3.2}
$$

with $\xi = +1$ for right moving fields and $\xi = -1$ for left moving fields. The spin index $s = \{\uparrow, \downarrow\}$. The Klein factors $\eta_{\xi,s}$ are responsible for reproducing the correct anticommutation relations between different Fermionic species and $\alpha$ is the short distance cutoff that is taken to zero at the end of the calculation. The fields $\Phi_{\xi,s}(x)$ are in turn combinations of the bosonic fields $\phi_\nu$ (charge) and $\phi_\sigma$ (spin) and their conjugate momenta $\partial_x \theta_\nu$ and $\partial_x \theta_\sigma$. It is expressed as

$$
\Phi_{\xi,s} = \sqrt{\frac{\pi}{2}} \left[ (\theta_\rho - \xi \phi_\rho) + s(\theta_\sigma - \xi \phi_\sigma) \right] \tag{3.3}
$$

where $\phi_\nu = (\phi_\uparrow \pm \phi_\downarrow)/\sqrt{2}$, $\theta_\nu = (\theta_\uparrow \pm \theta_\downarrow)/\sqrt{2}$, and $\nu = \rho, \sigma$ (charge and spin modes) correspond to the $\pm$ combinations respectively. The bosonic fields satisfy the commutation relation $[\phi_\nu(x), \partial_y \theta_{\nu'}(y)] = i\pi \delta(x - y)\delta_{\nu,\nu'}$. With the above identification we can cast the original fermionic Hamiltonian in the equivalent general bosonic form

$$
H = \frac{1}{2} \int dx \sum_{\nu=\rho,\sigma} v_\nu \left[ K_\nu (\partial_x \theta_\nu)^2 + \frac{(\partial_x \phi_\nu)^2}{K_\nu} \right] + H_{\text{int}} \tag{3.4}
$$

where $H_{\text{int}}$ are the bosonized interactions which may couple spin and charge as described in chapter 4, Eq. 4.13 or they may be completely decoupled. In the later case spin-charge separation can be formally defined as a statement where the Hamiltonian can be expressed as a sum of two pieces involving only charge or spin fields in the absence of interactions mixing spin and charge modes in the bosonic theory. The phenomenon of spin-charge separation holds for the spin-full problem even in the presence of forward and back-scattering fermionic interactions [25, 101].

Physically $\phi_\rho$ and $\phi_\sigma$ are the phases of the charge density wave (CDW) and spin density wave (SDW) fluctuations, and $\theta_\rho$ is the superconducting phase. The parameter $K_\nu$, a measure of the electron-electron interaction strength in the theory, is referred to as the Luttinger parameter, see appendix A. For $K = 1$, it refers to a non-interacting theory. The repulsive and attractive regimes are given by $K < 1$ and
$K > 1$ for repulsive and attractive interactions respectively. Furthermore, $K_{\sigma} = 1$ for systems in which there are no explicit spin symmetry breaking fields or spontaneous breakdown of spin-rotation invariance. The velocities for the charge and spin modes are given by $v_{\nu}$ where $\nu = \rho, \sigma$.

It is a salient feature of the 1D electron gas that all the properties of such systems, including fermionic correlation functions, can be expressed in terms of the bosonic fields (apart from the Klein factors) [101–103]. Any 1D problem involving only the forward scattering interactions can be solved exactly by using the boson representation in which it is non-interacting [25–27]. Furthermore it is advantageous that when spin-charge separation holds the Hamiltonian is separable, and so wavefunctions, and therefore correlation functions, factor.

The effects of some perturbations on the low energy properties of Luttinger liquids can be studied using the renormalization group idea. In considering the 1D AlAs QWR model, as described in chapter 4, where such a situation may arise we employ this scheme to study the phase diagram. We focus on the long distance physics

Figure 3.4. The momentum shell renormalization group process involves decomposing the field into fast and slow moving Fourier modes. All the fields with wavevector $q$ lying in the momentum shell $\Lambda/b < q < \Lambda$, with the scale factor $b$, are then integrated out leaving a reduced volume of radius $\lambda/b$. Next, the wavevectors are rescaled by $q' = bq$. As a result we recover the original volume in the momentum space [104–108].
that can be precisely derived from the effective bosonized field theory. The coupling
constants which appear in the problem are then effective parameters and implicitly
include much of the high energy physics. A weak coupling perturbative renormal-
ization group treatment \cite{25, 26, 42, 50, 57, 104, 105, 107–109} of all the interactions is
then employed to reveal the low energy, long wavelength physics. The procedure
involves in thinning the degrees of freedom followed by a rescaling of length scales.
The physics of the problem is then studied by investigating the dependence of the
coupling constants on the length scale. The momentum shell renormalization group
procedure carried out in this dissertation is described in Fig. 3.4.

3.2 Finite temperature spectral functions in Luttinger liquid

The finite temperature single hole correlation function, \( G^\xi_<(x, t; T) \), is defined as

\[
G^\xi_<(x, t; T) = \langle \psi^\dagger_{\xi,s}(x, t) \psi_{\xi,s}(0, 0) \rangle
\]

where \( \xi = \pm \) for the right and left moving fermionic fields \( \psi_{\xi,s} \) (refer Eq 3.1)
respectively. The spin index \( s = \{ \uparrow, \downarrow \} \). The spatial and temporal coordinates are denoted
by \( x \) and \( t \). The temperature is denoted by \( T \). Recently, explicit analytic expressions
for the above finite temperature correlation function in the Luttinger liquid have been
obtained under various conditions \cite{37}.

The spectral function, \( A^<(k, \omega) \), relevant for the ARPES experiments is obtained
from the above by Fourier transforming. In the spin-rotationally invariant case, the
finite-temperature single hole spectral function \cite{37} may be written in terms of the
scaled variables \( \tilde{k} = \frac{\omega_{\xi,s}}{\pi T} \) and \( \tilde{\omega} = \frac{\omega}{\pi T} \) with the Boltzmann constant \( k_B = 1 \)

\[
A^<(\tilde{k}, \tilde{\omega}) \propto \int_{-\infty}^{\infty} dq \ h_{\gamma_0}(\tilde{k} - 2rq) \times
h_{\gamma_0 + \frac{1}{2}} \left[ \tilde{\omega} - \frac{\tilde{k}}{2} + (1 + r)q \right] h_{\gamma_0} \left[ \tilde{\omega} - \frac{\tilde{k}}{2} - (1 - r)q \right]
\]

\[
(3.6)
\]
where \( k \) is the momentum measured with respect to the Fermi wavevector \( k_F \), \( \omega \) the energy relative to Fermi energy \( E_F \) and \( r = v_\sigma / v_\rho \) is the ratio between the spin velocity and the charge velocity and \( h_\gamma \) is related to the beta function,

\[
h_\gamma(k) = \Re \left[ (2i)\gamma B \left( \frac{\gamma - i k}{2}, 1 - \gamma \right) \right].
\]

The charge interaction strength \( \gamma_\rho \) is related to the charge Luttinger parameter \( K_\rho \) by \( \gamma_\rho = \frac{1}{8} (K_\rho + K_\rho^{-1} - 2) \), i.e. \( \gamma_\rho = 0 \) in the noninteracting case, and \( \gamma_\rho \) increases with increasing interaction strength. Because of spin rotation invariance, we use \( K_\sigma = 1 \) and \( \gamma_\sigma = 0 \). The scaled form of the spectral function arises from the critical nature of the Luttinger liquid model. The corresponding zero temperature expressions are also documented in the literature [25, 38, 39].
4. PHASE DIAGRAM OF THE ALUMINUM ARSENIDE QUANTUM WIRE

4.1 Introduction

In the usual realization of a QWR, transverse quantization leads to a succession of nested energy bands. While much of the attention has been focused on elucidating the theoretical properties of a single band QWR [65,84–87,110–112], there is a theoretical and practical urgency to focus on the novel phenomena which may arise in these systems when more than one energy band is involved. A theoretical attempt has been made in this direction by Starykh et.al. [110] where they examined and demonstrated

Figure 4.1. Aluminum arsenide quantum wire fabricated using the cleaved edge overgrowth technique. The notation 2DEG refers to the two dimensional electron gas which couples to the quantum wire from either side. *Picture courtesy of Dr. M. Rother, Ph.D Thesis (2000), Technische Universitaet Muenchen, Germany.*
the possibility of gapped phases in a QWR focusing on the nested bandstructure arrangement (see Fig. 4.2) which arises due to the quantum confinement. According to their theoretical proposal when the electronic density in such a system is tuned so that the lowest two successive energy levels are occupied, there are gapped phases possible, for e.g., an interband CDW, with anti-correlated charge density waves in each band, and a “Cooper phase” at zero pairing momenta with strong singlet superconducting fluctuations. However due to the possibility of density reorganization (see Fig 4.2) a mechanism in which it becomes energetically favorable for the two lowest subbands to match their densities, the interband CDW is the most likely state. The Cooper phase may exist just as the second band becomes occupied, when the difference in Fermi momenta is the largest [110].

In this regard one of the questions which could be posed is the following: Is there a possibility of a robust superconducting phase with a spin gap in a multiple Fermi point QWR? To answer the question we consider the theoretical treatment of an AlAs QWR which has been recently fabricated by Moser et.al. [89, 90] using the cleaved edge overgrowth technique [70] (see Fig. 4.1). Our calculations indicate that in the clean limit (i.e. no disorder) this QWR has the possibility to realize a spin gap with a stable SS phase with finite pairing momentum. The finite pairing of the Cooper pairs is an indication of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state which is known to lead to inhomogeneous superconductivity [93].

AlAs is a heavy mass semiconductor with three degenerate valleys in the first Brillouin zone and anisotropic mass [113]. The arrangement of the bands in momentum-space makes it an ideal candidate for a system where multiple Fermi points are present even at the lowest densities. There are two degenerate nonoverlapping bands separated in momentum-space by half an umklapp vector ($k_U$), as illustrated in Fig. 4.3. For low densities with only the lowest bands of transverse quantization occupied, the density-reorganizing interband CDW instability discussed above is forbidden. In addition, since the two (degenerate) band minima are connected by half an umklapp vector, there is a class of umklapp excitations unique to this bandstructure which
exist at all densities (see Fig. 4.5(e)) and which have the possibility to favor novel electronic phases.

Figure 4.2. Bandstructure of a quantum wire where there is only one band of lowest energy. When the first two bands are filled, interactions between the four Fermi points lead to gaps. The possibility of density reorganization is shown, in which it becomes energetically favorable for the first two subbands to match their Fermi momenta. This costs the kinetic energy of moving the densities away from the noninteracting values, but gains the CDW gap energy [110]. The notations $E$ and $k$ refer to energy and momentum respectively.

In this chapter, we use abelian bosonization and the weak coupling renormalization group scheme to theoretically characterize this QWR. We find that for repulsive interactions, the wire can be tuned so that the ground state has a spin gap which favors either a divergent CDW correlation function or a divergent singlet superconducting correlation function with finite pairing momenta for the Cooper pairs. Even though the original problem contains a repulsive electron-electron interaction, there is a possibility of generating an effective attraction between the electrons in the course of renormalization of the electron-electron interaction. Such a repulsion induced superconductivity is a novel realization in itself and the fact that a mesoscopic system such as the AlAs QWR discussed in this dissertation can allow for its physical realization is a great source of excitement. The final phase has one gapless (total) charge
mode with no gapless spin modes. In the literature this is also referred to as the C1S0 phase [42, 57, 64, 110].

The outline of this chapter is as follows. In section 4.2 we describe the AlAs bandstructure. In section 4.3 we state the model Hamiltonian used to describe the AlAs QWR and classify the low energy long wavelength fermionic interaction processes which are important. In section 4.4 we bosonize the Hamiltonian in a symmetric and an anti-symmetric basis of the bosonic fields constructed from the two bands A and B (see Fig. 4.3(b)). In section 4.5 we derive the renormalization group equations and discuss the electronic phase diagram. In section 4.6 we state the conclusions.

4.2 Quantum wire bandstructure

In bulk AlAs, conduction-band minima (or valleys) occur at the six equivalent X-points of the Brillouin zone. The constant energy surface consists of six half ellipsoids (three full ellipsoids in the first Brillouin zone), with their major axes along one of the \( \langle 100 \rangle \) directions. These valleys are highly anisotropic with an anisotropic effective mass of \( 1.1m_e \) in the longitudinal direction and \( 0.19m_e \) in the transverse direction, where \( m_e \) is the bare mass of the electron. Since a large effective mass leads to a reduced kinetic energy, many-body effects related to the Coulomb potential are expected to be enhanced in AlAs compared to the light-mass, \( 0.067m_e \), GaAs system.

In the AlAs QWR fabricated by the cleaved edge overgrowth process [70, 90], the initial growth direction is along \( [001] \) with the AlAs layer flanked by GaAs and AlGaAs on either side. This creates the two dimensional electron gas. To prepare the QWR the heterostructure is then cleaved in the perpendicular direction specified by \( [110] \) (the cleavage plane). The 1D channel thus formed at the edge of the cleaved plane together with the tantulum gate deposited on top of the two dimensional electron gas then helps to define the length of the QWR.

The bandstructure of the QWR can be estimated, approximately, by taking slices through the bandstructure of the corresponding two or three dimensional material.
For special systems such as CNTs, which have cylindrical boundary conditions one can just take slices with various transverse momenta which is a good quantum number in these systems. However, most other physical systems do not have such elegant boundary conditions, and in general there will be boundary reflections that mix states of different transverse momenta. The effect of this is that the dispersion of the lowest lying band, rather than corresponding to a slice along a particular constant transverse momentum, corresponds instead to a slice that tracks the minimum of the two or three dimensional dispersion relation.

For the cleaved edge AlAs QWR when one performs this analysis [115] we obtain the bandstructure arrangement as shown in Fig. 4.3(b). In the lowest lying band the transverse momentum has no role to play. The bandstructure consists of two degenerate bands $A$ and $B$, as shown in Fig. 4.3(b) referring to the degenerate X and Y valleys in the AlAs bandstructure (see Fig. 4.3(a)). Even at the lowest densities, there are two degenerate subbands. In addition, the band minima are separated by half an umklapp vector, $k_U/2$, giving rise to umklapp interactions which are present at all fillings and is not related to the commensurability of the electron gas with the underlying lattice. The four Fermi points, represented by black dots in Fig. 4.3(a) and Fig. 4.3(b) are at $k_{F}^{A \pm} = -\frac{k_{U}}{4} \pm k_{F}^{o}$ and $k_{F}^{B \pm} = \frac{k_{U}}{4} \pm k_{F}^{o}$ where $k_U$ is the umklapp vector, and $k_{F}^{o}$ is the magnitude of the Fermi wavevector measured from the bottom of each band.

We also note that the band structure of AlAs electrons is similar to Si, except that in Si there are six ellipsoids centered around six equivalent points along the $\Delta$-lines of the Brillouin zone, while in AlAs we have three (six half) ellipsoids at the $X$-points. Typically these valleys are denoted by the directions of their major axes: $X, Y,$ and $Z$ for the [100], [010], and [001] valleys, respectively. For our purposes a crucial difference between AlAs and Si is the manner in which the valleys are occupied in a quantum well from which eventually the QWRs are fabricated. When the electrons are confined along the [001] direction in a (001) Si-MOSFET or a Si/Si-Ge heterostructure, the two $Z$ valleys, with their major axes pointing out of plane, are
Figure 4.3. (a) The aluminum arsenide quantum wire bandstructure considered here has the four Fermi points indicated in the diagram. The two ellipses refer to the degenerate X and Y valleys [114] situated at the X-point (indicated by the open circle) of the Brillouin zone. Note the energy minimum for aluminum arsenide is not at the Γ-point. The distance between the two open circles is half an umklapp vector. (b) In our calculation the quantum wire bandstructure is modelled with the two degenerate bands labeled A and B referring to the degenerate X and Y valleys in an aluminum arsenide bandstructure. Even at the lowest densities, there are two degenerate subbands. In addition, the band minima are separated by half an umklapp vector, $k_U/2$, giving rise to new “umklapp” interactions which are present at all fillings. The Fermi points, represented by black dots on the figure, are at $k_F^{A\pm} = -k_F^o \pm k_F^o$ and $k_F^{B\pm} = k_F^o \pm k_F^o$ where $k_U$ is the umklapp vector, and $k_F^o$ is the magnitude of the Fermi wavevector measured from the bottom of each band. The notations $E$ and $k$ refer to energy and momentum respectively.
occupied because the larger mass of electrons along the confinement direction lowers their energy. In AlAs quantum wells grown on a (001) GaAs substrate, however, the $Z$ valley is occupied only if the well thickness is less than approximately 5 nm \[116\]. For larger well thicknesses, a biaxial compression of the AlAs layer, induced by the lattice mismatch between AlAs and GaAs, causes the $X$ and $Y$ valleys with their major axes lying in the plane to be occupied \[113\]. For the AlAs QWR fabricated by Moser et al. \[90\] using the cleaved edge overgrowth technique (see Fig. 4.3), the well thickness is 15 nm. As a result the $X$ and $Y$ valleys are lower in energy and provide the two degenerate conduction bands which can be occupied by electrons. For Si such a possibility is precluded as stated above.

There are also crucial differences between the AlAs QWR and the CNT bandstructure. In the CNTs the two bands, around the Dirac points, between which the electron-electron scattering processes take place are not separated by half an umklapp vector as in the AlAs QWR \[74\]. Furthermore, the umklapp interactions which are generated in the CNT systems are present only at half-fillings and not just at any electronic density. At half-filling, a metallic CNT maps to the Hubbard model also at half-filling. While the Hubbard model has umklapps at half-filling, these do not correspond to umklapps in the original CNT. Rather, they are merely extra interactions which are only allowed by symmetry at the Dirac points, i.e. at half-filling. Also, a metallic tube is unlike our QWR, in that the pseudospin which is equivalent to the sublattice quantum number prevents an electron from backscattering from one branch to another around the same Brillouin zone points. A doped semiconducting tube could perhaps do this. We in fact do include backscattering within the same subband which is strictly forbidden in a metallic CNT.

Furthermore, empirical evidence \[114, 116\] suggests that in an AlAs quantum well the spin degeneracy is not lifted in the absence of magnetic field leading us to conclude that spin-orbit coupling effects can be safely ignored in the theoretical formulation of the present problem.
4.3 The Fermionic Hamiltonian

In a QWR electrons are quantum mechanically confined to move along one direction with their motion in the remaining transverse directions confined via a potential \( V_{\text{conf}}(\vec{r}_\perp) \) where \( \vec{r}_\perp = (y, z) \) denotes the transverse coordinates of quantization. Electron-electron interactions within the wire are described by \( U(\vec{r}) \) which is purely repulsive. The Hamiltonian is a sum of two independent terms in the transverse and longitudinal directions with the result that the wavefunction (and therefore the correlation functions) can be decomposed as a product of \( \phi(\vec{r}_\perp) \) and \( \psi_s(x) \) where \( \phi(\vec{r}_\perp) \) is the orthogonal wavefunction of transverse quantization of the two degenerate bands (X and Y valleys) and \( \psi_s(x) \) the longitudinal part. In order to describe the physics along the longitudinal direction we now promote the wavefunction, \( \psi_s(x) \), to the level of a field operator (for a field theoretic description) responsible for creating and annihilating the electrons taking part in the various scattering processes. With this in mind the second quantized Hamiltonian suitable for our purposes of study is

\[
H = \sum_s \int d^3\vec{r} \Psi_s^\dagger(\vec{r}) \left( -\frac{1}{2m} \nabla_{\vec{r}}^2 - \mu + V_{\text{conf}}(\vec{r}_\perp) \right) \Psi_s(\vec{r}) + \frac{1}{2} \sum_{s,s'} \int d^3\vec{r} d^3\vec{r}' U(\vec{r} - \vec{r}') \Psi_s^\dagger(\vec{r}) \Psi_s^\dagger(\vec{r}') \Psi_{s'}(\vec{r}) \Psi_{s'}(\vec{r}') \tag{4.1}
\]

where \( \Psi_s(\vec{r}) = \phi(\vec{r}_\perp) \psi_s(x) \) is now the field operator for an electron species of spin \( s = \{\uparrow, \downarrow\} \), and \( \mu \) is the chemical potential in the leads. Because the low energy, long wavelength excitations occur around the vicinity of the Fermi points (see Fig. 4.3(b)) a further decomposition is possible with \( \Psi_s(\vec{r}) = \phi(\vec{r}_\perp)(\psi_{As}(x) + \psi_{Bs}(x)) \). The coordinate \( x \) is in the long direction of the wire. The longitudinal part of the field can be naturally expanded in terms of the right- and left-moving excitations, \( R_{ns}(x) \) and \( L_{ns}(x) \), respectively, residing around the Fermi points of the two bands (indicated by the black dots in Fig. 4.3(b)) with \( \psi_{As}(x) = R_{As}(x) e^{i k_{F}^{A+} x} + L_{As}(x) e^{i k_{F}^{A-} x} \) and \( \psi_{Bs}(x) = R_{Bs}(x) e^{i k_{F}^{B+} x} + L_{Bs}(x) e^{i k_{F}^{B-} x} \). The band index is \( n = A, B \) and the Fermi momenta are defined by \( k_{F}^{A\pm} = -\frac{k_{U}}{4} \pm k_{F}^{o} \) and \( k_{F}^{B\pm} = \frac{k_{U}}{4} \pm k_{F}^{o} \) where \( k_{U} \) is the umklapp
vector, and $k_F^o$ is the magnitude of the Fermi wavevector measured from the bottom of each band, as shown in Fig. 4.3(b).

The interaction part of the Hamiltonian reduces to a sum of two types of fermionic processes. The first type describes the interaction of electrons within the same band, $n = A, B$, and contains the forward ($U^F_{\text{intra}}$) and the backward scattering ($U^B_{\text{intra}}$) processes. These are referred to as the intraband interaction processes. The second type describes electron-electron scattering processes involving both bands, classified as interband interactions. The relevant interband interaction terms in the fermionic language include forward ($U^F$), backward ($U^B_d, U^B_x$ and $U^B_{\text{inter}}$), and inter-valley umklapp ($U_{\text{um}}$) scattering. The Fermionic interaction terms of the problem are expressed below via the right- and left- moving excitations, $R_{ns}(x)$ and $L_{ns}(x)$. In the interaction terms stated below the band index is $n = A, B$, the spin index is $s = \{\uparrow, \downarrow\}$, $k_U$ is the umklapp vector and $k_F^o$ is the magnitude of the Fermi wavevector measured from the bottom of each band as shown in Fig. 4.3(b). The notation $\xi_n = \delta_{nA} - \delta_{nB}$.

The matrix element $M$, which is the interaction kernel, is given by the expression

$$M(x - x') = \int U(\vec{r} - \vec{r}')\phi^2(\vec{r}_\perp)\phi^2(\vec{r}'_\perp)d\vec{r}_\perp d\vec{r}'_\perp. \quad (4.2)$$

The Fermionic interaction terms are as follows

**Intraband interaction** (see Fig. 4.4)

The intraband forward and backward scattering terms are shown in Fig. 4.4 and their expressions stated in Eqs. 4.3 and 4.4. The intraband forward scattering interaction term, $U^F_{\text{intra}}$, is

$$U^F_{\text{intra}} = \frac{1}{2} \sum_{n=A,B} \int dx dx' M(x - x') \sum_{s,s'} \left[ R^\dagger_{ns}(x) R_{ns}(x) + L^\dagger_{ns}(x) L_{ns}(x) \right] \times \left[ R^\dagger_{ns'}(x') R_{ns'}(x') + L^\dagger_{ns'}(x') L_{ns'}(x') \right] \quad (4.3)$$
Figure 4.4. Representative low energy long wavelength *intraband electron-electron scattering processes*. In each figure $E$ and $k$ refer to energy and momentum respectively. The open and filled dots represent electrons which are taking part in the scattering processes with the arrows depicting the direction of scattering. The Fermi points are at $k_F^{A\pm} = -\frac{k_U}{4} \pm k_F^\circ$ and $k_F^{B\pm} = \frac{k_U}{4} \pm k_F^\circ$ (as described in Fig. 4.3(b)) where $k_U$ is the umklapp vector, and $k_F^\circ$ is the magnitude of the Fermi wavevector measured from the bottom of each band.
and the intraband backscattering term, $U_{\text{intra}}^B$ is
\[
U_{\text{intra}}^B = \frac{1}{2} \sum_{n=A,B} \int \int dx \, dx' \, M(x-x') \sum_{s,s'} \left[ R_{ns'}^\dagger(x) L_{ns'}^\dagger(x') R_{ns'}(x') L_{ns}(x) e^{-2ik_F(x-x')} + L_{ns}^\dagger(x) R_{ns}^\dagger(x') L_{ns'}(x') R_{ns}(x) e^{2ik_F(x-x')} \right]
\] (4.4)

The interband scattering terms are shown in Fig. 4.5 and their expressions stated in Eqs. 4.5 – 4.9.

**Interband interaction** (see Fig. 4.5)

The forward scattering term, $U^F$, is
\[
U^F = \frac{1}{2} \sum_{n \neq m} \int \int dx \, dx' \, M(x-x') \sum_{s,s'} \left[ R_{ns}^\dagger(x) R_{ns}(x) + L_{ns}^\dagger(x) L_{ns}(x) \right] \times \left[ R_{ms'}^\dagger(x') R_{ms'}(x') + L_{ms'}^\dagger(x') L_{ms'}(x') \right]
\] (4.5)

The direct backscattering term, $U^B_d$, is
\[
U^B_d = \frac{1}{2} \sum_{n \neq m} \int \int dx \, dx' \, M(x-x') \sum_{s,s'} \left[ R_{ns}^\dagger(x) L_{ns}(x) L_{ms'}^\dagger(x') R_{ms'}(x') e^{-2ik_F(x-x')} + L_{ns}^\dagger(x) R_{ns}(x) R_{ms'}^\dagger(x') L_{ms'}(x') e^{2ik_F(x-x')} \right]
\] (4.6)

The exchange backscattering term, $U^B_x$, is
\[
U^B_x = -\frac{1}{2} \sum_{n \neq m} \int \int dx \, dx' \, M(x-x') e^{i\xi_0(x-x')} \sum_{s,s'} \left[ R_{ns}^\dagger(x) L_{ns'}(x') R_{ms'}^\dagger(x') R_{ms}(x) + L_{ns}^\dagger(x) R_{ns'}(x') R_{ms'}(x') L_{ms}(x) \right]
\] (4.7)

The interband backscattering term, $U^B_{\text{inter}}$, is
\[
U^B_{\text{inter}} = -\frac{1}{2} \sum_{n \neq m} \int \int dx \, dx' \, M(x-x') e^{i\xi_0(x-x')} \sum_{s,s'} \left[ R_{ns}^\dagger(x) R_{ns'}(x') R_{ms'}^\dagger(x') R_{ms}(x) + L_{ns}^\dagger(x) L_{ns'}(x') L_{ms}(x) + R_{ns}^\dagger(x) R_{ns'}(x') L_{ms}(x) e^{-2ik_F(x-x')} + L_{ns}^\dagger(x) L_{ns'}(x') R_{ms'}^\dagger(x') R_{ms}(x) e^{2ik_F(x-x')} \right]
\] (4.8)
and finally the inter-valley umklapp scattering term, $U_{um}$, is

$$U_{um} = \frac{1}{2} \sum_{n \neq m} \int dxdx' M(x - x') e^{ikU/2(x - x')} \xi_n \sum_{s,s'} \left[ R_{ns}^\dagger (x) L_{ns'}^\dagger (x') e^{-ikF(x - x')} + L_{ns}^\dagger (x) R_{ns'}^\dagger (x') e^{ikF(x - x')} \right]$$

(4.9)

The interband forward scattering term is shown in Fig. 4.5(a). The backscattering term has three types - direct, exchange and interband. We define direct backscattering, $U_{B_d}$, as an event where backscattering processes occur in each band separately (see Fig. 4.5(b)). Exchange backscattering, $U_{B_x}$, has the same initial and final states as direct backscattering, but the electrons switch bands (see Fig. 4.5(c)). Interband backscattering, $U_{B_{inter}}$, is backscattering between two electrons in different bands (see Fig. 4.5(d)). The inter-valley umklapp scattering is unique to this bandstructure (see Fig. 4.5(e)). It is a scattering process where two electrons starting, for e.g., in band A with total momentum $-k_U/2$ scatter into band B, with total momentum $k_U/2$. The momentum difference between the initial and final states is an umklapp vector which can be exchanged with the lattice. This is an umklapp process which is present at all densities and is not related to the commensurability of the electron gas with the underlying lattice. It is unique to the AlAs QWR bandstructure and as we shall see later will play an important role in classifying the phase diagram.

4.4 Bosonizing the Hamiltonian

The low energy properties of the interacting 1D electron gas can be conveniently described within the framework of the bosonization technique [7,25–27]. Within this approach one can associate with the right- and left- moving, $R_{ns}(x)$ and $L_{ns}(x)$, respectively, fermionic field operators a combination of bosonic fields $\phi_{n\nu} = (\phi_{n\uparrow} \pm \phi_{n\downarrow})/\sqrt{2}$ and $\theta_{n\nu} = (\theta_{n\uparrow} \pm \theta_{n\downarrow})/\sqrt{2}$, where $\nu = \rho, \sigma$ (the charge and spin modes) correspond to the $\pm$ combination, $s = \{\uparrow, \downarrow\}$ is the spin index and $n = A,B$ is the band in-
Figure 4.5. Representative low energy long wavelength interband electron-electron scattering processes. In each figure $E$ and $k$ refer to energy and momentum respectively. The open and filled dots represent electrons which are taking part in the scattering processes with the arrows depicting the direction of scattering. The Fermi points are at $k_F^{A\pm} = -\frac{k_U}{4} \pm k_F^\phi$ and $k_F^{B\pm} = \frac{k_U}{4} \pm k_F^\phi$ (as described in Fig. 4.3(b)) where $k_U$ is the umklapp vector, and $k_F^\phi$ is the magnitude of the Fermi wavevector measured from the bottom of each band. The inter-valley umklapp scattering (Fig. 4.5(e)) shown above is unique to this aluminum arsenide quantum wire bandstructure arrangement.
index. The bosonic fields satisfy the commutation relation 
\[ [\phi_{n\nu}(x), \partial_x \theta_{n',\nu'}(x')] = i\pi \delta(x - x') \delta_{n,\nu'} \delta_{n,\nu} \] with \( \hbar \) set equal to one. We then have
\[
R_{ns}(x) = \frac{\eta_{Rns}}{\sqrt{2\pi \alpha}} e^{i\sqrt{\frac{\pi}{2}}[\theta_{n\nu}(x) - \phi_{n\nu}(x) + s(\theta_{na}(x) - \phi_{na}(x))]} \tag{4.10}
\]
and,
\[
L_{ns}(x) = \frac{\eta_{Lns}}{\sqrt{2\pi \alpha}} e^{i\sqrt{\frac{\pi}{2}}[\theta_{n\nu}(x) + \phi_{n\nu}(x) + s(\theta_{na}(x) + \phi_{na}(x))]} \tag{4.11}
\]
where \( \alpha \) is the short distance cutoff, \( \eta_{Rns} \) and \( F_{Lns} \) are the Klein factors for the right- and left- moving fields of band \( n \) with species of spin \( s \). They are required to preserve the anti-commutation relations of the fermionic fields. The convenient field variables for the Hamiltonian in our problem will be a linear combination of the boson fields constructed out of the two bands. We define the transformation to a symmetric and an anti-symmetric basis as 
\[
\phi_{\nu}^\pm = \frac{1}{\sqrt{2}} (\phi_{A\nu} \pm \phi_{B\nu}) \quad \text{and} \quad \theta_{\nu}^\pm = \frac{1}{\sqrt{2}} (\theta_{A\nu} \pm \theta_{B\nu}).
\]
Upon bosonization and subsequent transformation the parts of the Hamiltonian corresponding to free motion produce the harmonic terms in the symmetric and the anti-symmetric bosonic fields (\( \phi_{\nu}^\pm \) and \( \theta_{\nu}^\pm \)) only. The intraband interactions and the interband interactions, however, generate both cosine interaction terms and harmonic terms. Furthermore while bosonizing we also used the fact that the exponential \( e^{ik_U x} = 1 \). This is true because the electrons in the QWR move in an underlying lattice and their spatial coordinate \( x = ma_x \), where \( a_x \) is the lattice spacing in the long direction of the wire and \( m \) is an integer. When multiplied with the umklapp vector, \( k_U = 2\pi/a_x \), and exponentiated the result is \( \exp[-2m\pi] = 1 \).

The Hamiltonian, \( H \), can be written in the following canonical form
\[
H = \frac{1}{2} \sum_{\mu=\pm, \nu=\rho,\sigma} \int dR \left[ v^\mu_\nu K^\rho_\nu (\partial_R \theta^\mu_\nu)^2 + \frac{v^\mu_\nu}{K^\rho_\nu} (\partial_R \phi^\mu_\nu)^2 \right] + H_{\text{int}} \tag{4.12}
\]
where the bosonic interaction terms, \( H_{\text{int}} \), are
\[
H_{\text{int}} = \frac{t_1}{2\pi^2 \alpha^2} \int dR \cos[\sqrt{4\pi} \phi^+_\sigma] \cos[\sqrt{4\pi} \phi^-_\sigma] \\
+ \frac{t_2}{2\pi^2 \alpha^2} \int dR \cos[\sqrt{4\pi} \phi^-_\rho] \cos[\sqrt{4\pi} \phi^+_\sigma] \\
+ \frac{t_3}{2\pi^2 \alpha^2} \int dR \cos[\sqrt{4\pi} \phi^-_\rho] \cos[\sqrt{4\pi} \phi^-_\sigma]
\]
with the coupling constants defined in terms of the Coulomb matrix element $M(a)$

\begin{align}
t_1 &= t_2 = 2 \int da M(a) \cos[2k_F a] \\
t_3 &= 2 \int da M(a) \left( \cos[2k_F a] - \cos \left( \frac{k_F a}{2} \right) \right) \\
t_4 &= t_5 = -t_{10} = -t_{11} = -2 \int M(a) \cos \left( \frac{k_F a}{2} \right) \\
t_6 &= -t_9 = -2 \int da M(a) \cos[2k_F a] \cos \left( \frac{k_F a}{2} \right) \\
t_7 &= -2 \int da M(a) \sin[2k_F a] \sin \left( \frac{k_F a}{2} \right) \\
t_8 &= 2 \int da M(a) \left( 1 - \cos[2k_F a] \right) \cos \left( \frac{k_F a}{2} \right) \\
t_9 &= 2 \int da M(a) \left( 1 - \cos[2k_F a] \right) \sin \left( \frac{k_F a}{2} \right)
\end{align}

(4.14)

In the Hamiltonian, $R = (x + x')/2$ is the center-of-mass coordinate of two electrons and $a = x - x'$ their relative coordinate in the long direction of the QWR. In the quadratic part the bare symmetric and anti-symmetric Luttinger parameters, $K_{\nu}^\pm$, quoted in appendix A, can be expressed in terms of the original Luttinger parameters $K_{\nu}$. Furthermore the Luttinger parameters which have been derived here starting from the Fermionic Hamiltonian, Eq. 4.1, are the bare effective parameters [25]. The symmetric and anti-symmetric velocities $v_{\nu}^\pm$, refer appendix A, can also be expressed in terms of the original velocities $v_{\nu}$.

The coupling constants of the problem are denoted by $t_i$, where $i = 1, \ldots, 11$. They are related to the fourier components of the interaction kernel, $M(a)$, with
the wavevectors of the problem - \( k_U \) and \( k_{F}^{o} \). It is instructive to observe that the umklapp vector is independent of the electron density in the QWR whereas \( k_{F}^{o} \) is not. This allows for the interesting possibility to tune \( k_{F}^{o} \) experimentally and control the initial conditions in the renormalization group equations itself and possibly get oneself into various electronic phases of matter as allowed in an interacting 1D electron gas problem. Also, the initial conditions depend on the QWR parameters - the width (\( w \)), the length (\( L \)), and the distance of the QWR from the back-gate (\( d \)).

The first bosonized interaction term with the coupling \( t_{1} \) arises from intraband backscattering type processes (refer Fig. 4.4(b)) with a coupling strength which depends on the \( 2k_{F}^{o} \) cosine fourier component of the interaction kernel \( M(a) \). The second is a result of the direct backscattering type interaction as shown in Fig. 4.5(b) and has a coupling strength equal to that of an intraband backscattering process. This is evident from the diagram of the scattering processes shown in Figs. 4.4(b) and 4.5(b). The third interaction term has contributions from both the direct and exchange backscattering processes, whereas the fourth term is exclusively generated from exchange backscattering. The exchange backscattering process has a strength which depends on the \( k_U/2 \) cosine fourier component of the interaction kernel \( M(a) \). The third interaction term is a combination of both and has the \( 2k_{F}^{o} \) and the \( k_U/2 \) cosine fourier components. These first four interaction terms have in their bosonized expressions the charge density wave phase \( \phi_{\rho}^{-} \) for the relative charge channel in the antisymmetric basis together with the spin fields \( \phi_{\sigma}^{+}, \phi_{\sigma}^{-} \), and \( \theta_{\sigma}^{-} \). The next three terms \( t_5, t_6, \) and \( t_7 \) are generated from the interband backscattering process shown in Fig. 4.5(d). They involve only the spin fields \( \phi_{\sigma}^{+}, \phi_{\sigma}^{-} \), and \( \theta_{\sigma}^{-} \). For \( t_6 \) and \( t_7 \) the coupling depends on both the \( 2k_{F}^{o} \) and \( k_U/2 \) cosine fourier component of the interaction kernel. The strength of \( t_5 \) is proportional to \( k_U/2 \).

Bosonization of the inter-valley umklapp scattering fermionic processes produce six bosonized interaction terms in total. Out of those, two are of the form

\[
\sim \cos[\sqrt{4\pi}\theta_{\rho}^{-}] \cos[\sqrt{4\pi}\phi_{\rho}^{-}] \cos[\sqrt{4\pi}\theta_{\sigma}^{-}] \cos[\sqrt{4\pi}\phi_{\sigma}^{-}]
\]

\[
\sim \sin[\sqrt{4\pi}\theta_{\rho}^{-}] \sin[\sqrt{4\pi}\phi_{\rho}^{-}] \sin[\sqrt{4\pi}\theta_{\sigma}^{-}] \sin[\sqrt{4\pi}\phi_{\sigma}^{-}]
\]

(4.15)
From a purely physical standpoint these terms involve self destructing competing dual fields. Furthermore the couplings associated with these interactions can never grow since the perturbations involved have a scaling dimension which is greater than two and makes them irrelevant in the renormalization group sense. We therefore ignore their contribution in computing the renormalization group equations. We retain only the remaining four interaction terms labeled as \( t_8, t_9, t_{10} \) and \( t_{11} \). All these terms involve the superconducting phase \( \theta_p^- \) for the relative charge channel in the antisymmetric basis together with the spin fields of the problem. Their coupling strength depends on the \( 2k_F^2 \) and \( k_U/2 \) cosine fourier component. Finally we note that the Hamiltonian remains quadratic in the total charge fields \( \phi_p^+ \) and \( \theta_p^+ \).

In summary, starting from the interacting 1D Hamiltonian (see Eq. 4.1) we have classified the important low energy long wavelength fermionic interaction processes and then bosonized them (see Eqs. 4.12 and 4.13). In the next section 4.5 we use a weak coupling renormalization group treatment, described earlier in chapter 3, to determine which of the coupling constants associated with the bosonized interaction terms diverge.

4.5 Analyzing the renormalization group equations

To analyze the low energy, long wavelength behavior of the interacting system, we employ the renormalization group approach. In this approach the shortwave-length modes are systematically eliminated leading to a set of coupled differential equations for the coupling constants. For the present problem, one can derive the appropriate renormalization group equations for the entire set of interactions, \( t_i \), where \( i = 1, \ldots, 11 \), in perturbation theory about the noninteracting fixed point, the quadratic Hamiltonian Eq. 4.12 using the momentum shell renormalization group procedure described in chapter 3. The renormalization group equations for these coupling constants (up to second order, \( O(2) \)) of the problem are quoted in appendix B.
We study the renormalization group equations for the regimes - $K_{\rho}^- < 1$ (repulsive) and $K_{\rho}^- > 1$ (attractive) of the bosonic theory in the relative charge channel. The $K_{\rho}^- < 1$ case is repulsive since it promotes the CDW phase, $\phi_{\rho}^-$. The $K_{\rho}^- > 1$ case is attractive because it promotes the SS phase, $\theta_{\rho}^-$. The equations are integrated numerically for some suitable initial conditions until one or more couplings grow to be of order one, $O(1)$. The order one $O(1)$ couplings are considered to be large and thus pin (gap) the appropriate bosonic modes. We then replace the gapped fields with their expectation value both in the Hamiltonian and in the bosonized version of the correlation functions. The correlation functions which do not vanish then help to determine the divergent susceptibilities and the possible thermodynamic phase for that regime.

The initial condition under which we begin the renormalization group flow is determined by evaluating the coupling constants, Eq. 4.14 for the QWR parameters width, length and the distance from the back-gate. The phenomenological form for the interaction kernel is $M(a) = \frac{e^2}{4\pi\epsilon_o \sqrt{w^2+a^2}} e^{-\frac{(a/d)}{\sqrt{w^2+a^2}}}$, which has the nature of a screened Coulomb potential where $e$ is the electronic charge and $\epsilon_o$ the permittivity of free space. The screening involves two length scales. The distance of the QWR to the back-gate, $d$, and the width, $w$, of the wire. The width $w$ provides the short-distance cutoff whereas the distance to the back-gate $d$ is the long-distance cutoff. Using these parameters and the expression for the coupling constants, Eq. 4.14 we can make an estimate for the initial conditions.

For the quantum wire of Moser et.al. [89,90] we have a transverse size of $w \sim 15\text{nm}$ separated from the metallic gate by a distance $d \sim 300\text{nm}$. The wire length is $L \sim 1\mu\text{m}$. We then have $w/d \sim 0.05$ and the ratio $L/d = 10/3$. The parameters used to estimate $k_F^D$ for the aluminum arsenide bandstructure are: density of the electrons in the quantum wire $\sim 10^8 \text{m}^{-1}$ and the effective mass of the electron $m^* = 0.33 m_e$ along the long direction where $m_e$ is the bare mass of the electron [90]. Furthermore, experimental evidence [114,116] suggests that spin rotational invariance is not broken.
in the AlAs quantum wells in the absence of a magnetic field. The problem is then $SU(2)$ invariant and we can set $K^\pm_\sigma = 1$ to begin the renormalization group flow.

The analysis, with the above initial conditions, for the repulsive regime in the relative charge channel, $K^-_\rho < 1$, shows that the coupling constants $t_2$ and $t_3$ diverge, in fact $(t_2, t_3) \to (\infty, \infty)$. The fields which get gapped are the antisymmetric charge field $\phi^-_\rho$ and the spin fields $\phi^\pm_\sigma$. Their possible acquired expectation values are $(\langle \phi^-_\rho \rangle, \langle \phi^+_\sigma \rangle, \langle \phi^-_\sigma \rangle) = (\pm \sqrt{\pi}/2, 0, 0)$ or $(0, \pm \sqrt{\pi}/2, \pm \sqrt{\pi}/2)$. The final phase in either case is a dominant divergent intraband (odd combination) $2k_F^\rho$-CDW. The corresponding CDW correlation function, $\hat{\chi}_{\text{CDW},2k_F^\rho}^{\text{intra,odd}}$ (refer appendix C), decays with the power law $\chi_{\text{CDW}} \sim (1/r)^{K^+\rho/2}$ where $K^+_\rho$ is the total charge Luttinger parameter.

Although the original screened Coulomb interaction is repulsive, in the course of renormalization it can be led to an effective attractive regime, $K^-_\rho > 1$. For this case the renormalization group flows indicate that the divergent coupling constants are $t_9$ and $t_{10}$ where both $(t_9, t_{10}) \to (\infty, \infty)$. From the interactions terms we can then deduce that the dual antisymmetric charge field $\theta^-_\rho$ gets gapped together with the spin fields $\phi^\pm_\sigma$. They acquire the expectation values of $(\langle \theta^-_\rho \rangle, \langle \phi^+_\sigma \rangle, \langle \phi^-_\sigma \rangle) = (\pm \sqrt{\pi}/2, 0, 0)$ or $(0, \pm \sqrt{\pi}/2, \pm \sqrt{\pi}/2)$. These gapped fields lead to a state with a divergent intraband SS correlation function $\Delta_{\text{intra,singlet}}^{\text{intra,odd}}$ (appendix C) with the power law $\chi_{\text{SS}} \sim (1/r)^{1/2K^+\rho}$.

We also find through our analysis that although for the finite sized wire with $L/d \sim 3.33$, the initial conditions for the renormalization group flows differ from the true 1D limit of $L/d \to \infty$, due to the screening of the back gate this is not a severe effect, and the system remains in the same basin of attraction as the infinite wire. The renormalization group results can now be summarized in the phase diagram shown in Fig. 4.6.

For the AlAs QWR bandstructure, due to the presence of four Fermi points we have in general eight fields, $\phi^\pm_\nu$ and their duals $\theta^\pm_\nu$ where $\nu = \rho, \sigma$ refer to the charge and spin modes. For a gapless system, Luttinger liquid, we would have a C2S2 phase where the notation refers to the number of gapless charge ($C$) and spin ($S$) modes. But in the present problem due to the presence of interactions certain modes as predicted
Figure 4.6. *Phase diagram*: Divergent correlation functions for the quantum wire in the presence of inter-valley umklapp scattering for the two regimes $K_\rho^- < 1$ (repulsive) and $K_\rho^- > 1$ (attractive). The notation CDW stands for charge density wave and SS for singlet superconductivity. In the diagram $k_p$ denotes the pairing momenta of the center-of-mass of the Cooper pairs. The finite pairing momentum is an indication of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state which is encouraged in this wire due to the presence of the umklapp interactions. Such a state is also known to lead to inhomogeneous superconductivity.

by the renormalization analysis get gapped. Furthermore, due to the absence of any bosonized interaction terms in the total charge mode we expect the total charge field to remain gapless. As a result we have the C1S0 phase [42, 64] where the notation refers to one gapless total charge mode $(\phi_\rho^+) \text{ with all other charge and spin modes gapped.}$

One of the novel aspects of this superconductivity is that it originated from a purely repulsive screened Coulomb interaction. In the process of renormalization, in the relative charge channel for $K_\rho^- > 1$, an attractive interaction was generated. This resulted in a pairing of up and down spins within a band and subsequent scattering of it from one band to another via the umklapp Cooper scattering process. Energetically the process can be understood as a competition between Coulomb repulsion of pairing and the kinetic energy of the pair where the latter wins. Such a kinetic energy driven mechanism for superconductivity has been proposed earlier in the context of high temperature superconductors [57].

Another unique aspect of this superconductivity is that the pairing momenta of the Cooper pairs is nonzero. It is half the umklapp vector. Being at a finite wavevector
one could think of this as a density modulated superconducting state where the superfluid density varies from one lattice site to another with the wavevector $\frac{k_F}{2}$. Such an inhomogeneous superconducting state is known to arise in the FFLO state [93].

4.6 Conclusion

QWRs provide an opportunity for technological innovation. In this context a phase diagram helps to understand what electronic phase the QWR may predominantly find itself in since it has an important effect on the transport properties. In this paper we have investigated the possibility of a spin gapped AlAs QWR. Using 1D field theoretic methods and perturbative renormalization group we are able to conclude that the novel AlAs QWR, fabricated by Moser et al. [89, 90] under investigation will have the possibility of a spin gapped state with divergent $2k_F$-CDW or SS fluctuations. While the CDW wave phase is robust deep in the repulsive region, there is a part of the phase diagram which promotes a non-trivial SS with finite-momentum Cooper pairing leading to an inhomogeneous superconducting state. The finite pairing momentum is an indication of a FFLO state.
5. LUTTINGER LIQUID KINK

5.1 Introduction

One of the most dramatic consequences of confining electrons to one spatial dimension is the prediction of spin-charge separation. That is, due to many-body interactions the electron is no longer a stable quasiparticle, but decays into separate spin and charge modes [29–31]. A direct experimental observation of spin-charge separation has proven difficult although evidence for Luttinger liquid behavior has been reported in many 1D systems, via, e.g., a suppression of the density of states near the Fermi level in ropes of carbon nanotubes [32] or power law behavior in the conductance vs. temperature in edge states of the fractional quantum Hall effect [33, 34] and carbon nanotubes [35]. Until now, very limited direct evidence for spin-charge separation has been reported. Tunneling measurements later provided evidence for explicit spin-charge separation in 1D systems, via real-space imaging of Friedel oscillations using scanning tunneling microscopy on single-walled carbon nanotubes [100] and momentum- and energy-resolved tunneling between two coupled QWRs [80], both of which observed multiple velocities indicative of spin-charge separation. More direct evidence of spin-charge separation would be to measure separate spin and charge dispersions in a single-particle spectral function. [36] Despite much effort in this area, this has only been achieved recently in an unambiguous way in the Mott-Hubbard insulator SrCuO$_2$. [36] Other claims of the detection of separately dispersing spin and charge peaks with ARPES [95, 96] have been overturned [97, 98], or lack independent verification of the spin and charge energy scales. [99]

Part of the difficulty in directly measuring spin and charge dispersions through measurements proportional to the single particle spectral function is that within Luttinger liquid theory, the spinon branch is muted compared to the holon branch. Finite
Figure 5.1. Schematic diagram of peak broadening due to interactions and finite temperature in the Luttinger liquid spectral function. The dashed lines denote the zero temperature dispersion tracking the charge part with velocity $v_\rho$ and the spin part with velocity $v_\sigma$. At $T \neq 0$, the peaks become thermally broadened as indicated by the shaded regions. In this case the effective dispersion now tracks the solid red line, so that the low energy part tracks the sum of the two broad spin and charge peaks, resulting in a low energy velocity $v_l$ which is between the spin and charge velocities. Note the high energy effective dispersion is parallel to the charge part but displaced, an effect due to finite temperature and interactions. This results in the high energy part extrapolating back to a value $k_{ex} \neq k_F$.

temperature and experimental resolution only compound the problem, making direct detection of the spinon branch in, e.g., ARPES difficult. In this chapter, we show how spin-charge separation can nevertheless be detected via the systematic temperature dependence of a kink in the effective electronic dispersion, even in cases where the spin peak is not directly resolvable.
5.2 Theory

Although the electron is not an elementary excitation of the Luttinger liquid because it is unstable to spin-charge separation, an effective electronic dispersion may still be defined by the existence of (generally broad) peaks in the spectral function. At zero temperature in 1D, there are two sharp peaks in the electronic spectral function, one dispersing at the velocity $v_\sigma$ of the collective spin modes (spinons) and the other at the velocity $v_\rho$ of the collective charge modes (holons) \cite{38,39}. However, at finite temperature, the spin and charge peaks are broadened, as shown schematically in Fig. 5.1. At low binding energy, this causes the two to merge into one broad peak with an effective dispersion which lies between the spin velocity $v_\sigma$ and the charge velocity $v_\rho$. Although the two peaks separate at higher binding energies, interactions and temperature strongly suppress the spin peak for repulsive interactions. As a result, the dominant (and most easily measurable) peak will disperse with the charge velocity at high energy. This gives rise to a kink in the effective electronic dispersion. Since the Luttinger liquid is quantum critical, the kink energy scales linearly with temperature, $E_{\text{kink}} \propto a(r, \gamma_\rho)T$, where $a$ is a function of the velocity ratio $r = v_\sigma/v_\rho$ and the interaction strength $\gamma_\rho = \frac{1}{5}(K_\rho + K_\rho^{-1} - 2)$ where $K_\rho$ is the charge Luttinger parameter. For $\gamma_\rho = 0.15 - 0.30$ and $r = 0.2 - 0.4$, the range of $a$ is $a = 3.3 - 3.9$. The kink is stronger for lower values of $r$, but diminishes again for strong enough interaction strength. Moreover, the high energy linear effective dispersion extrapolates to the Fermi energy at a wavevector $k_{ex} \neq k_F$ which is shifted from the Fermi wavevector by an amount which scales linearly with temperature. Recently explicit analytic expressions for correlation functions in the Tomonaga-Luttinger liquid at finite temperature were obtained under various conditions \cite{37}. We consider here the single hole spectral function, $A^<(k, \omega)$, since it is directly proportional to the intensity observed in ARPES experiments. In the spin-rotationally invariant case, the finite-
temperature single hole spectral function [37] may be written in terms of the scaled variables $\tilde{k} = \frac{\nu k}{\pi T}$ and $\tilde{\omega} = \frac{\omega}{\pi T}$ with the Boltzmann constant $k_B = 1$,

$$A^<(k, \tilde{\omega}) \propto \int_{-\infty}^{\infty} dq \ h_{\gamma_c + \frac{1}{2}} \left( \frac{\tilde{\omega} - k}{2} + (1 + r)q \right) h_{\gamma_c} \left[ \frac{\tilde{\omega} - k}{2} - (1 - r)q \right]$$

(5.1)

where $r = v_\sigma / v_\rho$ is the ratio between the spin velocity and the charge velocity and $h_{\gamma}$ is related to the beta function

$$h_{\gamma}(k) = \Re \left[ (2i)^{\gamma} B \left( \frac{\gamma - ik}{2}, 1 - \gamma \right) \right]$$

(5.2)

The charge interaction strength $\gamma_\rho$ is related to the charge Luttinger parameter $K_\rho$ by $\gamma_\rho = \frac{1}{8} (K_\rho + K_\rho^{-1} - 2)$, i.e. $\gamma_\rho = 0$ in the noninteracting case, and $\gamma_\rho$ increases with increasing interaction strength. Because of spin rotation invariance, we use $K_\sigma = 1$ and $\gamma_\sigma = 0$.

### 5.3 Results and Discussion

In order to define a single-hole effective dispersion, we use momentum distribution curves (MDC’s), i.e. the single hole spectral function $A^<(k, \omega_o)$ considered as a function of $k$ at a given value of the frequency $\omega_o$. The effective dispersion is identified by the position $k_o = k_o(\omega_o)$ of the maximum of $A^<_{\max}(k, \omega_o)$ with respect to $k$. This gives an implicit equation for the effective single hole dispersion $\omega_o(k_o)$. This method gives a more reliable definition of the effective dispersion than using energy distribution curves (EDC’s), i.e. the spectral function considered as a function of frequency at a given momentum $k_o$, $A^<(k_o, \omega)$. Whereas EDC’s can become quite broad with increasing interaction strength, MDC’s are always sharp due to kinematic constraints, [117] so that there is less experimental uncertainty in identifying the location of a peak in the MDC.

Fig. 5.2(a) shows representative intensity plots of the spectral function, $A^<(k, \omega)$. In the figure, we have used an interaction strength $\gamma_\rho = 0.15$, temperature $k_B T = \ldots$
Figure 5.2. Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_{\rho} = 0.15$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2$, 0.3, and 0.4. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2$, 0.3, and 0.4. In all cases the spin velocity $v_\sigma = 1\text{eV-Å}$ and the temperature $k_B T = 14\text{meV}$.
Figure 5.3. MDC’s for $\gamma_\rho = 0.15$. The spin velocity $v_\sigma = 1\text{eV}\cdot\text{Å}$ and the temperature $k_B T = 14\text{meV}$. The ratio of spin to charge velocity is $r = 0.2$.

As is evident from the figure, the effective dispersion is linear as expected at low energy and also at high energy, but with different velocities. This gives rise to a “kink” in the effective dispersion, i.e. a change in the effective velocity. While at zero temperature, there are two well-defined peaks in the MDC’s, one dispersing with the charge velocity and the other with the spin velocity, when the temperature is finite, the width of these MDC peaks is thermally broadened. (See Fig. 5.1.) At low energies and finite temperatures, the sum of the two broad peaks is itself one broad peak, as can be seen in panels (a)-(c) in Fig. 5.3, and the maximum in the MDC will track a velocity $v_l$ which is between the spin and charge velocities, $v_\sigma < v_l < v_\rho$. At high enough energies, the temperature broadened singularities due to the spin and charge part become sufficiently separated, and the spin peak is sufficiently muted, that the MDC peak tracks the charge velocity. The separation of the muted spin peak from the stronger charge peak can be seen in panels (d) and (e) of Fig. 5.3.
In panels (f)-(i), the charge and spin peaks have moved sufficiently apart that the peak in the MDC will track the charge part. Aside from the presence of a kink in the effective dispersion, the position of the high energy linear effective dispersion is another signature of Luttinger liquid behavior. In Fig. 5.2(a) the dotted line is an extrapolation of the high energy linear part of the effective dispersion back to the Fermi energy. As can be seen from the figure, the dotted line extrapolates to \( E = E_F \) at a wavevector \( k_{ex} = k_F + \alpha(r, \gamma_\rho)T \) which is shifted from the Fermi wavevector by an amount which scales linearly with temperature.

Fig. 5.2(b) shows the effective dispersion for each of the three values of \( r \), overlaid for comparison. As one might expect, as \( r \to 1 \), the kink vanishes, since then the charge and spin pieces disperse with the same velocity. As \( r \) is decreased, so that now \( v_\rho > v_\sigma \), a kink appears, and strengthens as \( r \) is further decreased. One can see the general features that the low energy part disperses with a velocity \( v_l \) which is between the spin and charge velocities, \( v_\sigma < v_l < v_\rho \), and that the high energy part disperses with the charge velocity. However, this high energy effective dispersion extrapolates back to the Fermi energy at a wavevector \( k_{ex} \neq k_F \). At higher interaction strengths, EDC’s broaden significantly, so that \( k_{ex} \) is smaller and the kink diminishes in strength. However, \( E_{kink} \) moves to deeper binding energy as the interaction strength is increased. Additional calculations exploring the dependence of the kink on various interaction strengths are shown in appendix D.

In Fig. 5.4 we show how the effective dispersion changes with temperature. Because the Luttinger liquid is quantum critical, the spectral function has a scaling form, and the only energy scale in the effective dispersion is the temperature itself. As a result, the kink energy depends linearly on the temperature, \( E_{kink} \propto T \). As can be seen in the figure, varying only the temperature merely moves the kink to deeper binding energy, leaving the low energy velocity \( v_l \) (and therefore the strength of the kink) unchanged. in addition, as temperature is increased, the high energy part extrapolates back to the Fermi energy at a higher value of \( k_{ex} \). Up until now, we have studied the Luttinger kink in a phenomenological manner, allowing \( \gamma_\rho \) and \( r \) to
vary independently of each other. It is also useful to consider the systematics of the kink strength and energy within the context of a microscopic model. As an example, we show in Fig. 5.5 results for a Luttinger liquid derived from an incommensurate repulsive 1D Hubbard model. We take the density to be away from half filling, \( n = 0.3 \). For a given value of \( U/t \), renormalized values of \( \gamma_c^* \) and \( r^* \) are taken from Ref. [118], where Bethe-ansatz was used to find the renormalized values of \( K_{\rho}^* \), \( v_{\rho}^* \), and \( v_{\sigma}^* \). In Fig. 5.5, we show the intensity plots of the spectral function along with the effective dispersion, for the values \( U/t = 16, 8, \) and \( 4 \) of the repulsive Hubbard model. This corresponds to renormalized values of \( \gamma_{\rho}^* = 0.05, 0.04, 0.02 \), and \( r^* = 0.1, 0.2, 0.4 \), respectively. Upon increasing the Hubbard interaction strength \( U \), the strength of the kink is enhanced due to the change in the renormalized velocity ratio \( r^* \). Notice that

\[
\begin{align*}
\text{Figure 5.4. Temperature variation of the effective dispersion. The temperature varies from } k_B T &= 4\text{meV to } k_B T = 14\text{meV, starting from the lower curve and moving to the upper curve. The interaction strength } \\
\gamma_{\rho} &= 0.15, \text{the spin velocity } v_{\sigma} &= 1\text{eV-Å, and the ratio of spin to charge velocity } r = 0.3. 
\end{align*}
\]
Figure 5.5. Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions for $U = 16, 8, \text{and} 4$ in units of the hopping integral $t$. The density $n = 0.3$. (a) The intensity of $A^<(k, \omega)$. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. (b) Comparison of the dispersions at different values of $U/t$. In all cases the spin velocity $v_\sigma = 1eV\cdot\text{Å}$ and the temperature $k_B T = 14meV$.

in this case, the kink is more pronounced, and there is a sharper distinction between the low energy and high energy linear parts.

It is worth noting that behavior reminiscent of this physics was recently reported in ARPES experiments on the quasi-one-dimensional Mott-Hubbard insulator SrCuO$_2$. [36] Being an insulating material, SrCuO$_2$ is gapped, whereas the Luttinger spectral functions presented here are not. Nevertheless, the effective dispersion (measured by
EDC’s) shows a single peak at energies close to the gap, which then separates into two peaks at higher binding energy.

5.4 Conclusion

In conclusion, we have shown the existence of a temperature-dependent kink in the effective electronic dispersion of a spin-rotationally invariant Luttinger liquid, due to spin-charge separation. At low energies, the effective dispersion is linear, with a velocity between the spin and charge velocities, $v_\sigma < v_l < v_\rho$. At high energies, the MDC peak disperses with the charge velocity. Because the Luttinger liquid is quantum critical, the kink between the high energy and low energy behavior has an energy set by temperature, $E_{\text{kink}} \propto T$. In addition, the high energy effective dispersion extrapolates back to the Fermi energy at a wavevector $k_{ex} \neq k_F$ which is shifted from the Fermi wavevector by an amount which is proportional to temperature. As interactions are increased, the kink diminishes in strength, and moves to higher binding energy. In cases where finite temperature and interactions along with experimental uncertainties obscure the detection of two separate peaks in the effective dispersion, the kink analysis presented here can be used as a signature of spin-charge separation in Luttinger liquids.
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APPENDICES
Appendix A: Luttinger parameters for the quantum wire

The symmetric and the anti-symmetric velocity \((v^\pm_\rho, v^\pm_\sigma)\) and the Luttinger parameters, \((K^\pm_\rho, K^\pm_\sigma)\) are expressed in terms of the original velocity and the Luttinger parameters as

\[
v^+_\rho K^+_\rho = v_\rho K_\rho + \frac{M(2k_F^\rho)}{2\pi} - \frac{b^-}{2\pi}
\]

\[
v^+_\rho K^-_\rho = \frac{v^+_\rho}{K^-_\rho} = \frac{v_\rho}{K_\rho} + \frac{8M(0)}{2\pi} - \frac{M(2k_F^\rho)}{2\pi} - \frac{b^+}{2\pi}
\]

\[
v^-_\rho K^-_\rho = v_\rho K_\rho - \frac{2\pi}{2\pi} - \frac{b^-}{2\pi}
\]

\[
v^-_\rho K^+_\rho = \frac{v^-_\rho}{K^+_\rho} = \frac{v_\rho}{K_\rho} - \frac{M(2k_F^\rho)}{2\pi} + \frac{b^+}{2\pi}
\]

\[
v^+_\sigma K^+_\sigma = v_\sigma K_\sigma + \frac{M(2k_F^\sigma)}{2\pi} - \frac{b^-}{2\pi}
\]

\[
v^+_\sigma K^-_\sigma = \frac{v^+\sigma}{K^-_\sigma} = \frac{v_\sigma}{K_\sigma} - \frac{M(2k_F^\sigma)}{2\pi} - \frac{b^+}{2\pi}
\]

\[
v^-_\sigma K^-_\sigma = v_\sigma K_\sigma + \frac{M(2k_F^\rho)}{2\pi} + \frac{b^-}{2\pi}
\]

where the \(b^\pm\) are defined as

\[
b^\pm = \frac{e^2}{4\pi\epsilon_o} \int da \frac{e^{-(a/d)} \cos \left(\frac{ka}{2}\right)}{\sqrt{w^2 + a^2}} (M(2k_F^\rho) \pm M(0))
\]

and \(M(0) = \int da M(a)\) and \(M(2k_F^\rho) = \int da M(a) \cos[2k_F^\rho a]\). The interaction kernel is \(M(a) = \frac{e^2}{4\pi\epsilon_o \sqrt{w^2 + a^2}}\) (see Eq. 4.2) where \(a\) is the distance along the long direction of the wire, \(e\) is the electronic charge, and \(\epsilon_o\) the permittivity of free space. The phenomenological charge and spin Luttinger parameters are \(K\rho\) and \(K\sigma\) respectively, and the charge and the spin velocities are \(v\rho\) and \(v\sigma\). The velocities are taken to be
identical for the two bands since they are degenerate. The explicit expressions for the bare Luttinger parameters and the bare velocities are given by

\[ K_\nu = \sqrt{\frac{2\pi v_F + 2g_{4,\nu} + g_\nu}{2\pi v_F + 2g_{4,\nu} - g_\nu}} \]  \hspace{1cm} (A.10)

and

\[ v_\nu = \sqrt{\left(\frac{v_F + g_{4,\nu}}{\pi}\right)^2 - \left(\frac{g_\nu}{2\pi}\right)^2} \]  \hspace{1cm} (A.11)

where \( g_\rho = g_1 - 2g_2, g_\sigma = g_1, g_{4,\rho} = g_4 \) and \( g_{4,\sigma} = 0 \). In terms of the forward and backscattering amplitudes the above g-ology coefficients are given by \( g_1 = M(2k_F^\rho), g_2 = M(0) - M(2k_F^\rho) \) and \( g_4 = M(0) \). The wavevectors \( k_U \) and \( k_F \), respectively, are the umklapp wavevector and the magnitude of the Fermi wavevector measured from the bottom of each band (see Fig. 4.3).

**Appendix B: Renormalization group equations**

The renormalization group equation for the coupling constants (see Eq. 4.13) of the problem are

\[ \frac{dt_1}{dL} = \left(2 - K_\sigma^+ - K_\sigma^-\right) t_1 - \frac{t_2t_3}{2\pi} - \frac{t_5t_6}{2\pi} - \frac{t_9t_{10}}{2\pi} \]  \hspace{1cm} (B.1)

\[ \frac{dt_2}{dL} = \left(2 - K_\rho^- - K_\sigma^-\right) t_2 - \frac{t_1t_3}{2\pi} - \frac{t_4t_6}{2\pi} - \frac{t_9t_{11}}{2\pi} \]  \hspace{1cm} (B.2)

\[ \frac{dt_3}{dL} = \left(2 - K_\rho^- - K_\sigma^-\right) t_3 - \frac{t_1t_2}{2\pi} - \frac{t_4t_5}{2\pi} - \frac{t_{10}t_{11}}{2\pi} \]  \hspace{1cm} (B.3)

\[ \frac{dt_4}{dL} = \left(2 - \frac{1}{K_\sigma^-} - K_\rho^-\right) t_4 - \frac{t_2t_6}{2\pi} - \frac{t_3t_5}{2\pi} - \frac{t_8t_{11}}{2\pi} \]  \hspace{1cm} (B.4)

\[ \frac{dt_5}{dL} = \left(2 - \frac{1}{K_\sigma^-} - K_\rho^-\right) t_5 - \frac{t_1t_6}{2\pi} - \frac{t_3t_4}{2\pi} - \frac{t_{8}t_{10}}{2\pi} \]  \hspace{1cm} (B.5)

\[ \frac{dt_6}{dL} = \left(2 - \frac{1}{K_\sigma^-} - K_\rho^-\right) t_6 - \frac{t_1t_5}{2\pi} - \frac{t_2t_4}{2\pi} - \frac{t_8t_9}{2\pi} \]  \hspace{1cm} (B.6)
\[
\frac{dt_7}{dL} = \left(2 - \frac{1}{K^\sigma_\rho} - K^\sigma_\rho^+\right) t_7 \quad (B.7)
\]

\[
\frac{dt_8}{dL} = \left(2 - \frac{1}{K^\rho_\rho} - \frac{1}{K^\rho_\rho^+}\right) t_8 - \frac{t_4 t_{11}}{2\pi} - \frac{t_5 t_{10}}{2\pi} - \frac{t_6 t_9}{2\pi} \quad (B.8)
\]

\[
\frac{dt_9}{dL} = \left(2 - \frac{1}{K^\rho_\rho} - K^\rho_\rho^+\right) t_9 - \frac{t_1 t_{10}}{2\pi} - \frac{t_2 t_{11}}{2\pi} - \frac{t_3 t_{8}}{2\pi} \quad (B.9)
\]

\[
\frac{dt_{10}}{dL} = \left(2 - K^-_\sigma - \frac{1}{K^\rho_\rho}\right) t_{10} - \frac{t_1 t_9}{2\pi} - \frac{t_2 t_{11}}{2\pi} - \frac{t_3 t_{8}}{2\pi} \quad (B.10)
\]

\[
\frac{dt_{11}}{dL} = \left(2 - K^-_\sigma - \frac{1}{K^\rho_\rho}\right) t_{11} - \frac{t_2 t_9}{2\pi} - \frac{t_3 t_{10}}{2\pi} - \frac{t_4 t_{8}}{2\pi} \quad (B.11)
\]

\[
\frac{d\ln K^\rho_\rho^-}{dL} = \frac{1}{8\pi^2} \left[- K^\rho_\rho^- \left(t_2^2 + t_3^2 + t_4^2\right) + \frac{1}{K^\rho_\rho^-} \left(t_8^2 + t_9^2 + t_{10}^2 + t_{11}^2\right)\right] \quad (B.12)
\]

\[
\frac{d\ln K^\sigma_\sigma^+}{dL} = - \frac{K^\sigma_\sigma^+}{8\pi^2} \left(t_1^2 + t_2^2 + t_6^2 + t_7^2 + t_9^2\right) \quad (B.13)
\]

\[
\frac{d\ln K^\sigma_\sigma^-}{dL} = \frac{1}{8\pi^2} \left[- K^\sigma_\sigma^- \left(t_1^2 + t_3^2 + t_{10}^2 + t_5^2\right) + \frac{1}{K^\sigma_\sigma^-} \left(t_4^2 + t_5^2 + t_6^2 + t_7^2 + t_8^2\right)\right] \quad (B.14)
\]

where \(L = \ln(\Lambda/\alpha)\), with length scale \(\Lambda\). The initial conditions of the problem are

\[
t_1(0) = t_2(0) = 2 \int daM(a) \cos[2k_F^0 a]
\]

\[
t_3(0) = 2 \int daM(a) \left( \cos[2k_F^0 a] - \cos \left(\frac{k_F^0 a}{2}\right)\right)
\]

\[
t_4(0) = t_5(0) = -t_{10}(0) = -t_{11}(0) = -2 \int M(a) \cos \left(\frac{k_F^0 a}{2}\right)
\]

\[
t_6(0) = -t_9(0) = -2 \int daM(a) \cos[2k_F^0 a] \cos \left(\frac{k_F^0 a}{2}\right)
\]

\[
t_7(0) = -2 \int daM(a) \sin[2k_F^0 a] \sin \left(\frac{k_F^0 a}{2}\right)
\]

\[
t_8(0) = 2 \int daM(a) \left(1 - \cos[2k_F^0 a]\right) \cos \left(\frac{k_F^0 a}{2}\right)
\] (B.15)
In the above equations the interaction kernel is \( M(a) = \frac{e^2}{4\pi\epsilon_0} \frac{e^{-(a/d)}}{\sqrt{w^2 + a^2}} \) (see Eq. 4.2) where \( a \) is the distance along the long direction of the wire. The coupling constants of the interaction terms (see Eq. 4.13) are denoted by \( t_i \), where \( i = 1, \ldots, 11 \). They are related to the fourier components of the interaction kernel, \( M(a) \). The wavevectors \( k_U \) and \( k_F^0 \), respectively, are the umklapp wavevector and the magnitude of the Fermi wavevector measured from the bottom of each band (see Fig. 4.3). The symmetric and anti-symmetric velocity \( (v^\pm, v^\pm) \) and Luttinger parameters, \( (K^\pm, K^\pm) \) are given by the expressions quoted in appendix A.

**Appendix C: Correlation functions for the quantum wire**

The fermionic definition together with the bosonized version of the correlation functions are stated below. The correlation functions have been classified into two categories - intraband and interband. In the expressions the band index is \( n = A, B \). The spin index is \( s = \{\uparrow, \downarrow\} \), and the Fermi momenta are defined by \( k_F^{A\pm} = -\frac{k_U}{4} \pm k_F^0 \) and \( k_F^{B\pm} = \frac{k_U}{4} \pm k_F^0 \) where \( k_U \) is the umklapp vector, and \( k_F^0 \) is the magnitude of the Fermi wavevector measured from the bottom of each band, as shown in Fig. 4.3(b). The correlation functions are expressed in terms of the right- and left- moving excitations, \( R_{ns}(x) \) and \( L_{ns}(x) \), respectively, residing around the Fermi points of the two bands (indicated by the black dots in Fig. 4.3(b)). The fields in the correlation function are the symmetric and the anti-symmetric fields defined as \( \phi^\nu_{\nu} = \frac{1}{\sqrt{2}}(\phi_{A\nu} \pm \phi_{B\nu}) \) and its dual \( \theta^\nu_{\nu} = \frac{1}{\sqrt{2}}(\theta_{A\nu} \pm \theta_{B\nu}) \) where \( \nu = \rho, \sigma \) are the charge and spin modes. The Klein factors are denoted by \( \eta_{R_{ns}} \) and \( \eta_{L_{ns}} \) for the right- and left- moving fermions, respectively, in band \( n \) with spin \( s \).
C.1 Charge density wave (CDW) correlation functions

Intraband CDW (even combination), $2k_F^o$ wavevector

\[
\hat{O}_{CDW,2k_F^o}^{\text{intra,even}}(x) = \left[ e^{i2k_F^o x} L_A^\dagger R_A^\dagger + e^{-i2k_F^o x} R_A^\dagger L_A \right] + (A \to B) \tag{C.1}
\]
\[
= \frac{2}{\pi \alpha} \sin[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\phi_\sigma^+ + \phi_\sigma^-)] \\
+ \frac{2}{\pi \alpha} \sin[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\phi_\sigma^+ - \phi_\sigma^-)] \tag{C.2}
\]

Intraband CDW (odd combination), $2k_F^o$ wavevector

\[
\hat{O}_{CDW,2k_F^o}^{\text{intra,odd}}(x) = \left[ e^{i2k_F^o x} L_A^\dagger R_A^\dagger + e^{-i2k_F^o x} R_A^\dagger L_A \right] - (A \to B) \tag{C.3}
\]
\[
= \frac{2}{\pi \alpha} \sin[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\phi_\sigma^+ + \phi_\sigma^-)] \\
- \frac{2}{\pi \alpha} \sin[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\phi_\sigma^+ - \phi_\sigma^-)] \tag{C.4}
\]

C.2 Spin density wave (SDW) correlation functions

Intraband SDW (even combination), $2k_F^o$ wavevector

\[
\hat{O}_{SDW,2k_F^o}^{\text{intra,even}}(x) = \left[ e^{i2k_F^o x} L_A^\dagger \left( \frac{\sigma}{2} \right)_{\alpha,\beta} R_A^\dagger + e^{-i2k_F^o x} R_A^\dagger \left( \frac{\sigma}{2} \right)_{\alpha,\beta} L_A \right] + (A \to B) \tag{C.5}
\]
\[
[\hat{O}_{SDW,2k_F^o}^{\text{intra,even}}(x)]_z = -\frac{1}{\pi \alpha} \cos[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^o x] \sin[\sqrt{\pi}(\phi_\sigma^+ + \phi_\sigma^-)] \\
- \frac{1}{\pi \alpha} \cos[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^o x] \sin[\sqrt{\pi}(\phi_\sigma^+ - \phi_\sigma^-)] \tag{C.6}
\]
\[
[\hat{O}_{SDW,2k_F^o}^{\text{intra,even}}(x)]_y = q_1 \frac{1}{\pi \alpha} \cos[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\theta_\sigma^+ + \theta_\sigma^-)] \\
+ \frac{1}{\pi \alpha} \cos[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\theta_\sigma^+ - \theta_\sigma^-)] \tag{C.7}
\]
\[
[\hat{O}_{SDW,2k_F^o}^{\text{intra,even}}(x)]_x = \frac{1}{\pi \alpha} \cos[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\theta_\sigma^+ + \theta_\sigma^-)] \\
+ \frac{1}{\pi \alpha} \cos[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^o x] \cos[\sqrt{\pi}(\theta_\sigma^+ - \theta_\sigma^-)] \tag{C.8}
\]
Intraband SDW (odd combination), $2k_F^0$ wavevector

$$\hat{O}_{SDW,2k_F^0}^{\text{intra,odd}}(x) = [e^{i2k_F^0x}L^\dagger_{A\alpha}\left(\frac{\sigma}{2}\right)_{\alpha,\beta}R_A^\dagger + e^{-i2k_F^0x}R^\dagger_{A\alpha}\left(\frac{\sigma}{2}\right)_{\alpha,\beta}L_{A\beta}] - (A \rightarrow B) \quad (C.9)$$

$$[\hat{O}_{SDW,2k_F^0}^{\text{intra,odd}}(x)]_x = -\frac{1}{\pi}\cos[\sqrt{\pi}(\phi_\sigma^+ + \phi_\sigma^-) - 2k_F^0x] \sin[\sqrt{\pi}(\phi_\sigma^+ - \phi_\sigma^-)]$$

$$+ \frac{1}{\pi}\cos[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^0x] \sin[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-)] \quad (C.10)$$

$$[\hat{O}_{SDW,2k_F^0}^{\text{intra,odd}}(x)]_y = \frac{1}{\pi}\cos[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^0x] \cos[\sqrt{\pi}(\theta_\sigma^+ + \theta_\sigma^-)]$$

$$- \frac{1}{\pi}\cos[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^0x] \cos[\sqrt{\pi}(\theta_\sigma^+ - \theta_\sigma^-)] \quad (C.11)$$

$$[\hat{O}_{SDW,2k_F^0}^{\text{intra,odd}}(x)]_z = \frac{1}{\pi}\cos[\sqrt{\pi}(\phi_\rho^+ + \phi_\rho^-) - 2k_F^0x] \sin[\sqrt{\pi}(\theta_\sigma^+ + \theta_\sigma^-)]$$

$$- \frac{1}{\pi}\cos[\sqrt{\pi}(\phi_\rho^+ - \phi_\rho^-) - 2k_F^0x] \sin[\sqrt{\pi}(\theta_\sigma^+ - \theta_\sigma^-)] \quad (C.12)$$

C.3 Interband CDW

Interband CDW (even combination), $\frac{kU}{2}$ wavevector

$$\hat{O}_{CDW,kU}^{\text{inter,even}}(x) = [e^{i\frac{kU}{2}x}(R^\dagger_{A\alpha}R_{B\beta} + L^\dagger_{A\alpha}L_{B\beta}) + e^{-i\frac{kU}{2}x}(A \rightarrow B) \quad (C.13)$$

$$= -\frac{in_{RA}n_{RB}}{\pi}\sin[\sqrt{\pi}(\theta_\rho^- + \theta_\sigma^- - \phi_\rho^- - \phi_\sigma^-)] - \frac{kU}{2}x]$$

$$-\frac{in_{RA}n_{RB}}{\pi}\sin[\sqrt{\pi}(\theta_\rho^- - \theta_\sigma^- - \phi_\rho^- + \phi_\sigma^-) - \frac{kU}{2}x] + (R \rightarrow L) \quad (C.14)$$

Interband CDW (odd combination), $\frac{kU}{2}$ wavevector

$$\hat{O}_{CDW,kU}^{\text{inter,odd}}(x) = (e^{i\frac{kU}{2}x}(R^\dagger_{A\alpha}R_{B\beta} + L^\dagger_{A\alpha}L_{B\beta}) - e^{-i\frac{kU}{2}x}(A \rightarrow B) \quad (C.15)$$

$$= -\frac{n_{RA}n_{RB}}{\pi}\cos[\sqrt{\pi}(\theta_\rho^- + \theta_\sigma^- - \phi_\rho^- - \phi_\sigma^-) - \frac{kU}{2}x]$$

$$-\frac{n_{RA}n_{RB}}{\pi}\cos[\sqrt{\pi}(\theta_\rho^- - \theta_\sigma^- - \phi_\rho^- + \phi_\sigma^-) - \frac{kU}{2}x] + (R \rightarrow L) \quad (C.16)$$
Interband CDW (even combination), $\frac{k_F}{2} + 2k_F^0$ wavevector

$$\tilde{\chi}_{\text{inter, even}}^{\text{CDW,} \frac{k_F}{2} + 2k_F^0} (x) = e^{i(\frac{k_F}{2} + 2k_F^0)x} L_{As}^\dagger R_{Bs} + e^{-i(\frac{k_F}{2} + 2k_F^0)x} R_{Bs}^\dagger L_{As}$$ \hspace{1cm} (C.17)

$$= -\frac{i\hbar \Lambda \eta_{A}}{\pi \alpha} \sin[\sqrt{\pi}(\theta^\rho + \theta^\sigma + \phi^+_\rho + \phi^+_\sigma) - (\frac{k_F}{2} + 2k_F^0)x]$$

$$-\frac{i\hbar \Lambda \eta_{B}}{\pi \alpha} \sin[\sqrt{\pi}(\theta^\rho - \theta^\sigma + \phi^+_\rho - \phi^+_\sigma) - (\frac{k_F}{2} + 2k_F^0)x]$$ \hspace{1cm} (C.18)

Interband CDW (odd combination), $\frac{k_F}{2} + 2k_F^0$ wavevector

$$\tilde{\chi}_{\text{inter, odd}}^{\text{CDW,} \frac{k_F}{2} + 2k_F^0} (x) = e^{i(\frac{k_F}{2} + 2k_F^0)x} L_{As}^\dagger R_{Bs} - e^{-i(\frac{k_F}{2} + 2k_F^0)x} R_{Bs}^\dagger L_{As}$$ \hspace{1cm} (C.19)

$$= \frac{\eta_{A} \eta_{B}}{\pi \alpha} \cos[\sqrt{\pi}(\theta^\rho + \theta^\sigma + \phi^+_\rho + \phi^+_\sigma) - (\frac{k_F}{2} + 2k_F^0)x]$$

$$+\frac{\eta_{A} \eta_{B}}{\pi \alpha} \cos[\sqrt{\pi}(\theta^\rho - \theta^\sigma + \phi^+_\rho - \phi^+_\sigma) - (\frac{k_F}{2} + 2k_F^0)x]$$ \hspace{1cm} (C.20)

Interband CDW (even combination), $\frac{k_F}{2} - 2k_F^0$ wavevector

$$\tilde{\chi}_{\text{inter, even}}^{\text{CDW,} \frac{k_F}{2} - 2k_F^0} (x) = e^{i(\frac{k_F}{2} - 2k_F^0)x} R_{As}^\dagger L_{Bs} + e^{-i(\frac{k_F}{2} - 2k_F^0)x} L_{Bs}^\dagger R_{As}$$ \hspace{1cm} (C.21)

$$= -\frac{i\hbar \Lambda \eta_{A}}{\pi \alpha} \sin[\sqrt{\pi}(\theta^\rho + \theta^\sigma - \phi^+_\rho - \phi^+_\sigma) - (\frac{k_F}{2} - 2k_F^0)x]$$

$$-\frac{i\hbar \Lambda \eta_{B}}{\pi \alpha} \sin[\sqrt{\pi}(\theta^\rho - \theta^\sigma - \phi^+_\rho + \phi^+_\sigma) - (\frac{k_F}{2} - 2k_F^0)x]$$ \hspace{1cm} (C.22)

Interband CDW (odd combination), $\frac{k_F}{2} - 2k_F^0$ wavevector

$$\tilde{\chi}_{\text{inter, odd}}^{\text{CDW,} \frac{k_F}{2} - 2k_F^0} (x) = e^{i(\frac{k_F}{2} - 2k_F^0)x} R_{As}^\dagger L_{Bs} - e^{-i(\frac{k_F}{2} - 2k_F^0)x} L_{Bs}^\dagger R_{As}$$ \hspace{1cm} (C.23)

$$= \frac{\eta_{A} \eta_{B}}{\pi \alpha} \cos[\sqrt{\pi}(\theta^\rho + \theta^\sigma - \phi^+_\rho - \phi^+_\sigma) - (\frac{k_F}{2} - 2k_F^0)x]$$

$$+\frac{\eta_{A} \eta_{B}}{\pi \alpha} \cos[\sqrt{\pi}(\theta^\rho - \theta^\sigma - \phi^+_\rho + \phi^+_\sigma) - (\frac{k_F}{2} - 2k_F^0)x]$$ \hspace{1cm} (C.24)
C.4 Interband SDW

Interband SDW (even combination), $k_U/2$ wavevector

\[
\hat{O}_{\text{SDW}, \frac{k_U}{2}}(x) = e^{i\frac{k_U x}{2}}(R_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} R_{B\beta} + L_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} L_{B\beta})
\]

\[
+ e^{-i\frac{k_U x}{2}}(R_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} R_{B\beta} + L_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} L_{B\beta})
\]

\[
\hat{O}_{\text{SDW, even}, \frac{k_U}{2}}(x) = -\frac{i\eta_{RA}\eta_{RB}}{2\pi\alpha} \sin[\sqrt{\pi}(\theta_\rho + \theta_\sigma - \phi_\rho - \phi_\sigma) - \frac{k_U}{2} x] + (R \rightarrow L)
\]

\[
\hat{O}_{\text{SDW, odd}, \frac{k_U}{2}}(x) = -\frac{i\eta_{RA}\eta_{RB}}{2\pi\alpha} \sin[\sqrt{\pi}(\theta_\rho + \theta_\sigma - \phi_\rho - \phi_\sigma) - \frac{k_U}{2} x] + (R \rightarrow L)
\]

Interband SDW (odd combination), $k_U/2$ wavevector

\[
\hat{O}_{\text{SDW, odd}, \frac{k_U}{2}}(x) = e^{i\frac{k_U x}{2}}(R_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} R_{B\beta} + L_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} L_{B\beta})
\]

\[
- e^{-i\frac{k_U x}{2}}(R_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} R_{B\beta} + L_{A\alpha}^\dagger \left( \frac{\alpha}{2} \right)_{\alpha,\beta} L_{B\beta})
\]

\[
\hat{O}_{\text{SDW, odd}, \frac{k_U}{2}}(x) = \frac{\eta_{RA}\eta_{RB}}{2\pi\alpha} \cos[\sqrt{\pi}(\theta_\rho + \theta_\sigma - \phi_\rho - \phi_\sigma) - \frac{k_U}{2} x] + (R \rightarrow L)
\]

\[
\hat{O}_{\text{SDW, odd}, \frac{k_U}{2}}(x) = -\frac{\eta_{RA}\eta_{RB}}{2\pi\alpha} \cos[\sqrt{\pi}(\theta_\rho + \theta_\sigma - \phi_\rho - \phi_\sigma) - \frac{k_U}{2} x] + (R \rightarrow L)
\]

\[
\hat{O}_{\text{SDW, odd}, \frac{k_U}{2}}(x) = \frac{\eta_{RA}\eta_{RB}}{2\pi\alpha} \sin[\sqrt{\pi}(\theta_\rho + \theta_\sigma - \phi_\rho - \phi_\sigma) - \frac{k_U}{2} x] + (R \rightarrow L)
\]

\[
\hat{O}_{\text{SDW, odd}, \frac{k_U}{2}}(x) = \frac{\eta_{RA}\eta_{RB}}{2\pi\alpha} \sin[\sqrt{\pi}(\theta_\rho + \theta_\sigma - \phi_\rho - \phi_\sigma) - \frac{k_U}{2} x] + (R \rightarrow L)
\]
Interband SDW (even combination), $\frac{k_U}{2} + 2k_F^0$ wavevector

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) = e^{i(\frac{k_U}{2} + 2k_F^0)x} L_{\alpha \beta}^\dagger \left( \frac{\theta}{2} \right)_{\alpha \beta} R_{B \beta} + e^{-i(\frac{k_U}{2} + 2k_F^0)x} R_{B \alpha}^\dagger \left( \frac{\theta}{2} \right)_{\alpha \beta} L_{A \beta} \] (C.33)

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) \big|_z = -\frac{\eta_{LA1} \eta_{RB1}}{2\pi \alpha} \sin \left[ \sqrt{\pi} (\theta^- + \theta^+ + \phi_\rho^+ + \phi_\sigma^+) - \left( \frac{k_U}{2} + 2k_F^0 \right)x \right] \] (C.34)

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) \big|_y = -\frac{\eta_{LA1} \eta_{RB1}}{2\pi \alpha} \cos \left[ \sqrt{\pi} (\theta^- + \theta^+ + \phi_\rho^+ + \phi_\sigma^+) - \left( \frac{k_U}{2} + 2k_F^0 \right)x \right] \] (C.35)

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) \big|_x = -\frac{\eta_{LA1} \eta_{RB1}}{2\pi \alpha} \sin \left[ \sqrt{\pi} (\theta^- + \theta^+ + \phi_\rho^+ + \phi_\sigma^+) - \left( \frac{k_U}{2} + 2k_F^0 \right)x \right] \] (C.36)

Interband SDW (odd combination), $\frac{k_U}{2} + 2k_F^0$ wavevector

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) = e^{i(\frac{k_U}{2} + 2k_F^0)x} L_{\alpha \beta}^\dagger \left( \frac{\theta}{2} \right)_{\alpha \beta} R_{B \beta} - e^{-i(\frac{k_U}{2} + 2k_F^0)x} R_{B \alpha}^\dagger \left( \frac{\theta}{2} \right)_{\alpha \beta} L_{A \beta} \] (C.37)

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) \big|_z = \frac{\eta_{LA1} \eta_{RB1}}{2\pi \alpha} \cos \left[ \sqrt{\pi} (\theta^- + \theta^+ + \phi_\rho^+ + \phi_\sigma^+) - \left( \frac{k_U}{2} + 2k_F^0 \right)x \right] \] (C.38)

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) \big|_y = -\frac{\eta_{LA1} \eta_{RB1}}{2\pi \alpha} \sin \left[ \sqrt{\pi} (\theta^- + \theta^+ + \phi_\rho^+ + \phi_\sigma^+) - \left( \frac{k_U}{2} + 2k_F^0 \right)x \right] \] (C.39)

\[ \hat{O}_{SDW, \frac{k_U}{2} + 2k_F^0}(x) \big|_x = \frac{\eta_{LA1} \eta_{RB1}}{2\pi \alpha} \cos \left[ \sqrt{\pi} (\theta^- + \theta^+ + \phi_\rho^+ + \phi_\sigma^+) - \left( \frac{k_U}{2} + 2k_F^0 \right)x \right] \] (C.40)
Interband SDW (even combination), $\frac{k_U}{2} - 2k_F^o$ wavevector

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) = e^{i\frac{k_U}{2} - 2k_F^o} x R_A^\dagger \left( \frac{\pi}{2} \right)_{\alpha,\beta} L_B^\dagger \left( \frac{\pi}{2} \right)_{\alpha,\beta} R_A^\dagger$$  \hspace{1cm} (C.41)

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) \bigg|_z = \frac{-in_{R(\alpha)} - in_{L(\beta)}}{2\pi\alpha} \sin\sqrt{\pi}(\theta^+ - \theta^+ - \phi^+ + \phi^+ - \frac{(k_U}{2} - 2k_F^o) x]$$

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) \bigg|_y = \frac{-in_{R(\alpha)} + in_{L(\beta)}}{2\pi\alpha} \cos\sqrt{\pi}(\theta^+ - \theta^+ - \phi^+ + \phi^+ - \frac{(k_U}{2} - 2k_F^o) x]$$

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) \bigg|_x = \frac{-in_{R(\alpha)} - in_{L(\beta)}}{2\pi\alpha} \sin\sqrt{\pi}(\theta^+ - \theta^+ - \phi^+ + \phi^+ - \frac{(k_U}{2} - 2k_F^o) x]$$

Interband SDW (odd combination), $\frac{k_U}{2} - 2k_F^o$ wavevector

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) = e^{i\frac{k_U}{2} - 2k_F^o} x R_A^\dagger \left( \frac{\pi}{2} \right)_{\alpha,\beta} L_B^\dagger \left( \frac{\pi}{2} \right)_{\alpha,\beta} R_A^\dagger$$  \hspace{1cm} (C.45)

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) \bigg|_z = \frac{in_{R(\alpha)} + in_{L(\beta)}}{2\pi\alpha} \cos\sqrt{\pi}(\theta^+ - \theta^+ - \phi^+ + \phi^+ - \frac{(k_U}{2} - 2k_F^o) x]$$

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) \bigg|_y = \frac{-in_{R(\alpha)} + in_{L(\beta)}}{2\pi\alpha} \sin\sqrt{\pi}(\theta^+ - \theta^+ - \phi^+ + \phi^+ - \frac{(k_U}{2} - 2k_F^o) x]$$

$$\hat{O}_{SDW, \frac{k_U}{2} - 2k_F^o} (x) \bigg|_x = \frac{in_{R(\alpha)} - in_{L(\beta)}}{2\pi\alpha} \sin\sqrt{\pi}(\theta^+ - \theta^+ - \phi^+ + \phi^+ - \frac{(k_U}{2} - 2k_F^o) x]$$
C.5 Superconducting correlation functions

Intraband singlet

\[
\Delta^{\text{intra,singlet}}(x) = (L_{A_1} R_{A_1} - L_{A_1} R_{A_1}) e^{-i \frac{\eta x}{2}} + (A \rightarrow B) e^{i \frac{\eta x}{2}} \tag{C.49}
\]

\[
\Delta^{\text{intra,singlet}}_{\text{d}}(x) = -\frac{2}{\pi} e^{i \sqrt{\eta} \frac{x}{2}} \cos[\sqrt{\eta} \theta_\rho^- - \frac{\eta x}{2}] \cos[\sqrt{\eta} \phi_\sigma^+] \cos[\sqrt{\eta} \phi_\sigma^-] + \frac{\pi}{\pi} e^{i \sqrt{\eta} \frac{x}{2}} \sin[\sqrt{\eta} \theta_\rho^- - \frac{\eta x}{2}] \sin[\sqrt{\eta} \phi_\sigma^+] \sin[\sqrt{\eta} \phi_\sigma^-] \tag{C.50}
\]

\[
\Delta^{\text{intra,singlet}}_{\text{d}}(x) = (L_{A_1} R_{A_1} - L_{A_1} R_{A_1}) e^{-i \frac{\eta x}{2}} - (A \rightarrow B) e^{i \frac{\eta x}{2}} \tag{C.51}
\]

Intraband \( \eta \)-pairing operators at \( \frac{\eta}{2} \pm 2k^0_F \) wavevectors

\[
\Delta^{\text{intra,} \eta_{\frac{\eta}{2} - 2k^0_F}}(x) = R_{A_1} R_{A_1} e^{-i (\frac{\eta}{2} - 2k^0_F) x} \pm L_{B_1} L_{B_1} e^{i (\frac{\eta}{2} - 2k^0_F) x} \tag{C.53}
\]

\[
\Delta^{\text{intra,} \eta_{\frac{\eta}{2} - 2k^0_F}}(x) = -\frac{i}{\pi} e^{i \sqrt{\eta} (\theta_\rho^+ - \phi_\rho^-)} \left\{ \begin{array} {l}
\cos[\sqrt{\eta} (\theta_\rho^- + \phi_\rho^+) - (\frac{\eta}{2} - 2k^0_F) x] \\
\frac{\eta}{2} - 2k^0_F \end{array} \right\} \tag{C.54}
\]

\[
\Delta^{\text{intra,} \eta_{\frac{\eta}{2} + 2k^0_F}}(x) = L_{A_1} L_{A_1} e^{-i (\frac{\eta}{2} + 2k^0_F) x} \pm R_{B_1} R_{B_1} e^{i (\frac{\eta}{2} + 2k^0_F) x} \tag{C.55}
\]

\[
\Delta^{\text{intra,} \eta_{\frac{\eta}{2} + 2k^0_F}}(x) = \frac{i}{\pi} e^{i \sqrt{\eta} (\theta_\rho^+ + \phi_\rho^-)} \left\{ \begin{array} {l}
\cos[\sqrt{\eta} (\theta_\rho^- + \phi_\rho^+) - (\frac{\eta}{2} + 2k^0_F) x] \\
\frac{\eta}{2} + 2k^0_F \end{array} \right\} \tag{C.56}
\]

where the upper row refers to the even combination and the lower to the odd.

Intraband Triplet

\[
\Delta^{\text{intra,triplet}}(x) = (L_{A_1} R_{A_1} + L_{A_1} R_{A_1}) e^{-i \frac{\eta x}{2}} + (A \rightarrow B) e^{i \frac{\eta x}{2}} \tag{C.57}
\]
where the upper row refers to the even combination and the lower to the odd.

**Interband singlet at \( k = 0 \) wavevector**

\[
\Delta_{\text{inter,singlet}}(x) = (L_{A1} R_{A1} - L_{A1} R_{B1}) \pm (A \rightarrow B) \quad \text{(C.65)}
\]

\[
\Delta_{\text{inter,singlet}}(x) = \frac{\eta_{A1} \eta_{B1}}{2\pi \alpha} e^{i \sqrt{2\pi} (\theta_{\rho}^+ + \theta_{\sigma}^+ + \phi_{\sigma}^+ + \phi_{\rho}^+)} \pm \frac{\eta_{A1} \eta_{B1}}{2\pi \alpha} e^{i \sqrt{2\pi} (\theta_{\rho}^- - \theta_{\sigma}^- - \phi_{\sigma}^- - \phi_{\rho}^-)} + (A \rightarrow B) \quad \text{(C.66)}
\]

**Interband singlet at \( 2k_F^0 \) wavevector**

\[
\Delta_{\text{inter,singlet}}(x) = [R_{A1} R_{B1} - (\uparrow \rightarrow \downarrow)] e^{i 2k_F^0 x} \pm [L_{A1} L_{B1} - (\uparrow \rightarrow \downarrow)] e^{-i 2k_F^0 x} \quad \text{(C.67)}
\]

\[
\Delta_{\text{inter,singlet}}(x) = \left[ \frac{\eta_{A1} \eta_{B1}}{2\pi \alpha} e^{i \sqrt{2\pi} (\theta_{\rho}^+ + \theta_{\sigma}^+ - \phi_{\rho}^+ - \phi_{\sigma}^+)} e^{i 2k_F^0 x} - \frac{\eta_{A1} \eta_{B1}}{2\pi \alpha} e^{i \sqrt{2\pi} (\theta_{\rho}^- - \theta_{\sigma}^- + \phi_{\rho}^- + \phi_{\sigma}^-)} e^{i 2k_F^0 x} \right] \\
\pm \left[ \frac{\eta_{A1} \eta_{B1}}{2\pi \alpha} e^{i \sqrt{2\pi} (\theta_{\rho}^+ + \theta_{\sigma}^+ + \phi_{\rho}^+ + \phi_{\sigma}^+)} e^{-i 2k_F^0 x} - \frac{\eta_{A1} \eta_{B1}}{2\pi \alpha} e^{i \sqrt{2\pi} (\theta_{\rho}^- - \theta_{\sigma}^- + \phi_{\rho}^- - \phi_{\sigma}^-)} e^{-i 2k_F^0 x} \right] \quad \text{(C.68)}
\]
Interband triplet at $k = 0$ wavevector

\[
\Delta^{\text{inter,triplet}}(x) = (L_A R_{B_1} + L_{A_1} R_{B_1}) \pm (A \rightarrow B)
\]

\[
= \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x + \theta^+_y + \phi^+_x)} + \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x - \theta^+_y + \phi^+_x)} \pm (A \rightarrow B)
\]  

Inter-band triplet at $2k_F^0$ wavevector

\[
\Delta^{\text{inter,triplet}}(x) = [R_{A_1} R_{B_1} + (\uparrow \downarrow)] e^{2k_F^0 x} \pm [L_{A_1} L_{B_1} + (\uparrow \downarrow)] e^{-2k_F^0 x}
\]

\[
= \left[ \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x + \theta^+_y + \phi^+_x)} e^{2k_F^0 x} + \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x - \theta^+_y + \phi^+_x)} e^{2k_F^0 x} \right]
\]

\[
\pm \left[ \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x + \theta^+_y + \phi^+_x)} e^{-2k_F^0 x} + \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x - \theta^+_y + \phi^+_x)} e^{-2k_F^0 x} \right]
\]  

\[
\Delta^{\text{inter,triplet}}(x) = R_{A_1} R_{B_1} e^{2i k_F^0 x} \pm L_{A_1} L_{B_1} e^{-2i k_F^0 x}
\]

\[
= \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x + \theta^+_y + \phi^+_x)} e^{2i k_F^0 x} \pm \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x + \theta^+_y + \phi^+_x)} e^{-2i k_F^0 x}
\]  

\[
\Delta^{\text{inter,triplet}}(x) = R_{A_1} R_{B_1} e^{2i k_F^0 x} \pm L_{A_1} L_{B_1} e^{-2i k_F^0 x}
\]

\[
= \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x - \theta^+_y + \phi^+_x)} e^{2i k_F^0 x} \pm \frac{\eta_{RA} \eta_{RB}}{2\pi \alpha} e^{i\sqrt{2\pi} (\theta^+_x - \theta^+_y + \phi^+_x)} e^{-2i k_F^0 x}
\]  

\[
\Delta^{\text{inter,triplet}}(x) = R_{A_1} R_{B_1} e^{2i k_F^0 x} \pm L_{A_1} L_{B_1} e^{-2i k_F^0 x}
\]
Appendix D: Variation of Luttinger liquid kink with interaction strength

Figure D.1. Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.20$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2$, 0.3, and 0.4. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2$, 0.3, and 0.4. In all cases the spin velocity $v_\sigma = 0.7eV\cdot\AA$ and the temperature $k_BT = 14meV$. 
Figure D.2. Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_{\rho} = 0.25$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2$, 0.3, and 0.4. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2$, 0.3, and 0.4. In all cases the spin velocity $v_\sigma = 0.7eV$-Å and the temperature $k_B T = 14meV$. 
Figure D.3. Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.30$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2$, 0.3, and 0.4. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2$, 0.3, and 0.4. In all cases the spin velocity $v_\sigma = 0.7\text{eV}\cdot\angstrom$ and the temperature $k_B T = 14\text{meV}$. 
Figure D.4. Intensity of the spectral function $A^<(k, \omega)$ and effective dispersions at an interaction strength $\gamma_\rho = 0.35$. (a) The intensity of $A^<(k, \omega)$ is shown for three different ratios of the spin to charge velocity, $r = 0.2$, 0.3, and 0.4. The black lines are the effective electronic dispersions derived from MDC peaks, as described in the text. The dashed line in the first panel shows that the high energy part of the effective dispersion does not extrapolate back to the Fermi wavevector, $k_F$. (b) Comparison of the dispersions at different values of the velocity ratio, $r = 0.2$, 0.3, and 0.4. In all cases the spin velocity $v_\sigma = 0.7eV-\AA$ and the temperature $k_B T = 14meV$. 

(a) $A^<(k, \omega)$ at $\gamma_\rho = 0.35$

(b) Effective dispersion at $\gamma_\rho = 0.35$
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VITA

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