SYMMETRIES, INTERACTIONS AND PHASE TRANSITIONS ON GRAPHENE HONEYCOMB LATTICE

by

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Abstract

Graphene, a monolayer of graphite, opened a new frontier in physics with reduced dimensionality. Due to the Dirac nature of the quasi particles it exhibits interesting experimental phenomena. It is believed that electron-electron interactions also play important role in graphene. We derive here a generalized theory of short ranged interactions consistent with the various discrete symmetries present on the lattice. Restrictions on the theory imposed by the atomic limit are also discussed. Within the framework of this model we calculated the beta functions governing the renormalization flow of the couplings to sub-leading order in 1/N. Our calculations show that charge density wave and anti-ferromagnetic quantum critical points are in the Gross-Neveu universality class even beyond mean-field level. Thereafter we use the extended Hubbard model to extract the phase diagram. It shows that the semimetallic ground state is stabilized once we include corrections to sub-leading order in 1/N.

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Chapter 1

Introduction

Carbon is the prime material for life on the planet and the basis of the entire organic chemistry. Because of the flexibility in its bonding, carbon-based systems show a large variety of structures with versatile physical properties. Depending on the dimensionality of the system, physical properties of carbon-based materials vary widely. Among the systems with only carbon atoms, graphene is a two-dimensional (2D) allotrope of carbon. In graphene, carbon atoms are arranged on a honeycomb structure made out of hexagons. This structure is similar to benzene rings stripped of hydrogen atoms. Graphite, which became well known to mankind after the invention of lead pencil in 1564, is a 3D allotrope of carbon Fig. [1.1]. The usefulness of graphite as a writing instrument comes from the fact that graphite is made out of stacks of graphene layers, weakly coupled by van der Waals forces. Hence, one produces various layers of graphene on paper while writing on it. Although one produces multiple layers of graphene on paper while writing, it took 440 years to isolate a single layer. Graphene, a 2D layer of graphite was first fabricated successfully by Novoselov et al.[1]. The reason behind this delay is not a lack of experimental tools to produce an atomicly thick layer of graphene but rather the persistence to confirm success [2]. Thin graphite or Graphene was eventually spotted due to subtle optical effects that it produces on top of a SiO_2 substrate [1].

It was P.R. Wallace [3] who first studied the band structures of graphene and discovered the semi-metallic nature of this material. Further theoretical developments came up with the most interesting properties that its low energy excitations are massless, chiral, Dirac fermions. This prescription, valid only on energy scales much smaller than the band width,

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Figure 1.1: Graphene (top left) consists of hexagonal honeycomb lattice of carbon atoms. Top right one showing Graphite consists of graphene layers. In bottom it is carbon nanotube in the left and 3-D allotrope of carbon on a spherical surface in right [4].

mimics the physics of Quantum Electrodynamics(QED) of massless fermions. On the other hand Dirac fermions in graphene move with a Fermi velocity v_F , which is 300 times smaller than the velocity of light [5],[6],[7]. Hence many unusual properties of QED can show up in graphene but at much smaller velocities. It is the Dirac fermions that behave quite differently compared to normal electrons in the presence of a magnetic field [8], [9] that lead to the frontier of new physics of graphene, e.g. anomalous integer quantum Hall effect(IQHE) [10],[11], which is quite different than the IQHE observed on Si- heterostructures or in normal 2D electron gas [12]. In fact, the anomalous IQHE is the trademark of Dirac nature of the quasiparticles present in graphene.

Let us begin our discussion on graphene from its crystallographic structure. Graphene

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Figure 1.2: Figure shows the anomalous quantum hall plateaus for single layer graphene. Inset diagram is for bilayer graphene [10].

indeed is made out of carbon atoms arranged in hexagonal honeycomb lattice as shown in Fig.[1.4]. The Bravais lattice of this structure is the triangular lattice and the honeycomb lattice be described as two interlocked triangular sub-lattices labelled A and B depicted in Fig. [1.2]. The sub-lattice \vec{A} is generated by the linear combination of the basis vectors $\vec{a_1} = (\sqrt{3}, -1)a$, $\vec{a_1} = (0, 1)a$ whereas the sub-lattice \vec{B} is then at $\vec{B} = \vec{A} + \vec{b}$, with \vec{b} being $\vec{b_1} = (1/\sqrt{3}, 1)a/2$, $\vec{b_2} = (1/\sqrt{3}, -1)a/2$, or $\vec{b_3} = (-1/\sqrt{3}, 0)a$, where a is the lattice spacing = 2.5A. Therefore the reciprocal lattice in momentum space is described by the vectors $\vec{R_1} = \frac{4\pi}{\sqrt{3}a}(1,0)$ and $\vec{R_2} = \frac{4\pi}{\sqrt{3}a}(\frac{1}{2}, \frac{\sqrt{3}}{2})$ and hence the Brillouin zone is also a hexagon.

Let us now consider the electrons present on the honeycomb lattice and review their behavior on it. An excellent model to start with is the tight binding model which mimics almost all the relevant physics. In this model only the nearest-neighbor hopping is taken into account. On the other hand probability amplitude for next nearest neighbor hopping and further remote hopping decays exponentially and therefore can be neglected. We further consider this model for a general diatomic system with different energies of electrons localized



Figure 1.3: Lattice structure of graphene honeycomb lattice showing sublattices A(red) and B(blue) with different lattice vectors that generate two interlocked triangular sublattices.

on site A and B. Let t be the hopping parameter related to the probability amplitude for electron transfer among nearest-neighbor sites and β be the difference in energies of electrons localized on site A and B. An example of a layered diatomic material described by this lattice is boron nitride [13]. The electronic structure of Carbon is $1s^22s^22p^2$. Therefore it has 4 electrons in the outer shell. Out of these 3 electrons form bonds with nearest neighbor sites by sp^2 hybridization and the fourth electron in the p_z orbital can hop through the system. Due to strong overlap of the wave functions on nearest neighbor sites t is large for graphene ~ 2.5 eV. Therefore the Hamiltonian corresponding to the model reads

$$H_{t} = - t \sum_{\vec{A}, i, \sigma = \pm 1} [u_{\sigma}^{\dagger}(\vec{A})v_{\sigma}(\vec{A} + \vec{b_{i}}) + H.c.] + \beta \sum_{\vec{A}, \sigma = \pm 1} [u_{\sigma}^{\dagger}(\vec{A})u_{\sigma}(\vec{A}) - v_{\sigma}^{\dagger}(\vec{A} + \vec{b_{1}})v_{\sigma}(\vec{A} + \vec{b_{1}})]$$
(1.1)

where u^{\dagger} and u (v^{\dagger} and v) are the electron creation and annihilation operators on the sublattice A (B) of the honeycomb lattice. Ignoring the spin for the sake of simplicity, we can write down the Hamiltonian as

$$H_{t} = \int \frac{d^{2}k}{(2\pi)^{2}} (u^{\dagger}(\vec{k}), v^{\dagger}(\vec{k})) \\ \times \begin{pmatrix} \beta & -t(e^{i\vec{k}\cdot\vec{b_{1}}} + e^{i\vec{k}\cdot\vec{b_{2}}} + e^{i\vec{k}\cdot\vec{b_{3}}}) \\ -t(e^{i\vec{k}\cdot\vec{b_{1}}} + e^{i\vec{k}\cdot\vec{b_{2}}} + e^{i\vec{k}\cdot\vec{b_{3}}}) & -\beta \end{pmatrix} \\ \times \begin{pmatrix} u(\vec{k}) \\ v(\vec{k}) \end{pmatrix}$$
(1.2)



Figure 1.4: The Brillouin zone. The reciprocal-lattice vectors are $\vec{R_1} = (4\pi/\sqrt{3}a)(1,0)$, $\vec{R_2} = (4\pi/\sqrt{3}a)(1/2,\sqrt{3}/2)$. The degeneracy points occur at the corners *ijklmn*, of the Brillouin zone [14].

using the fourier transforms

$$u(\vec{A}) = \int \frac{d^2k}{(2\pi)^2} e^{i\vec{k}\cdot\vec{A}} u(\vec{k}), \quad v(\vec{B}) = \int \frac{d^2k}{(2\pi)^2} e^{i\vec{k}\cdot\vec{B}} v(\vec{k}).$$
(1.3)

Therefore within the framework of the tight binding model the energy spectrum $E(k) = \pm (\beta^2 + t^2|e^{i\vec{k}\cdot\vec{b_1}} + e^{i\vec{k}\cdot\vec{b_2}} + e^{i\vec{k}\cdot\vec{b_3}}|^2)^{1/2}$, is doubly degenerate. With one electron per site, the negative energy states constitute the filled valence band and positive energy states form the empty conduction band. The separation between these bands is minimal at the zeros of the function $f(k) = (e^{i\vec{k}\cdot\vec{b_1}} + e^{i\vec{k}\cdot\vec{b_2}} + e^{i\vec{k}\cdot\vec{b_3}})$, which happens to occur at the six corners of the Brillouin zone but out of those only two at $\vec{q_1} = (4\pi/\sqrt{3}a)(1/2, 1/2\sqrt{3})$ and $\vec{q_2} = -\vec{q_1}$ are non-equivalent. Hereafter we restrict our discussion to the monatomic system for which $\beta = 0$ i.e. electrons on different sub-lattices have equal energy. For such a system, e.g. graphene with carbon atoms sitting at every site, the valence and conduction bands touch each other at these points [14]. Therefore within the frame work of the tight binding model

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graphene exhibits a semi-metallic ground state and a large value of t gives the semi-metallic state extra protection against interactions. Hence only electrons near these two points take part in the dynamics at low energies. Considering the low energy limit expansion of f(k)about $\vec{q_1}$ gives

$$f(\vec{q_1} + \vec{k}) = -i\frac{t\sqrt{3}}{2}e^{-i\frac{2\pi}{3}}k_x + i\frac{t}{2}(e^{i\frac{2\pi}{3}} - 1)k_y.$$
(1.4)

A similar expansion of f(k) about $\vec{q_2} = -\vec{q_1}$ can be obtained by using the relation

$$f(\vec{q_2} + \vec{k}) = -f^*(\vec{q_1} + \vec{k}).$$
(1.5)

Hence the dispersion relation $\omega^2 = t^2 |f(k)|^2$ near these two point becomes

$$\omega^2 = \frac{3t^2}{4}(k_x^2 + k_y^2) + O(k^3). \tag{1.6}$$

Therefore the valence and the conduction bands look like linear isotopic cones near these two points in the low energy limit. Thus the Hamiltonian H_t in the low energy limit reduces to

$$H_{t} = -\frac{t\sqrt{3}}{2} \sum_{\sigma=\pm} \int_{\vec{q}_{1}+\vec{p}}^{\Lambda} \frac{d^{2}\vec{p}}{(2\pi)^{2}} (u_{\sigma}^{\dagger}(\vec{q}_{1}+\vec{p}), v_{\sigma}^{\dagger}(\vec{q}_{1}+\vec{p})) \mathcal{P}_{+} \begin{pmatrix} u_{\sigma}(\vec{q}_{1}+\vec{p}) \\ v_{\sigma}(\vec{q}_{1}+\vec{p}) \end{pmatrix}$$
$$- \frac{t\sqrt{3}}{2} \sum_{\sigma=\pm} \int_{\vec{q}+\vec{p}}^{\Lambda} \frac{d^{2}\vec{p}}{(2\pi)^{2}} (u_{\sigma}^{\dagger}(\vec{q}_{2}+\vec{p}), v_{\sigma}^{\dagger}(\vec{q}_{2}+\vec{p})) \mathcal{P}_{-} \begin{pmatrix} u_{\sigma}(\vec{q}_{2}+\vec{p}) \\ v_{\sigma}(\vec{q}_{2}+\vec{p}) \end{pmatrix}$$
(1.7)

where $\mathcal{P}_{\pm} = \pm p_x \sigma_x - p_y \sigma_y$, and σ_x , σ_y are Pauli matrices. Here the frame of reference is conveniently rotated to $p_x = \vec{p} \cdot \vec{q}/q$ and $p_y = (\vec{q} \times \vec{p}) \times \vec{q}/q^2$, where $\vec{q} = \vec{q_1}$ and $\vec{q_2}(= -\vec{q_1})$ are the momenta associated with the Dirac points. Therefore the Hamiltonian H_t in the low energy limit is a Dirac-like Hamiltonian near these two points. Thus we dub these two points Dirac points and electrons near the two Dirac points behaves like relativistic fermions. On the other hand, if we include further remote hopping that won't affect the Dirac behavior of the quasi-particles but the Dirac cone will be shifted towards higher energy.

1.1 Outline of the work

Therefore within the framework of the tight-binding model we recognize the Dirac nature of the pseudo-relativistic quasi particles. We hereafter exploit this feature to develop the interacting theory of electrons on the honeycomb lattice. We will construct the interacting theory on honeycomb lattice consistent with the discrete symmetries present on it.

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Figure 1.5: Energy dispersion relation is conical near Dirac point. The valence band(blue) and conduction band(red) touch each other at the Dirac point point.

Chapter 2

Symmetries and interactions in graphene honeycomb lattice

In the introductory discussion we have noticed some interesting characteristics of electrons on graphene's honeycomb lattice, especially in the low energy regime. In that regime, we find that electrons behave like Dirac fermions near two non-equivalent Dirac points located at the corners of the Brillouin zone of the honeycomb lattice. Thus the electrons near these two points have dynamical importance in the low energy sector. Therefore we construct the free electron theory in the continuum limit which also allows us to define the so called 'valley representation' of γ - matrices by considering the electrons only near these two points. Going beyond the free electron model we here develop the interacting theory of electrons on honeycomb lattice consistent with the various discrete symmetries present on it. Furthermore, we consider only the four-fermion interactions and spinless fermions. The restriction on the interactions due to the 'atomic limit' is also presented here. At last, we reintroduce the spin degrees of freedom to generalize our discussion.

2.1 Free Lagrangian

Before describing interactions on the honeycomb lattice it is useful to study the free electron theory to define the representation for both the Dirac spinor and the matrices. Here we construct the four component spinors as

$$\psi_{\sigma}(\vec{x}) = T \sum_{\omega_n} \int^{\Lambda} \frac{d^2 \vec{p}}{(2\pi)^2} e^{i\omega_n \tau + i\vec{p}\cdot\vec{x}} \begin{pmatrix} u_{\sigma}(\vec{q_1} + \vec{p}, \omega_n) \\ v_{\sigma}(\vec{q_1} + \vec{p}, \omega_n) \\ u_{\sigma}(\vec{q_2} + \vec{p}, \omega_n) \\ v_{\sigma}(\vec{q_2} + \vec{p}, \omega_n) \end{pmatrix},$$
(2.1)

after conveniently rotating the frame of reference to $p_x = \vec{p} \cdot \vec{q}/q$ and $p_y = (\vec{q} \times \vec{p}) \times \vec{q}/q^2$, where $\vec{q} = \vec{q_1}$ and $\vec{q_2}(= -\vec{q_1})$ are the momenta associated with the Dirac points, T is temperature, τ is the imaginary time and $\omega_n =$ are the fermionic Matsubara frequencies which form a continuum in the zero temperature limit. Hence we can write down the quantum mechanical action corresponding to H_t as

$$S = \sum_{\sigma} \int_{0}^{\beta} d\tau \int d^{2}\vec{x} \,\psi_{\sigma}^{\dagger}(\vec{x},\tau) (\partial_{\tau} + M_{x}\partial_{x} + M_{y}\partial_{y})\psi_{\sigma}(\vec{x},\tau), \qquad (2.2)$$

where

$$M_x = -i\left(\begin{array}{c|c} \sigma_x & 0\\ \hline 0 & -\sigma_x \end{array}\right), M_y = i\left(\begin{array}{c|c} \sigma_y & 0\\ \hline 0 & \sigma_y \end{array}\right).$$

Here we have taken the Fermi velocity $v_F = \frac{t\sqrt{3}}{2} = 1$ and $\hbar = k_B = 1$ for convenience. We can also write M_x, M_y in terms of other matrices as

$$M_x = i\gamma_0\gamma_1, M_y = i\gamma_0\gamma_2, \tag{2.3}$$

satisfying the following Clifford algebra

$$\{\gamma_{\mu}, \gamma_{\nu}\} = 2\delta_{\mu,\nu}, \quad for \quad \mu, \nu = 0, 1, 2,$$
 (2.4)

so that

$$\{M_x, M_y\} = 0. \tag{2.5}$$

Hence the quantum mechanical action at zero temperature can be written as

$$S = \int_0^\beta d\tau \int d^2 \vec{x} \sum_{\sigma=\pm 1} \overline{\psi}_\sigma(\vec{x},\tau) \gamma_\mu \partial_\mu \psi_\sigma(\vec{x},\tau).$$
(2.6)

where $\overline{\psi}_{\sigma}(\vec{x},\tau) = \psi^{\dagger}(\vec{x},\tau)\gamma_0$ and we define the γ matrices as

$$\gamma_{0} = \begin{pmatrix} \sigma_{z} & 0 \\ \hline 0 & \sigma_{z} \end{pmatrix} , \quad \gamma_{1} = \begin{pmatrix} \sigma_{y} & 0 \\ \hline 0 & -\sigma_{y} \end{pmatrix},$$
$$\gamma_{2} = \begin{pmatrix} \sigma_{x} & 0 \\ \hline 0 & \sigma_{x} \end{pmatrix}$$
(2.7)

so that they satisfy the anti-commutation relation (2.4). We further define

$$\gamma_3 = \begin{pmatrix} 0 & \sigma_y \\ \hline \sigma_y & 0 \end{pmatrix}, \quad \gamma_5 = -i \begin{pmatrix} 0 & \sigma_y \\ \hline -\sigma_y & 0 \end{pmatrix}, \quad (2.8)$$

which anticommute with all the other γ - matrices and also $\{\gamma_3, \gamma_5\} = 0$. Finally we construct

$$\gamma_{35} = i\gamma_3\gamma_5 = \left(\begin{array}{c|c} -I & 0\\ \hline 0 & I \end{array}\right),$$

which commutes with γ_{μ} , $\mu = 0, 1, 2$ but anti-commutes with γ_3 and γ_5 . Together these define the so called 'valley representation' of γ matrices. Therefore the quantum mechanical action, $S = \int_0^{1/T} d\tau d\vec{x} L_0$, defines the free Lagrangian as

$$L_0 = \sum_{\sigma=\pm 1} \overline{\psi}_{\sigma} \gamma_{\mu} \partial_{\mu} \psi_{\sigma}.$$
(2.9)

The free Lagrangian L_0 obviously respects relativistic invariance. Apart from that it also exhibits a global U(4) symmetry generated by $\{I_2, \vec{\sigma}\} \otimes \{I, \gamma_3, \gamma_5, \gamma_{35}\}$.

2.2 Interactions and symmetries

Let us now consider electron-electron interactions on graphene's honeycomb lattice. We will focus here only on four fermion interactions which in general are defined by the Hamiltonian

$$H_{int} = \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta \mid V \mid \gamma\delta \rangle r_{\alpha}^{\dagger} r_{\beta}^{\dagger} r_{\delta} r_{\gamma}, \qquad (2.10)$$

where r^{\dagger} and r are fermionic creation and annihilation operators, satisfying the relation $\{r_{\alpha}, r_{\beta}^{\dagger}\} = \delta_{\alpha\beta}$, and the matrix element corresponding to the interaction potential $V(\vec{k})$ is $\langle \alpha\beta | V | \gamma\delta \rangle$ is given by

$$\langle \alpha\beta \mid V \mid \gamma\delta \rangle = \int d\vec{x} d\vec{y} \varphi_{\alpha}^{*}(\vec{x}) \varphi_{\beta}^{*}(\vec{y}) V(\vec{x} - \vec{y}) \varphi_{\gamma}(\vec{x}) \varphi_{\delta}(\vec{y}).$$
(2.11)

Here we can take $\varphi(\vec{x})$ to be localized p-orbital wave-functions that belong to either A or B sublattice. In general, there is no restriction on the overlap of the wave-functions, and all the matrix elements $\langle \alpha\beta | V | \gamma\delta \rangle$ are finite. In the following we consider only short-ranged interactions, which are defined by the potential $V(\vec{x})$ with regular Fourier component $V(\vec{k})$ at $\vec{k} = 0$. We further restrict the interaction potential to be a contact potential, i.e.

 $V(\vec{x} - \vec{y}) = V(\vec{x})\delta(\vec{x} - \vec{y})$. Therefore at low energies we can write down the interacting Lagrangian for spinless fermions corresponding to H_{int} as

$$L_{int} = (\psi^{\dagger}(\vec{x},\tau)A\psi(\vec{x},\tau))(\psi^{\dagger}(\vec{x},\tau)B\psi(\vec{x},\tau)), \qquad (2.12)$$

where A and B are 4×4 Hermitian matrices. Therefore the interacting Lagrangian contains 16^2 parameters. However, the number of parameters in L_{int} is restricted by the symmetries present on the lattice. Two discrete symmetries present on the lattice are mirror symmetry and time reversal symmetry.

2.2.1 "Mirror" symmetry (S)

The labelling of the two sublattices is arbitrary, and therefore L_{int} should be invariant under the exchange of sublattice labeling $(A \leftrightarrow B)$ implying that L_{int} has to be invariant under the exchange of components $(u_i \leftrightarrow v_i)$, within the same valley. In the valley representation we recognize the mirror symmetry operator as

$$S = \gamma_2 = \left(\begin{array}{cc} \sigma_x & 0\\ 0 & \sigma_x \end{array}\right).$$

and therefore

$$S\begin{pmatrix}u_{\sigma}(\vec{q_{1}})\\v_{\sigma}(\vec{q_{1}})\\u_{\sigma}(\vec{q_{2}})\\v_{\sigma}(\vec{q_{2}})\end{pmatrix} = \begin{pmatrix}v_{\sigma}(\vec{q_{1}})\\u_{\sigma}(\vec{q_{1}})\\v_{\sigma}(\vec{q_{2}})\\u_{\sigma}(\vec{q_{2}})\end{pmatrix}.$$
(2.13)

Invariance of L_{int} under mirror symmetry requires both A and B to be either even, i.e.

$$SAS^{-1} = A$$
 and $SBS^{-1} = B$ (even)

or odd, i.e

$$SAS^{-1} = -A$$
 and $SBS^{-1} = -B$ (odd)

under S.

2.2.2 Time reversal symmetry (TRS)

Invariance of the Hamiltonian under TRS requires $I_t H I_t^{-1} = H$, where I_t is the TRS operator, defined as $I_t = TK$. Here T is the unitary operator and K is the complex conjugate operator. We here consider the Hamiltonian

$$H = i\gamma_0\gamma_i p_i + m_1\gamma_0, \tag{2.14}$$

where the mass m_1 arises due to the imbalance in chemical potential on two sub-lattices A and B [?]. The mass term m_1 give rise to charge density wave ordering on the lattice and thus m_1 is real. Therefore it is invariant under time reversal symmetry. On the other hand time reversal symmetry of the free Hamiltonian originates in the tight binding model from the fact that its elements are real. Recall that momentum changes sign under the transformation $I_t p_i I_t^{-1} = -p_i$. Therefore, invariance of H under TRS implies

$$\{T, i\gamma_0\gamma_1\} = [T, i\gamma_0\gamma_2] = [T, \gamma_0] = 0.$$
(2.15)

Hence $T \in \{i\gamma_1\gamma_3, i\gamma_1\gamma_5\}$. Therefore within the framework of the tight binding model with uniform hopping time reversal symmetry is not uniquely defined. Hence we need to consider a generalized tight binding model with anisotropic hopping defined as

$$H_{aniso} = -\sum_{\vec{r} \in A} \sum_{i=1}^{3} (t + \delta t_{\vec{r},i}) u_{\vec{r}}^{\dagger} v_{\vec{r}+\vec{b}_{i}} + H.c., \qquad (2.16)$$

where

$$\delta t_{\vec{r},i} = \frac{1}{3} \Delta(\vec{r}) e^{i\vec{K_{+}} \cdot \vec{b_{i}}} e^{i\vec{G} \cdot \vec{r}} + c.c. = \frac{2}{3} \Delta(\vec{r}) \cos(\vec{K} \cdot \vec{b_{i}} + \vec{G} \cdot \vec{r})$$
(2.17)

represents non-uniform hopping and 't' is the uniform one. Here, K_{\pm} are the momenta associated with the Dirac points K and K' respectively and $\vec{G} = \vec{K_{+}} - \vec{K_{-}}$. Therefore \vec{G} couples the two non-equivalent Dirac points at $\vec{K_{\pm}}$. Let us consider the affect of the non-uniform hopping on lattice. The non-uniform hopping can generates a so called Kekule texture on the lattice. We will discuss this issue latter in the context of parity symmetry. On a length scale much larger than the lattice spacing a, the Hamiltonian to the leading order in the gradient expansion, subject to a Kekule texture is given by

$$H_{aniso} = \int d^2 \vec{r} \Psi^{\dagger}(\vec{r}) \mathcal{K}_D \Psi(\vec{r}), \qquad (2.18)$$

with

$$\Psi^{\dagger}(\vec{r}) = (v^{\dagger}_{+}(\vec{r}), u^{\dagger}_{+}(\vec{r}), u^{\dagger}_{-}(\vec{r}), v^{\dagger}_{-}(\vec{r})), \qquad (2.19)$$

where \pm denotes the Dirac points at \vec{K}_{\pm} and u, v have their usual significance. Notice here that for convenience we have chosen a different definition of the spinor $\psi(\vec{r})$ from (2.1). The kernel in the Hamiltonian (2.18) is defined as

$$\mathcal{K}_D = \begin{pmatrix} 0 & -2i\partial_z & \Delta(\vec{r}) & 0\\ -2i\partial_{\overline{z}} & 0 & 0 & \Delta(\vec{r})\\ \overline{\Delta}(\vec{r}) & 0 & 0 & 2i\partial_z\\ 0 & \overline{\Delta}(\vec{r}) & 2i\partial_{\overline{z}} & 0 \end{pmatrix}, \qquad (2.20)$$

where z = x + iy and therefore $\partial_z = (\partial_x - i\partial_y)/2$, where overline denotes complex conjugation. With a Kekule structure $\Delta(\vec{r}) = \Delta_0$, the dispersion takes the simple form $\epsilon_{\pm}(\vec{p}) = \pm \sqrt{|\vec{p}|^2 + |\Delta_0|^2}$, i.e., a single particle mass gap $|\Delta_0|$ opens up. The Dirac kernel \mathcal{K}_D respects time reversal symmetry originating from the real elements in tight-binding model. Although the order parameter Δ_0 is relaxed to be complex its phase is redundant because the spectral mass gap is real. In fact it can be removed from the kernel (\mathcal{K}_D) with a chiral transformation that rotates the phases of \pm species by opposite angles. On the other hand this is not true any more if the phase in the order parameter $\Delta(\vec{r})$ varies in space, and in particular, if it contains vortices [15].

In the limit $\Delta_0 = 0$ the Hamiltonian H_{aniso} reduces to

$$H_0 = -i\partial_x \sigma_z \otimes \sigma_x - i\partial_y \sigma_z \otimes \sigma_y, \tag{2.21}$$

where H_0 is the free Hamiltonian. We can also write down the free Hamiltonian in terms of other matrices by defining

$$\gamma_0 \gamma_1 = -i\sigma_z \otimes \sigma_x, \gamma_0 \gamma_2 = -i\sigma_z \otimes \sigma_y, \tag{2.22}$$

so that these matrices also satisfy the anti-commuting algebra (2.4). Choosing $\gamma_0 = \sigma_z \otimes \sigma_z$, one finds $\gamma_1 = I_2 \otimes \sigma_y$ and $\gamma_2 = -I_2 \otimes \sigma_x$. We further chose $\gamma_3 = \sigma_x \otimes \sigma_z$ and $\gamma_5 = \sigma_y \otimes \sigma_z$. This representation of the γ - matrices is unitarily equivalent to the valley representation, where the transformation is generated by

$$U = i\sigma_x \oplus I_2. \tag{2.23}$$

In the continuum limit the Hamiltonian with anisotropic hopping reduces to

$$H_{aniso} = i\gamma_0\gamma_i p_i + m_2 i\gamma_0\gamma_3 + m_3 i\gamma_0\gamma_5, \qquad (2.24)$$

where $m_2 = Im(\Delta(\vec{r}))$ and $m_3 = Re(\Delta(\vec{r}))$. These two masses are generated from the Kekule pattern on the lattice and are therefore real. Hence the Hamiltonian is time reversal symmetric. Therefore in the valley representation the mass terms become

$$UH_m U^{-1} = im_2 \gamma_0 \gamma_5 + im_3 \gamma_0 \gamma_3, \tag{2.25}$$

where $H_m = m_2 i \gamma_0 \gamma_3 + m_3 i \gamma_0 \gamma_5$. Therefore time reversal symmetry of the Hamiltonian requires

$$[T, i\gamma_0\gamma_3] = \{T, i\gamma_0\gamma_5\} = 0.$$
(2.26)

Hence the unitary part of the time reversal symmetry operator is defined by

$$T=i\gamma_1\gamma_5=\left(egin{array}{cc} 0&I_2\ I_2&0\end{array}
ight),$$

in the valley representation.

Therefore, time reversal operator T exchanges the two non-equivalent Dirac points K and K' [4] and therefore invariance of H_{int} under TRS reflects that the labeling of the two Dirac points is arbitrary. In terms of field components

$$I_t r_1 I_t = r_2, I_t r_1^{\dagger} I_t = r_2^{\dagger}, \qquad (2.27)$$

and vice-versa, where $r_i = u_i$ or v_i . Therefore, for L_{int} to be invariant under TRS both A and B need to be either even i.e.,

$$TAT^{-1} = A$$
 and $TBT^{-1} = B$

or odd i.e.,

$$TAT^{-1} = -A$$
 and $TBT^{-1} = -B$

under TRS.

After defining these two discrete symmetries of the lattice we can group the interactions in four categories:

1. Even-even (Even under S and even under T): $\{I, \gamma_2, i\gamma_0\gamma_3, i\gamma_1\gamma_5\} \equiv \vec{A}$

- 2. Even-odd: $\{i\gamma_0\gamma_1, i\gamma_0\gamma_5, i\gamma_1\gamma_3, i\gamma_3\gamma_5\} \equiv \vec{B}$
- 3. Odd-even: $\{\gamma_0, \gamma_3, i\gamma_0\gamma_2, i\gamma_3\gamma_2\} \equiv \vec{C}$
- 4. Odd-odd: $\{\gamma_1, \gamma_5, i\gamma_1\gamma_2, i\gamma_5\gamma_2\} \equiv \vec{D}$

Hence the interacting Lagrangian which is symmetric under mirror symmetry (S) and TRS (I_t) is required to be of the following form

$$L_{int} = a_{1i}a_{2j}(\psi^{\dagger}A_{i}\psi)(\psi^{\dagger}A_{j}\psi) + b_{1i}b_{2j}(\psi^{\dagger}B_{i}\psi)(\psi^{\dagger}B_{j}\psi) + c_{1i}c_{2j}(\psi^{\dagger}C_{i}\psi)(\psi^{\dagger}C_{j}\psi) + d_{1i}d_{2j}(\psi^{\dagger}D_{i}\psi)(\psi^{\dagger}D_{j}\psi)$$

$$(2.28)$$

Where $\vec{a_i}, \vec{b_i}, \vec{c_i}, \vec{d_i}, i = 1, 2$ are the coupling constants. We further notice that all the interactions e.g. the first one, $a_{1i}a_{2j}(\psi^{\dagger}A_i\psi)(\psi^{\dagger}A_j\psi)$ are symmetric under the exchange of indices i, j. Therefore the number of interactions allowed by "Mirror" symmetry and TRS is 40.

2.3 Translational invariance

Apart from these two discrete lattice symmetries, the interactions conserve the momentum at two Dirac points. The couplings that are allowed by the momentum conservation or alternatively translational invariance have the form $\{r_{\pm}^{\dagger}r_{\pm}r_{\pm}^{\dagger}r_{\pm}, r_{\pm}^{\dagger}r_{+}r_{-}^{\dagger}r_{-}\}$, corresponding to block-diagonal matrices in the interacting Lagrangian, while $\{r_{\pm}^{\dagger}r_{\pm}r_{\pm}^{\dagger}r_{\pm}, r_{\pm}^{\dagger}r_{\pm}r_{\pm}r_{\pm}^{\dagger}r_{\pm}\}$, corresponds to block off diagonal matrices in the interacting Lagrangian (2.28). Here \pm labels the two Dirac points. The block off diagonal matrices from $\vec{A}, \vec{B}, \vec{C}, \vec{D}$ are

$$i\gamma_{1}\gamma_{5} = \begin{pmatrix} 0 & | I \\ -I & | 0 \end{pmatrix}, i\gamma_{0}\gamma_{3} = \begin{pmatrix} 0 & | \sigma_{x} \\ \sigma_{x} & | 0 \end{pmatrix} \in \vec{A}$$
$$i\gamma_{0}\gamma_{5} = \begin{pmatrix} 0 & | -i\sigma_{x} \\ i\sigma_{x} & | 0 \end{pmatrix}, i\gamma_{1}\gamma_{3} = i\begin{pmatrix} 0 & | I \\ -I & | 0 \end{pmatrix} \in \vec{B}$$
$$\gamma_{3} = \begin{pmatrix} 0 & | \sigma_{y} \\ \sigma_{y} & | 0 \end{pmatrix}, i\gamma_{2}\gamma_{3} = \begin{pmatrix} 0 & | \sigma_{z} \\ \sigma_{z} & | 0 \end{pmatrix} \in \vec{C}$$

$$\gamma_5 = \left(\begin{array}{c|c} 0 & -i\sigma_y \\ \hline i\sigma_y & 0 \end{array}\right), i\gamma_2\gamma_5 = \left(\begin{array}{c|c} 0 & i\sigma_z \\ \hline -i\sigma_z & 0 \end{array}\right) \in \vec{D}$$

Therefore two block-diagonal matrices from each group $\vec{A}, \vec{B}, \vec{C}, \vec{D}$ and the remaining eight block off-diagonal matrices altogether define the translationally invariant interacting Lagrangian as

$$L_{int} = \psi^{\dagger}(a_{1} + a_{2}\gamma_{2})\psi\psi^{\dagger}(a_{3} + a_{4}\gamma_{2})\psi$$

$$+ \psi^{\dagger}(b_{1}\gamma_{0} + b_{2}i\gamma_{0}\gamma_{2})\psi\psi^{\dagger}(b_{3}\gamma_{0} + b_{4}i\gamma_{0}\gamma_{2})\psi$$

$$+ \psi^{\dagger}(c_{1}i\gamma_{0}\gamma_{1} + c_{2}i\gamma_{3}\gamma_{5})\psi\psi^{\dagger}(c_{3}i\gamma_{0}\gamma_{1} + c_{4}i\gamma_{3}\gamma_{5})\psi$$

$$+ \psi^{\dagger}(d_{1}\gamma_{1} + d_{2}i\gamma_{1}\gamma_{2})\psi\psi^{\dagger}(d_{3}\gamma_{1} + b_{4}i\gamma_{1}\gamma_{2})\psi$$

$$+ g_{A}\psi^{\dagger}(i\gamma_{1}\gamma_{3} + \gamma_{1}\gamma_{5})\psi\psi^{\dagger}(i\gamma_{1}\gamma_{3} - \gamma_{1}\gamma_{5})\psi$$

$$+ g_{B}\psi^{\dagger}(i\gamma_{0}\gamma_{3} + \gamma_{0}\gamma_{5})\psi\psi^{\dagger}(i\gamma_{0}\gamma_{3} - \gamma_{0}\gamma_{5})\psi$$

$$+ g_{D}\psi^{\dagger}(i\gamma_{2}\gamma_{3} + \gamma_{2}\gamma_{5})\psi\psi^{\dagger}(i\gamma_{2}\gamma_{3} - \gamma_{2}\gamma_{5})\psi$$

$$(2.29)$$

Hence all the symmetries present on the lattice restricts the number of allowed interactions to 16 and this is the most general interaction allowed by symmetry. Note that L_{int} is invariant under the U(1) symmetry generated by $i\gamma_3\gamma_5 = \sigma_z \otimes I_2$. This is same as imposing translational invariance and can be used as an alternative way to generate(2.29) from (2.28).

2.4 Parity symmetry

For the sake of completeness we here also examine how the interactions transform under the parity (P). Once again let us begin with the free Hamiltonian

$$H_t = i\gamma_0\gamma_i p_i. \tag{2.30}$$

This Hamiltonian is invariant under the parity transformation since honeycomb lattice with uniform hopping is invariant under space inversion. Recall that the momentum changes sign under the parity transformation, i.e.,

$$Pp_i P^{-1} = -p_i. (2.31)$$

Thus the invariance of the free Hamiltonian under parity implies

$$\{P, i\gamma_0\gamma_1\} = \{P, i\gamma_0\gamma_2\} = 0.$$
(2.32)

There are four matrices that anti-commute with both $i\gamma_0\gamma_1$ and $i\gamma_0\gamma_2$, thus

$$P \in \{\gamma_0, i\gamma_0\gamma_3, i\gamma_1\gamma_2, i\gamma_0\gamma_5\}.$$

Let us now incorporate a mass term generating from the charge density wave ordering on lattice. We have already found that this mass in continuum limit reads as $m\gamma_0$. This mass is invariant under parity also since it is real on lattice. On the other hand the charge density wave ordering generates from the imbalance in chemical potential on the two sub-lattices, therefore $m \rightarrow -m$ under the parity. This imposes further restriction $\{P, \gamma_0\} = 0$, for the Hamiltonian to be invariant under parity (P) and thus $P \in \{i\gamma_0\gamma_3, i\gamma_0\gamma_5\}$. Therefore, one can define the parity operator as

$$P = i\gamma_0(\gamma_3\cos\theta + \gamma_5\sin\theta), \qquad (2.33)$$

where the parameter $\theta(0 \le \theta \le 2\pi)$ is to be determined to define P uniquely. Note that this definition of parity operator (P) in (2.33) is independent of representation of γ - matrices. On the other hand θ depends on the representation. However, tight binding model with uniform hopping restricts the scope to determine θ uniquely. Therefore to determine θ and uniquely define the parity operator we impose anisotropy in the hopping amplitude [15]. Kekule pattern generating from anisotropic hopping and its transformation under space inversion is depicted in Fig.[2.1] and Fig.[2.2]. The Hamiltonian with anisotropic hopping is already defined in (2.16). Here without any loss of generality we here choose $\Delta(\vec{r}) = \Delta_0$, where Δ_0 is real. Therefore in continuum limit the Hamiltonian reads as

$$H = i\gamma_0\gamma_i p_i + \Delta_0 i\gamma_0\gamma_5. \tag{2.34}$$

The pattern (c) in Fig. [2.2] corresponds to the mass $\Delta_0 i \gamma_0 \gamma_3$ and this is invariant under the space inversion with the inversion center located at the center of a hexagon. On the other hand masses corresponding to (a) and (b) transforms into each other under space inversion or parity. Therefore $P\Delta_0 P^{-1} = \Delta_0$ and invariance of H under the parity transformation requires

$$\theta = \frac{\pi}{2}, \frac{3\pi}{2}.\tag{2.35}$$



Figure 2.1: Kekule pattern arising on lattice due to anisotropic hopping. The electronic hopping amplitude is enhanced on thick red bonds while it is reduced on the blue bonds relative to the uniform hopping amplitude t [15].

Therefore the parity operator in this representation is defined as,

$$P_C = \pm i\gamma_0\gamma_5 = \sigma_x \otimes I_2. \tag{2.36}$$

On the other hand it is already noticed that this representation is unitary equivalent to the valley representation, where

$$U = i\sigma_x \oplus I_2. \tag{2.37}$$

Hence the parity operator in the valley representation is defined by

$$P = U^{\dagger} P_C U = \sigma_x \otimes \sigma_x = \pm i \gamma_0 \gamma_3. \tag{2.38}$$

It turns out that the interacting Lagrangian (2.29) invariant under parity transformation, i.e., $PL_{int}P^{-1} = L_{int}$. Comparing S with Charge conjugation symmetry (C), it turns out that L_{int} is CPT invariant, as it should be.

2.5 Atomic limit and interactions

We now impose the 'atomic limit' on the interacting theory. In this approximation all the matrix elements with $\alpha \neq \gamma$ and $\beta \neq \delta$ in (2.11) can be neglected since the overlap will be



Figure 2.2: Kekule pattern in fig. [2.2] can be considered as a superposition (a) and (b). Kekule pattern can be generated by repeating (a). Here'C' is the space inversion center. Under the space inversion (a) and (b) transforms into each other while (c) is invariant under it.

small. Therefore in this approximation

$$\langle \alpha\beta \mid V \mid \gamma\delta \rangle = \delta_{\alpha\gamma}\delta_{\beta\delta} \int d\vec{x}d\vec{y} |\varphi_{\alpha}(\vec{x})|^{2}V(\vec{x}-\vec{y})||\varphi_{\beta}(\vec{y})|^{2}$$

= $\delta_{\alpha\gamma}\delta_{\beta\delta}V_{\alpha\beta},$ (2.39)

and thus the lattice Hamiltonian for interactions reads

$$H_{int} = \sum_{\alpha\beta} V_{\alpha\beta} n_{\alpha} n_{\beta}.$$
(2.40)

In the continuum model therefore all the quartic interactions are required to have equal numbers of u, u^{\dagger} and v, v^{\dagger} . Therefore interactions containing unequal numbers of u and u^{\dagger} and v and v^{\dagger} will drop out e.g.

$$(\psi^{\dagger}\psi)(\psi^{\dagger}\gamma_{2}\psi) = (u_{1}^{\dagger}u_{1} + v_{1}^{\dagger}v_{1} + u_{2}^{\dagger}u_{2} + v_{2}^{\dagger}v_{2})(u_{1}^{\dagger}v_{1} + v_{1}^{\dagger}u_{1} + u_{2}^{\dagger}v_{2} + v_{2}^{\dagger}u_{2})$$
(2.41)

$$(\psi^{\dagger}\gamma_{0}\psi)(\psi^{\dagger}\gamma_{0}\gamma_{3}\psi) = (u_{1}^{\dagger}u_{1} - v_{1}^{\dagger}v_{1} + u_{2}^{\dagger}u_{2} - v_{2}^{\dagger}v_{2})(-u_{1}^{\dagger}v_{1} + v_{1}^{\dagger}u_{1} - u_{2}^{\dagger}v_{2} + v_{2}^{\dagger}u_{2})$$
(2.42)

$$(\psi^{\dagger}\gamma_{0}\gamma_{1}\psi)(\psi^{\dagger}\gamma_{3}\gamma_{5}\psi) = -(u_{1}^{\dagger}v_{1} + v_{1}^{\dagger}u_{1} - u_{2}^{\dagger}v_{2} - v_{2}^{\dagger}u_{2})(u_{1}^{\dagger}u_{1} + v_{1}^{\dagger}v_{1} + u_{2}^{\dagger}u_{2} + v_{2}^{\dagger}v_{2}) \quad (2.43)$$

$$(\psi^{\dagger}\gamma_{1}\psi)(\psi^{\dagger}\gamma_{1}\gamma_{2}\psi) = (u_{1}^{\dagger}v_{1} - v_{1}^{\dagger}u_{1} - u_{2}^{\dagger}v_{2} + v_{2}^{\dagger}u_{2})(u_{1}^{\dagger}u_{1} - v_{1}^{\dagger}v_{1} + u_{2}^{\dagger}u_{2} - v_{2}^{\dagger}v_{2})$$
(2.44)

and equivalently for the interactions corresponding to g_B and g_C . Therefore under this restriction the allowed quartic interactions define the interacting Lagrangian as

$$L_{int} = g_1(\overline{\psi}i\gamma_1\psi)^2 + g_2(\overline{\psi}i\gamma_2\psi)^2 + g_3(\overline{\psi}\gamma_0\psi)^2 + g_4(\overline{\psi}\psi)^2 + g_5(\overline{\psi}\gamma_0\gamma_1\psi)^2 + g_6(\overline{\psi}\gamma_0\gamma_2\psi)^2 + g_7(\overline{\psi}i\gamma_3\gamma_5\psi)^2 + g_8(\overline{\psi}i\gamma_0\gamma_3\gamma_5\psi)^2 + g_9((\overline{\psi}i\gamma_0\gamma_1\gamma_3\psi)^2 + (\overline{\psi}i\gamma_0\gamma_1\gamma_5\psi)^2) + g_{10}((\overline{\psi}i\gamma_0\gamma_2\gamma_3\psi)^2 + (\overline{\psi}i\gamma_0\gamma_2\gamma_5\psi)^2).$$
(2.45)

Therefore, the atomic limit restricts the number of allowed couplings to 10. Out of these 10 interactions the first 8 correspond to intra-valley scattering, whereas the rest correspond to inter-valley scattering. The strength of these coupling are completely determined by the microscopic lattice model.

Here we recognize $(\overline{\psi}\gamma_0\psi,\overline{\psi}\gamma_1\psi,\overline{\psi}\gamma_2\psi)$ as scalar under chiral SU(2) and $\overline{\psi}\gamma_3\gamma_5\psi$ as another scalar under SU(2) generated by $\{\gamma_3,\gamma_5,\gamma_{35}\}$, where $\gamma_{35} = i\gamma_3\gamma_5$. Whereas, $(\psi^{\dagger}\gamma_1\psi,\psi^{\dagger}\gamma_1\gamma_3\psi,\psi^{\dagger}\gamma_1\gamma_5\psi) = \vec{B_1}$ and $(\psi^{\dagger}\gamma_2\psi,\psi^{\dagger}\gamma_2\gamma_3\psi,\psi^{\dagger}\gamma_2\gamma_5\psi) = \vec{B_2}$ transform as vectors under chiral SU(2). On the other hand $(\overline{\psi}\gamma_0\gamma_3\gamma_5\psi)$ and $(\overline{\psi}\psi)$ are the components of $\vec{B_0}$ and \vec{A} respectively, which transform as vectors under chiral SU(2). The rest of the components from $\vec{B_0}$ and \vec{A} are present in L_{int} before we impose the 'atomic limit' on it [16].

We can carry on the same symmetry arguments as we did for the spinless electrons, including its spin degrees of freedom. It turns out that once we consider the spin of the electrons the number of interactions is doubled due to the extra two degrees of freedom. Therefore incorporating the spin degrees of freedom in our theory we get the interacting Lagrangian as

$$\begin{split} L_{int} &= g_1 \left(\sum_{\sigma} \overline{\psi}_{\sigma} i \gamma_1 \psi_{\sigma} \right)^2 + g_1' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_1 \psi_{\sigma} \right)^2 + g_2 \left(\sum_{\sigma} \overline{\psi}_{\sigma} i \gamma_2 \psi_{\sigma} \right)^2 \right) \\ &+ g_2' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_2 \psi_{\sigma} \right)^2 + g_3 \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_0 \psi_{\sigma} \right)^2 + g_3' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_0 \psi_{\sigma} \right)^2 \right) \\ &+ g_4 \left(\sum_{\sigma} \overline{\psi}_{\sigma} \psi_{\sigma} \right)^2 + g_4' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \psi_{\sigma} \right)^2 + g_5 \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_0 \gamma_1 \psi_{\sigma} \right)^2 \\ &+ g_5' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_0 \gamma_1 \psi_{\sigma} \right)^2 + g_6 \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_0 \gamma_2 \psi_{\sigma} \right)^2 + g_8' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_0 \gamma_3 \gamma_5 \psi_{\sigma} \right)^2 + g_7 \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_0 \gamma_3 \gamma_5 \psi_{\sigma} \right)^2 + g_9 \left\{ \left(\sum_{\sigma} \overline{\psi}_{\sigma} i \gamma_0 \gamma_1 \gamma_3 \psi_{\sigma} \right)^2 \right)^2 \\ &+ g_8' \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_0 \gamma_1 \gamma_5 \psi_{\sigma} \right)^2 \right\} + g_9' \left\{ \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_0 \gamma_2 \gamma_3 \psi_{\sigma} \right)^2 \right)^2 \\ &+ \left(\sum_{\sigma} \overline{\psi}_{\sigma} i \gamma_0 \gamma_2 \gamma_5 \psi_{\sigma} \right)^2 \right\} + g_{10}' \left\{ \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_0 \gamma_2 \gamma_3 \psi_{\sigma} \right)^2 \\ &+ \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} i \gamma_0 \gamma_2 \gamma_5 \psi_{\sigma} \right)^2 \right\},$$
 (2.46)

in the atomic limit. Although the couplings of the following form

$$(\sum_{\sigma} \overline{\psi}_{\sigma} M \psi_{\sigma})^2, \quad (\sum_{\sigma} \sigma \overline{\psi}_{\sigma} M \psi_{\sigma})^2,$$

where M is any matrix specifying the interaction, are symmetric their strength may be different depending on the individual lattice model. This issue will be discussed in detail in the context of Hubbard model latter.

2.6 Outline of the work

In this chapter we have discussed the symmetries present on the graphene honeycomb lattice. We have also derived the complete structure of the interactions allowed by those those symmetries. Restrictions on the interactions due to the atomic limit are also discussed. Within the frame work of this model we will study the possible phase transitions by using a renormalization group analysis in the next chapter.

Chapter 3

Renormalization and phase transition

In our earlier discussions we developed the interacting theory of electrons on graphene's honeycomb lattice that is consistent with discrete lattice symmetries. There we considered only short ranged four-fermion interactions. From that calculation it was determined that the theory contains 16 interactions for spinless electrons and this number gets double when we incorporate the spin of the electrons into the theory. The number of allowed interactions reduces to 10 once we impose the atomic limit on the spinless interactions. Constructing the interacting theory of electrons on the honeycomb lattice it is necessary to study the phase transitions to gapped insulating states within this model. This issue will be examined in the following discussion. Therefore we calculate the renormalization group (RG) flows of various couplings and present a detailed analysis on the various phase transitions from the semimetallic ground state. Our calculations show that there exist continuous phase transitions to charge-density-wave and anti-ferromagnetic gapped insulating ground states with a staggered pattern in either charge or spin respectively for large enough couplings. The transitions into these gapped insulating states generate a mass in the spectrum of the electrons. This mechanism of generating mass through dynamical symmetry breaking is similar to the Higg's mechanism in particle physics. Moreover we study the universality class of those continuous quantum phase transitions and found them to be in the Gross-Neveu universality class within and also beyond the mean-field approximation. Finally, for the Hubbard model it is shown that these two quantum critical phase transitions can be

achieved by tuning repulsive Hubbard onsite interactions and nearest neighbor Coulomb interactions to sufficiently large values. Considering the RG flows beyond the mean-field approximation it is found that corrections to the sub-leading order in 1/N provide the semimetal state an additional protection against interactions.

3.1 Wilson's one loop renormalization

Let us now compute the flow of the couplings applying Wilson's renormalization procedure. The usual power counting arguments imply that all short-ranged interactions are irrelevant at the Gaussian fixed point. To gain some control over the RG flow we first deform the Lagrangian by including N flavors of Dirac field. Therefore,

$$\overline{\Psi}\Psi \to \sum_{j=i}^{N} \overline{\Psi}_{j} \Psi_{j}.$$
(3.1)

and the couplings are redefined as $g_i \rightarrow 2g_i/N$ [17].

In the Wilsonian renormalization procedure, the fast modes are confined within the momentum shell $\Lambda < k < \Lambda/b$, where $b(\gg 1)$ is the renormalization parameter, whereas the slow modes correspond to momenta $k < \Lambda/b$. Thereafter integrating out the fast modes $\Lambda < k < \Lambda/b$ and over the Matsubara frequencies $-\infty < \omega_n < \infty$ [18], we get the flow of the different couplings at zero temperature to the sub-leading order in 1/N expansion as

$$\beta_{g_1} = -g_1 - (2 - \frac{1}{N})g_1^2 - \frac{2}{N}(g_7g_2 - g_5g_4) + \frac{1}{N}(-g_2 - g_3 + g_4 + g_5 - g_6) - g_8 + g_7)g_1 + \frac{1}{N}(g_3g_7 - g_4g_8),$$
(3.2)

$$\beta_{g_2} = -g_2 - (2 - \frac{1}{N})g_2^2 - \frac{2}{N}(g_7g_1 - g_6g_4) + \frac{1}{N}(-g_1 - g_3 + g_4 - g_5 + g_6) - g_8 + g_7)g_2 + \frac{1}{N}(g_3g_7 - g_4g_8),$$
(3.3)

$$\beta_{g_3} = -g_3 - \frac{1}{N} \left(g_4 g_5 + g_4 g_6 + g_7 g_1 + g_7 g_2 \right), \qquad (3.4)$$

$$\beta_{g_4} = -g_4 - (4 - \frac{2}{N})g_4^2 - \frac{2}{N}(g_3 - g_1 - g_2 - g_5 - g_6 + g_7 + g_8)g_4$$

$$- \frac{1}{N}(-2g_5g_1 - 2g_6g_2 + g_3g_5 + g_3g_6 + g_1g_3 + g_2g_3 + g_8g_1 + g_8g_2)$$

$$- \frac{4}{N}(g_9g_{10} - g_4g_9 - g_4g_{10}), \qquad (3.5)$$

$$\beta_{g_5} = -g_5 - (2 - \frac{1}{N})g_5^2 + \frac{2}{N}(g_7g_6 - g_1g_4) + \frac{1}{N}(-g_6 - g_7 - g_1 + g_2 + g_3)$$

$$- g_4 + g_8)g_5 - \frac{1}{N}(g_8g_7 + g_4g_3) - \frac{1}{N}(g_9^2 + g_{10}^2) - \frac{2}{N}(g_9g_{10} + g_5g_9 + g_5g_{10}),$$
(3.6)

$$\beta_{g_6} = -g_6 - (2 - \frac{1}{N})g_6^2 + \frac{2}{N}(g_7g_5 - g_2g_4) + \frac{1}{N}(-g_5 - g_7 + g_1 - g_2 + g_3) - g_4 + g_8)g_6 - \frac{1}{N}(g_8g_7 + g_4g_3) - \frac{1}{N}(g_9^2 + g_{10}^2) - \frac{2}{N}(g_9g_{10} + g_6g_9 + g_6g_{10}),$$
(3.7)

$$\beta_{g_7} = -g_7 - (4 - \frac{2}{N})g_7^2 + \frac{2}{N}(g_3 - g_1 - g_2 - g_5 - g_6 + g_4 + g_8)g_7 - \frac{1}{N}(-2g_5g_6 + g_8g_5 + g_8g_6) + \frac{2}{N}(g_9g_{10} - 2g_7g_9 - g_7g_{10}),$$
(3.8)

$$\beta_{g_8} = -g_8 - \frac{1}{N}(g_7g_5 + g_7g_6 - g_4g_1 - g_4g_2) + \frac{2}{N}(g_9^2 + g_{10}^2), \qquad (3.9)$$

$$\beta_{g_9} = -g_9 - 2g_9^2 - \frac{1}{N}g_9^2 - \frac{g_9}{N}(g_3 + g_4 - g_5 - g_6 - g_7 - g_8 + g_{10}) + \frac{1}{N}(g_1g_{10} + g_9g_5 + g_9g_6 - g_7g_{10} + g_5g_{10} + g_6g_{10}), \qquad (3.10)$$

$$\beta_{g_{10}} = -g_{10} - 2g_{10}^2 - \frac{1}{N}g_{10}^2 - \frac{g_{10}}{N}(g_3 + g_4 - g_5 - g_6 - g_7 - g_8 + g_9) + \frac{1}{N}(g_2g_9 + g_9g_5 + g_9g_6 - g_7g_9 + g_5g_9 + g_6g_9),$$
(3.11)

where $\beta_{g_i} = \frac{dg_i}{d \ln b}$ and the couplings are rescaled as $g_i \Lambda / \pi \rightarrow g_i$. Since the model with $N = \infty$ is exactly solvable by saddle-point methods, the leading order β - functions may also be understood as guaranteeing that the solution is cut-off independent. It is also noticed that the renormalization with couplings g_i , $i = 1, \ldots, 8$ does not generate any new couplings in a one loop calculation. It is also noticed that the interacting Lagrangian L_{int} described by these 8 couplings is closed under renormalization in any order in a perturbative expansion. On the other hand, once we incorporate g_9 and g_{10} , which correspond to inter-valley scattering L_{int} in the 'atomic limit' is no longer closed under renormalization. In fact the one loop renormalization generates new terms like $(\overline{\psi}i\gamma_3\psi)^2$, $(\overline{\psi}i\gamma_5\psi)^2$, $(\overline{\psi}\gamma_0\gamma_3\psi)^2$, $(\overline{\psi}\gamma_0\gamma_3\psi)^2$. In the large N approximation β -functions for different couplings do not mix as expected at the mean-field level, but the mixing occurs when corrections of the order 1/N are included. Notice also that g_i^2 term is absent in the β -function for the coupling g_j , where $i \neq j$ [16] and the coefficient of g_i^2 in the β -function for g_i vanishes for N = 1/2 [19], [20] for $i, j = 1, \ldots, 8$. Moreover, the leading order contribution for g_4 and g_7 is maximal. A detailed discussion on this issue is presented in Appendix C.

3.2 Phase transitions

Different phase transitions and also the order of that transition on the honeycomb lattice can be determined by studying the stability of the fixed points exhibited by the flow equations. Let us consider the mean field flow equations first. This will provide both motivation and a guide to study the flow equations beyond the mean-field approximation. The mean-field flow equation is obtained by setting $N = \infty$ in the above flow equations. Therefore the mean-field flow equations are

$$\beta_{g_i} = -g_i - 2g_i^2, \tag{3.12}$$

for i = 1, 2, 5, 6, 9, 10,

$$\beta_{g_i} = -g_i - 4g_i^2, \tag{3.13}$$

for i = 4, 7 and

$$\beta_{g_i} = -g_i \tag{3.14}$$

for i = 3, 8. Therefore from the mean-field analysis it is found that the fixed point at $g_4 = -1/4$; $g_1 = g_2 = g_3 = g_5 = g_6 = g_7 = g_8 = 0$ is indeed a critical point, i.e. the stability matrix M defined as $M_{ij} = \frac{d\beta_{g_i}}{dg_j}$, has only one unstable direction around this point. This critical point corresponds to a continuous quantum phase transition to the charge density wave phase from the semimetal ground state. This critical point is found to be in the Gross-Neveu universality class [21]. Besides the charge-density-wave quantum critical point there is another critical point at $g_7 = -1/4$; $g_1 = g_2 = g_3 = g_4 = g_5 = g_6 = g_8 = 0$ that also corresponds to a continuous phase transition. The order parameter in this insulating phase, $\langle \bar{\psi}i\gamma_3\gamma_5\psi \rangle$, spontaneously breaks the time reversal symmetry [22]. Recently, the existence of this phase was also predicted for strong enough next nearest-neighbor Coulomb repulsion [23]. Other critical points corresponding to the couplings g_i , i = 1, 2, 5, 6, 9, 10 are found to be at larger couplings. Therefore any phase transition corresponding to these critical

points is prevented by the gap in either of these two channels. On the other hand the g_1 and g_2 couplings corresponds to the effective (2+1)-dimensional Thirring model for spinors [25],[24]. It is equally interesting to study the characteristics of this phase transition beyond mean field calculation when $N = \infty$, in particular N = 2.



Figure 3.1: Mean field $(N = \infty)$ flow diagram shows the quantum critical points at C, A. G and B are the Gaussian and bi-critical fixed point. The U- line in this diagram is the line of initial condition V = 0 in Hubbard model.

Besides the fully attractive Gaussian fixed point at $g_i = 0$, β -functions in Eqs. (3.2) – (3.11) exhibit a critical point at $g_4 = -1/3$; $g_1 = g_2 = g_3 = g_5 = g_6 = g_7 = g_8 = 0 = g_9 = g_{10}$ for N = 2. This critical point (CP) corresponds to a continuous phase transition from a semimetallic phase to a charge density wave (CDW) with a staggered pattern in charge. This state is characterized by the order parameter $C = \langle \overline{\psi}\psi \rangle (\neq 0)$. The CDW quantum critical point (QCP) exists at the mean-field level and also survives when sub-leading corrections in 1/N are included. Besides the CDW QCP the fixed point at $g_7 = -1/3$, $g_1 = g_2 =$ $g_3 = g_4 = g_5 = g_6 = g_8 = g_9 = g_{10} = 0$ also survives as a critical point. On the other hand the critical points corresponding to g_5, g_6, g_9, g_{10} are no longer critical point once we include the corrections to the sub-leading order in 1/N. The fixed points corresponding to $g_i = -2/3, g_j = g_3 = g_4 = g_5 = g_6 = g_7 = g_8 = g_9 = g_{10} = 0$, where i, j = 1, 2 but $i \neq j$ are critical points too. Their physical significance is somewhat unclear at the moment.

We now introduce the spin degrees of freedom of the electrons to extend our discussion on various possible phase transitions to different broken symmetry phases in spin and charge.



Figure 3.2: Flow diagram shows various phase separatrix. Dotted line is the Hubbard U line with V = 0. Addition of V shifts the line in downward direction. The intersection of this line with the separatrix determines the various phase boundaries presented in Fig. [2].

As argued earlier a similar symmetry argument taking spin in account shows that there are 20 short ranged interactions in the interacting Lagrangian after one imposes the 'atomic limit'. On the other hand deformation of the Lagrangian for N flavor of Dirac fermions is achieved by the following redefinition

$$\overline{\psi}_{+}\psi_{+} \to \sum_{\sigma=1}^{N/2} \overline{\psi}_{\sigma}\psi_{\sigma}; \quad \overline{\psi}_{-}\psi_{-} \to \sum_{\sigma=(N/2)+1}^{N} \overline{\psi}_{\sigma}\psi_{\sigma}.$$
(3.15)

The RG analysis can now be performed analogously to the spinless case showing that there are indeed two QCPs corresponding to phase transition either to an anti-ferromagnetic(AF) phase with staggered pattern in spin density or to a CDW. The order parameters in these two phases are defined as $A = \langle \sum_{\sigma} \sigma \overline{\psi}_{\sigma} \psi_{\sigma} \rangle$ and $C = \langle \sum_{\sigma} \overline{\psi}_{\sigma} \psi_{\sigma} \rangle$, respectively. At the mean-field level $(N = \infty)$ these two QCPs are in the Gross-Neveu universality class [21] and as our calculation shows they remain in the same universality class even after corrections of the order 1/N are included [17].

To gain a further insight into the properties of the anti-ferromagnetic and charge density wave quantum critical points it is sufficient to consider the restricted interacting Lagrangian

$$\widetilde{L}_{int} = g_a (\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \psi_{\sigma})^2 + g_c (\sum_{\sigma} \overline{\psi}_{\sigma} \psi_{\sigma})^2.$$
(3.16)

This only includes coupling in the anti-ferromagnetic and charge density wave channels denoted by g_a and g_c respectively since these are the two QCPs (CDW and AF) exhibited by L_{int} . Thus all the other couplings in L_{int} are irrelevant for further discussion and therefore set to zero. In the (g_a, g_c) attractive plane, the QCPs corresponding to the transition from semimetal to anti-ferromagnet(A) and charge density wave(C) are at (-1/3, 0) and (0, -1/3)respectively, beside the Gaussian fixed point(G) at (0,0) as depicted in the flow diagram. There is also a bi-critical(B) fixed point at (-1/2, -1/2), which directs the flow towards either the anti-ferromagnetic or charge density wave QCP. The sub-leading corrections of the order 1/N in the beta-functions affect the flow of the couplings, resulting in the shift of the fixed points towards the stronger coupling regime in comparison to the mean-field counterpart. Therefore the 1/N corrections lead to the stabilization of the semimetallic ground state. We further notice that the sign change of the block of the matrix γ_0 acting on the lower component of the spinor Ψ , $\gamma_0 = I_2 \otimes \sigma_z \rightarrow \sigma_z \otimes \sigma_z$, together with the exchange of couplings $g_a \leftrightarrow g_c$ leaves \widetilde{L}_{int} invariant and thus the charge-density wave and anti-ferromagnetic critical points appear symmetrically in the (g_a, g_c) attractive plane. The symmetric appearance of these two critical points can also be argued by considering the characteristics of the order parameters in these two phases. It is because of the preferential axis of spin, both the charge-density wave and anti-ferromagnetic order parameter breaks the Ising like symmetry. Hence these two quantum critical point belongs to the same universality class, Gross-Neveu in this case.

3.3 Extended Hubbard model

Let us now consider a specific lattice model that will allow us to achieve different phase transitions mentioned earlier by tuning some interactions already present on the lattice. The analysis is based on a useful decomposition of Hubbard's on-site interaction on a bipartite lattice into a sum of squares of average and staggered densities, and average and staggered magnetizations. The Hubbard model is defined by the Hamiltonian H_1 , where

$$H_{1} = \sum_{\vec{X}, \vec{Y}, \sigma, \sigma'} n_{\sigma}(\vec{X}) \left[\frac{U}{2} \delta_{\vec{X}, \vec{Y}} + \frac{e^{2}(1 - \delta_{\vec{X}, \vec{Y}})}{4\pi |\vec{X} - \vec{Y}|} \right] n_{\sigma'}(\vec{Y}),$$
(3.17)

where the first term represent on-site repulsive interaction and the second term corresponds to the Coulomb interaction. Hereafter we will decompose the Coulomb interaction into two parts consisting of the nearest-neighbor repulsive Coulomb interaction denoted by V and its long ranged tail. Even though the long ranged part of the Coulomb interaction can be represented by a massless scalar gauge field, its main effect on the lattice scale is to provide the repulsion between nearest-neighbors. Thus for our purposes here, consider only the nearest-neighbor part of the Coulomb interaction. Such a decomposition of the interaction into a short ranged and long ranged part is exact for an infinitely long-ranged one, but this is only an approximation for the Coulomb interaction.

Generalizing the Hamman's decomposition, the first term in H_1 can also be written exactly as

$$\frac{U}{8} \sum_{\vec{A}} [(n(\vec{A}) + n(\vec{A} + \vec{b}))^2 + (n(\vec{A}) - n(\vec{A} + \vec{b}))^2] - [(m(\vec{A}) + m(\vec{A} + \vec{b}))^2 + (m(\vec{A}) - m(\vec{A} + \vec{b}))^2],$$
(3.18)

where $n(\vec{A}), m(\vec{A}) = u_{+}^{\dagger}(\vec{A})u_{+}(\vec{A}) \pm u_{-}^{\dagger}(\vec{A})u_{-}(\vec{A})$, are the particle number and the magnetization at the site \vec{A} . Variables at the second sublattice (\vec{B}) are analogously defined in terms of $v_{\sigma}(\vec{B})$. Therefore the first term in the decomposition corresponds to the average density on sub-lattices A and B and the second term to the difference on electron number in those two sublattices, the third term to the average magnetization and the fourth term to the staggered magnetization. On the other hand, the short ranged part of Coulomb interaction, with strength $V(\vec{b})$ can be cast in the following form

$$\frac{1}{2} \sum_{\vec{X}\neq\vec{Y}} n(\vec{X})V(\vec{X}-\vec{Y})n(\vec{Y})$$

$$= \frac{V(\vec{b})}{4} \sum_{\vec{X}} \{ [n(\vec{A}) + n(\vec{A}+\vec{b})]^2 - [n(\vec{A}) - n(\vec{A}+\vec{b})]^2 \}.$$
(3.19)

Hence the first term of the nearest-neighbor Coulomb interaction is just the density-density interaction and the second term is the *negative* interaction in the CDW channel. Thus the strength of the interaction in CDW channel is softened by the nearest-neighbor Coulomb interaction.

Hereafter we cast the problem in the continuum limit suitable in the low energy regime. Defining the two *slow* components of fields as

$$r_{\sigma}^{1,2}(\vec{x},\tau) = \int_{|\vec{k}\pm\vec{K}|<\Lambda} \frac{d\vec{k}}{(2\pi)^2} e^{i\vec{k}\cdot\vec{x}} r_{\sigma}(\vec{k},\tau), \qquad (3.20)$$

with r = u, v, the Dirac field becomes

$$\psi_{\sigma}^{\dagger}(\vec{x},\tau)e^{i(\vec{k}.\vec{x})\gamma_{35}} = \left(u_{\sigma}^{1\dagger}(\vec{x},\tau), \ v_{\sigma}^{1\dagger}(\vec{x},\tau), u_{\sigma}^{2\dagger}(\vec{x},\tau), v_{\sigma}^{2\dagger}(\vec{x},\tau)\right),$$
(3.21)

where 1, 2 are the Dirac point indices. Therefore in terms of Dirac fields the average density, staggered density, average magnetization and staggered magnetization read as

$$n(\vec{A}) + n(\vec{B}) = \sum_{\sigma} \overline{\Psi}_{\sigma} \left(\frac{\sigma_z}{\sigma_z e^{-i2kx}} \frac{\sigma_z e^{i2kx}}{\sigma_z} \right) \Psi_{\sigma},$$
$$n(\vec{A}) + n(\vec{B}) = \sum_{\sigma} \overline{\Psi}_{\sigma} \left(\frac{I}{Ie^{-i2kx}} \frac{Ie^{i2kx}}{I} \right) \Psi_{\sigma},$$
$$n(\vec{A}) + n(\vec{B}) = \sum_{\sigma} \sigma \overline{\Psi}_{\sigma} \left(\frac{\sigma_z}{\sigma_z e^{-i2kx}} \frac{\sigma_z e^{i2kx}}{\sigma_z} \right) \Psi_{\sigma},$$

$$n(\vec{A}) + n(\vec{B}) = \sum_{\sigma} \sigma \overline{\Psi}_{\sigma} \left(\frac{I}{Ie^{-i2kx}} \middle| \frac{Ie^{i2kx}}{I} \right) \Psi_{\sigma},$$

respectively. Noting that

$$\left(\begin{array}{c|c} 0 & I \\ \hline 0 & 0 \end{array}\right) = \frac{1}{2}\gamma_1(i\gamma_5 + \gamma_3),$$

 $\quad \text{and} \quad$

$$\left(egin{array}{c|c} 0 & \sigma_z \ \hline 0 & 0 \end{array}
ight) = rac{1}{2} \gamma_0 \gamma_1 (i \gamma_5 + \gamma_3),$$

in 'valley representation', we write down the Hubbard U-model in continuum limit as

$$H_{1} = g_{d} \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_{0} \psi\right)^{2} - \frac{\widetilde{g}_{d}}{2} \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_{0} \gamma_{1} \gamma_{5} \psi\right)^{2} - \frac{\widetilde{g}_{d}}{2} \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_{0} \gamma_{1} \gamma_{3} \psi\right)^{2} + g_{f} \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_{0} \psi\right)^{2} - \frac{\widetilde{g}_{f}}{2} \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_{0} \gamma_{1} \gamma_{5} \psi\right)^{2} - \frac{\widetilde{g}_{f}}{2} \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_{0} \gamma_{1} \gamma_{3} \psi\right)^{2} + g_{c} \left(\sum_{\sigma} \overline{\psi}_{\sigma} \psi\right)^{2} - \frac{\widetilde{g}_{c}}{2} \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_{1} \gamma_{5} \psi\right)^{2} - \frac{\widetilde{g}_{c}}{2} \left(\sum_{\sigma} \overline{\psi}_{\sigma} \gamma_{1} \gamma_{3} \psi\right)^{2} + g_{a} \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \psi\right)^{2} - \frac{\widetilde{g}_{a}}{2} \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_{1} \gamma_{5} \psi\right)^{2} - \frac{\widetilde{g}_{a}}{2} \left(\sum_{\sigma} \sigma \overline{\psi}_{\sigma} \gamma_{1} \gamma_{3} \psi\right)^{2}.$$

$$(3.22)$$

Hence in the Hubbard U-model $g_d = -2\tilde{g_d} - e^2/4K = (U+V)a^2/8$, $g_c = -2\tilde{g_c} = (U-V)a^2/8$, $g_f = g_a = -2\tilde{g_f} = -2\tilde{g_a} = -Ua^2/8$, where the *d* and *c* couplings correspond to the first (average density) and the second (staggered density), whereas *f* and *a* couplings represent the third (magnetization) and the fourth (staggered magnetization) terms in H_1 . The short ranged Coulomb interaction is represented by the following: (i) the intra-unit-cell, nearest neighbor repulsion $V = e^2\sqrt{3}/a\pi$ and the $2\vec{K}$ Fourier component $e^2/2K$. Therefore the Hubbard model in the continuum limit dissolves into 12 couplings and all these couplings are allowed by the symmetry present on lattice. Moreover the mean-field renormalization calculation shows that the short ranged interactions renormalize as

$$\beta_{g_x} = -g_x - C_x g_x^2, \tag{3.23}$$

$$\beta_{\widetilde{g}_{\widetilde{x}}} = -\widetilde{g}_{\widetilde{x}} + 2\widetilde{g}_{\widetilde{x}}^{2}, \qquad (3.24)$$

where $C_{c,a} = 4$ and $C_{d,f} = 0$, where the couplings renormalize as $g_x \Lambda/\pi \rightarrow g_x$. Therefore the \tilde{g}_x couplings require larger interactions to open the gap in comparison to that for g_x . Hence existing gaps for finite g_c, g_a will prevent other gaps from opening. Therefore we can drop all the \tilde{g}_x for any further discussion. Therefore the semimetal-anti-ferromagnet transition is continuous at the N = 2 Gross-Neveu critical point at which

$$\langle \overline{\Psi}_{\sigma}(\vec{q},\omega)\Psi_{\sigma}(\vec{q},\omega)\rangle \sim (q^2 + \omega^2)^{(\eta_{\Psi}-1)/2},$$
(3.25)

with the fermion's anomalous dimension $\eta_{\Psi} = [2/3\pi^2 N] + O(1/N^2)$ [26],[27]. The order parameter correlation function at the critical point also decays as

$$\langle A(\vec{x},\tau)A(0,0)\rangle \sim (x^2 + \tau^2)^{-(1+\eta)/2},$$
(3.26)



Figure 3.3: The large N(blue) and N = 2(red) phase diagram for graphene. This clearly indicates that the semimettalic ground state is stabilized beyond mean-field. Here the axis are in units of $8/a^2$. The critical value of the Hubbard onsite repulsive interaction is $U_c = 0.25$ for $N = \infty$ and 0.3 for N = 2. On the other hand, the critical value of nearestneighbor Coulomb interaction for direct transition to the CDW phase is $V_c = U_c$ for $N = \infty$, but for N = 2 it is 0.33.

where η is the standard anomalous dimension, and $\eta = 1 - 16/(3\pi^2 N) + O(1/N^2)$. The correlation length diverges at the critical point with the exponent $\nu = 1 + 8/(3\pi^2 N) + O(1/N^2)$. The critical exponents are even calculated to the order $1/N^2$ [26],[27], as well as determined via exact renormalization group calculations [19],[20], Monte Carlo simulations, and the ϵ expansion, [28],[29]. In summary, for N = 2, one finds $\eta_{\Psi} = 0.038 \pm 0.006$, $\nu = 0.97 \pm 0.07$ and $\eta = 0.770 \pm 0.0016$ [19][20].

Even though the long ranged nature of the Coulomb interaction is found to be marginally irrelevant to the first order in 1/N [30],[31],[32] as

$$\beta_e = \frac{de^2}{dlnb} = (z-1)e^2,$$
(3.27)

where z is the dynamical critical exponent found to be

$$z = 1 - \frac{e^2}{2\pi N} + O(1/N^2), \qquad (3.28)$$

similar to the bosonic case, it leaves its imprint on the bare value of the coupling g_c . For a sufficiently large value of the nearest-neighbor repulsion V, when the line of initial condition

i.e. $g_a = -g_c$ for V = 0 reaches the left of the critical point C, a semimetal- charge density wave transition occurs. This gives an alternative mechanism to that of Ref. [33],[34] for charge density wave formation. On the other hand for a sufficiently large V when the line of initial condition comes to the left of the bi-critical point B, a direct transition between gapped insulating anti-ferromagnet and charge density wave state happens. This transition is discontinuous. The phase diagram depicted in Fig[3.3] both for $N = \infty$ and N = 2 shows that the semimetallic state is stabilized beyond the mean-field approximation.

Chapter 4

Conclusions

Within the framework of the tight-binding model it is found that at half-filling the valence and conduction bands touch each other at the Dirac points, located at the corners of the Brillouin zone and electron behaves like massless pseudo-relativistic Dirac fermion, where the Fermi velocity ($\sim 10^6$ m/s) plays the role of the velocity of light. It also turns out that out of six such Dirac points only two are non-equivalent. Therefore at energy scales much lower than the bandwidth only electrons near these points carry dynamical importance. Hence we construct the interacting theory of electrons on the honeycomb lattice in terms of Dirac fields by considering the four-fermionic short ranged interactions.

Discrete symmetries of the honeycomb lattice allow us to restrict the number of short ranged interactions in the continuum limit. Interchange of the labeling of two triangular sub-lattices of the honeycomb lattice presents a discrete symmetry of the lattice daubed as 'mirror symmetry'. Another discrete symmetry comes from relabeling of two non-equivalent Dirac points. We recognize this symmetry as the time-reversal symmetry of the problem. We argued here that the labeling of the two sub-lattices and the Dirac points is completely arbitrary and therefore the theory should remain invariant under relabeling.

Further restriction on the interactions is achieved by considering momentum conservation at the two Dirac points. Altogether these symmetries restrict the interacting theory to 16 couplings when we suppress the spin degrees of freedom of the electrons. Here we also considered the parity symmetry on the lattice and found an explicit representation in the continuum limit. It turns out that all the interactions are invariant under the mirror, time reversal, and parity symmetries combined. The number of interactions defining the interacting Lagrangian is further reduced by imposing the atomic limit. In the atomic limit the interacting Lagrangian is defined by 10 couplings for spinless electrons. When we incorporate the spin degrees of freedom into our theory the number of interactions allowed by the symmetry and atomic limit both gets double. This can be achieved by generalizing the discussion on symmetry for spinless electron after including the spin degrees of freedom.

Furthermore, analyzing the renormalization group flows, derived by using Wilson's one loop method with the interacting model in the atomic limit, we found that there exists a continuous phase transition to a charge density wave phase from the semimetallic ground state for spinless electrons. Considering the spin of the electrons we found that there exists an additional continuous phase transition to the anti-ferromagnetic phase. These two quantum phase transitions exist at the mean-field level and also survive when we consider sub-leading corrections in 1/N. These two quantum phase transitions are found to be in the Gross- Neveu universality class for large N and remains in the same universality class for finite number of fermionic species on the lattice. On the other hand, corrections to the sub-leading order in 1/N provide an extra protection to the semi-metallic ground state against interactions by slowing down the flow of the couplings towards the critical points. It is also argued that the interactions corresponding to intra-valley scattering are closed under renormalization to any order in perturbation theory. On the other hand, once we incorporate the interactions corresponding to inter-valley scattering the model in the atomic limit is no longer closed under renormalization.

Beside the charge-density wave quantum critical point the spinless interacting model also exhibits another critical point that corresponds to a continuous phase transition into a gapped insulating phase. The order parameter in this phase spontaneously breaks time reversal symmetry.

Finally we consider the extended Hubbard model with both an on-site (U) and a nearestneighbor (V) Coulomb repulsive potential. Neglecting the long ranged part of the Coulomb interaction we found that it is defined by 12 short ranged couplings. Parameterizing the couplings with U and V we thereafter extract the phase diagram showing the semimetalcharge density wave and anti-ferromagnet transition for sufficiently large U and V. In that

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phase diagram we also found a discontinuous transition between the charge density wave and anti-ferromagnet for large enough V.

Appendix A

Momentum shell integration in one loop Wilsonian renormalization

Let us consider the model with only two couplings

$$L = g_1 (\overline{\psi} M_1 \psi)^2 + g_2 (\overline{\psi} M_2 \psi)^2, \qquad (A.1)$$

where M_1 and M_2 are some Dirac matrices. To calculate the β -function to leading order in 1/N we have to compute the following integral

$$R_1 = \int_{\Lambda/b}^{\Lambda} \frac{kdk}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \quad Tr(M_i \gamma_{\mu} M_j \gamma_{\nu}) \quad \frac{k_{\mu} k_{\nu}}{\left(k^2 + \omega^2\right)^2},\tag{A.2}$$

where $\mu, \nu = 0, 1, 2$ and i, j = 1, 2 at one loop level. Because of the cyclic property of the trace we need i = j, otherwise the trace vanishes. Therefore to leading order in 1/N the two different couplings do not mix and we found

$$R_1 = \frac{\Lambda}{\pi} \ln b, \tag{A.3}$$

for $M = I, \gamma_3 \gamma_5$,

$$R_1 = \pm \frac{\Lambda}{2\pi} \ln b, \tag{A.4}$$

for $M = \gamma_1, \gamma_2, \gamma_0 \gamma_1, \gamma_0 \gamma_2$ (upper sign), $M = \gamma_1 \gamma_3, \gamma_1 \gamma_5, \gamma_0 \gamma_1 \gamma_3, \gamma_0 \gamma_1 \gamma_5$ (lower sign) and

$$R_1 = 0, \tag{A.5}$$

for $M = \gamma_0, \gamma_0 \gamma_3 \gamma_5$. On the other hand we will encounter the following integral

$$R_2 = \int_{\Lambda/b}^{\Lambda} \frac{kdk}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \quad (M_i \gamma_\mu M_j \gamma_\nu) \quad \frac{k_\mu k_\nu}{(k^2 + \omega^2)^2}, \tag{A.6}$$

in calculating the β functions to sub-leading order in 1/N. This integral may give a nontrivial result depending M_i and M_j explicitly. In a diagrammatic calculation this contribution is generated by the particle-hole diagram. On the other hand if we consider the particle-particle diagram it will leave us with the following integral

$$R_3 = \int_{\Lambda/b}^{\Lambda} \frac{kdk}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \quad (M_j \gamma_\mu M_i \gamma_\nu) \quad \frac{k_\mu (-k_\nu)}{\left(k^2 + \omega^2\right)^2}.$$
 (A.7)

The minus sign in front of the momentum k_{ν} comes from momentum conservation in the loop. For i = j, it is trivial to check that R_2 and R_3 cancel each other but these two may add for $i \neq j$ and generate new couplings. For example if we consider $M_1 = I$ and $M_2 = \gamma_0$ then the contributions from two such diagrams will add and generate the following two new couplings

$$(\overline{\psi}\gamma_0\gamma_1\psi)^2, (\overline{\psi}\gamma_0\gamma_2\psi)^2.$$

We can generalize these arguments after including the spin degree of freedom.



Figure A.1: Particle-hole and particle-particle diagrams at the one loop level without spin degrees of freedom may generate new coupling to sub-leading order in 1/N depending on the integrals R_2 and R_3 .

Appendix B

Flow equations

In this discussion we present the renormalization flow of the couplings defined the interacting Lagrangian (L_{int}) including the spin degree of freedom of electron. In Chapter 2, we found that when we incorporate the spin of the electrons, L_{int} is defined in terms of 16 coupling constants in the atomic limit. Even though in the mean-field approximation all the couplings are decoupled from each other, mixing may appear non-trivially at sub-leading order in 1/N.

On the other hand, when we take the spin degrees of freedom into account an additional complication arises since all the couplings become two-fold degenerate in bilinear space and it is thus impossible to determine after the fast mode and frequency integration which coupling gets renormalized if we consider the mixing of couplings g_i and g_i' , for i = 1, ..., 8. Therefore special care is required. Here we present the solution of this problem by considering the mixing of g_4 and g_4' couplings as follows

$$g_{4}\left(\sum_{\sigma=\pm}\sigma\overline{\psi}_{\sigma}\psi_{\sigma}\right)^{2} + g_{4}'\left(\sum_{\sigma=\pm}\overline{\psi}_{\sigma}\psi_{\sigma}\right)^{2}$$

$$= g_{+}\left[\left(\overline{\psi}_{\uparrow}\psi_{\uparrow}\right)^{2} + \left(\overline{\psi}_{\downarrow}\psi_{\downarrow}\right)^{2}\right] + 2g_{-}\overline{\psi}_{\uparrow}\psi_{\uparrow}\overline{\psi}_{\downarrow}\psi_{\downarrow},$$
(B.1)

where, $g_+ = g_4 + g_4'$ and $g_- = g_4 - g_4'$. The flow equations in terms of these two couplings read

$$\beta_{g_{+}} = -g_{+} - \left(2 - \frac{2}{N}\right)g_{+}^{2} - 2g_{-}^{2}, \tag{B.2}$$

$$\beta_{g_{-}} = -g_{-} - \left(4 - \frac{2}{N}\right)g_{+}g_{-}.$$
(B.3)

This procedure can easily be extended for other such pairs of couplings. This complication does not appear if we consider the mixing of two couplings with different order parameters.

Flow equations

In the Wilsonian one loop calculation the flow equation of different couplings in L_{int} is given by

$$\beta_{g_{1}} = -g_{1} - (2 - \frac{1}{N})g_{1}^{2} + \frac{1}{N}g_{1}(-g_{2} - g_{3} + g_{4} + g_{5} - g_{6} + g_{7} - g_{8} + g_{1}'$$

$$-g_{2}' - g_{3}' + g_{4}' + g_{5}' - g_{6}' + g_{7}' - g_{8}') + \frac{1}{N}(g_{3}g_{7} + g_{3}'g_{7}' - g_{4}g_{8} - g_{4}'g_{8}')$$

$$-\frac{2}{N}(g_{7}g_{2} + g_{7}'g_{2}' - g_{5}g_{4} - g_{5}'g_{4}'), \qquad (B.4)$$

$$\beta_{g_{1}'} = -g_{1}' - (2 - \frac{1}{N})g_{1}'^{2} + \frac{1}{N}g_{1}'(g_{1} - g_{2} - g_{3} + g_{4} + g_{5} - g_{6} + g_{7} - g_{8}$$

$$-g_{2}' - g_{3}' + g_{4}' + g_{5}' - g_{6}' + g_{7}' - g_{8}') + \frac{1}{N}(g_{3}'g_{7} + g_{3}g_{7}' - g_{4}'g_{8} - g_{4}g_{8}')$$

$$-\frac{2}{N}(g_{7}g_{2}' + g_{7}'g_{2} - g_{5}'g_{4} - g_{5}g_{4}'), \qquad (B.5)$$

$$\beta_{g_2} = -g_2 - (2 - \frac{1}{N})g_2^2 + \frac{1}{N}g_2(-g_1 - g_3 + g_4 - g_5 + g_6 + g_7 - g_8 - g_1' + g_2' - g_3' + g_4' - g_5' + g_6' + g_7' - g_8') + \frac{1}{N}(g_3g_7 + g_3'g_7' - g_4g_8 - g_4'g_8') - \frac{2}{N}(g_7g_1 + g_7'g_1' - g_6g_4 - g_6'g_4'),$$
(B.6)

$$\beta_{g_{2'}} = -g_{2'} - (2 - \frac{1}{N})g_{2'}^{2} + \frac{1}{N}g_{2'}^{2}(-g_{1} + g_{2} - g_{3} + g_{4} - g_{5} + g_{6} + g_{7} - g_{8}$$

$$-g_{1'} - g_{3'}^{2} + g_{4'}^{2} - g_{5'}^{2} + g_{6'}^{2} + g_{7'}^{2} - g_{8'}^{2}) + \frac{1}{N}(g_{3'}g_{7} + g_{3}g_{7'}^{2} - g_{4'}g_{8} - g_{4}g_{8'}^{2})$$

$$-\frac{2}{N}(g_{7}g_{1'}^{2} + g_{7'}g_{1} - g_{6'}g_{4} - g_{6}g_{4'}^{2}), \qquad (B.7)$$

$$\beta_{g_3} = -g_3 - \frac{1}{N}(g_4g_5 + g_4g_6 + g_4'g_5' + g_4'g_6') - \frac{1}{N}(g_7g_1 + g_7'g_1' + g_7g_2 + g_7'g_2'), \quad (B.8)$$

$$\beta_{g_{3'}} = -g_3 - \frac{1}{N}(g_4g_5' + g_4g_6' + g_4'g_5 + g_4'g_6) - \frac{1}{N}(g_7g_1' + g_7'g_1 + g_7g_2' + g_7'g_2), \quad (B.9)$$

$$\beta_{g_4} = -g_4 - (4 - \frac{2}{N})g_4^2 + \frac{2}{N}g_4(-g_1 - g_2 + g_3 - g_5 - g_6 + g_7 + g_8 - g_1' - g_2' + g_3' + g_4' - g_5' - g_6' + g_7' + g_8') + \frac{2}{N}(g_1g_5 + g_1'g_5' + g_2g_6 + g_2'g_6') - \frac{1}{N}(g_3g_5 + g_3g_6 + g_3'g_5' + g_3'g_6' + g_3g_1 + g_3g_2 + g_3'g_1' + g_3'g_2' + g_8g_1 + g_8'g_1' + g_8g_2 + g_8'g_2') (B.10)$$

Flow equations

$$\beta_{g_{4'}} = -g_{4'} - (4 - \frac{2}{N})g_{4'}^{2} + \frac{2}{N}g_{4'}(-g_{1} - g_{2} + g_{3} + g_{4} - g_{5} - g_{6} + g_{7} + g_{8} - g_{1'} - g_{2'} + g_{3'} - g_{5'} - g_{6'} + g_{7'} + g_{8'}) + \frac{2}{N}(g_{1}g_{5'} + g_{1'}g_{5} + g_{2}g_{6'} + g_{2'}g_{6}) - \frac{1}{N}(g_{3}g_{5'} + g_{3}g_{6'} + g_{3'}g_{5} + g_{3}g_{6} + g_{3}g_{1'} + g_{3}g_{2'} + g_{3'}g_{1} + g_{3'}g_{2} + g_{8}g_{1'} + g_{8}g_{1} + g_{8}g_{2'} + g_{8'}g_{2})$$
(B.11)

$$\beta_{g_5} = -g_5 - (2 - \frac{1}{N})g_5^2 + \frac{1}{N}g_5(-g_1 + g_2 + g_3 - g_4 - g_6 - g_7 + g_8 - g_1' + g_2' + g_3' - g_4' + g_5' - g_6' - g_7' + g_8') - \frac{1}{N}(g_3g_4 + g_3'g_4' + g_7g_8 + g_7'g_8') + \frac{2}{N}(g_7g_6 + g_7'g_6' - g_1g_4 - g_1'g_4')$$
(B.12)

$$\beta_{g_{5'}} = -g_{5'} - (2 - \frac{1}{N})g_{5'^2} + \frac{1}{N}g_{5'}(-g_1 + g_2 + g_3 - g_4 + g_5 - g_6 - g_7 + g_8)$$

$$-g_{1'} + g_{2'} + g_{3'} - g_{4'} - g_{6'} - g_{7'} + g_{8'}) - \frac{1}{N}(g_3g_4 + g_3'g_{4'} + g_7g_8)$$

$$+g_{7'}g_{8'}) + \frac{2}{N}(g_7g_6 + g_{7'}g_{6'} - g_1g_4 - g_1'g_{4'})$$
(B.13)

$$\beta_{g_{6}} = -g_{6} - (2 - \frac{1}{N})g_{6}^{2} + \frac{1}{N}g_{6}(g_{1} - g_{2} + g_{3} - g_{4} - g_{5} - g_{7} + g_{8} + g_{1}'$$

$$-g_{2}' + g_{3}' - g_{4}' - g_{5}' + g_{6}' - g_{7}' + g_{8}') - \frac{1}{N}(g_{3}g_{4} + g_{3}'g_{4}' + g_{7}g_{8} + g_{7}'g_{8}')$$

$$+ \frac{2}{N}(g_{7}g_{5} + g_{7}'g_{5}' - g_{2}g_{4} - g_{2}'g_{4}')$$
(B.14)

$$\beta_{g_{6}'} = -g_{6}' - (2 - \frac{1}{N})g_{6}'^{2} + \frac{1}{N}g_{6}'(g_{1} - g_{2} + g_{3} - g_{4} - g_{5} + g_{6} - g_{7} + g_{8}$$

+ $g_{1}' - g_{2}' + g_{3}' - g_{4}' - g_{7}' + g_{8}') - \frac{1}{N}(g_{3}'g_{4} + g_{3}g_{4}' + g_{7}'g_{8}$
+ $g_{7}g_{8}') + \frac{2}{N}(g_{7}g_{5}' + g_{7}'g_{5} - g_{2}'g_{4} - g_{2}g_{4}')$ (B.15)

$$\beta_{g_7} = -g_7 - (4 - \frac{2}{N})g_7^2 + \frac{2}{N}g_7(-g_1 - g_2 + g_3 + g_4 - g_5 - g_6 + g_8 - g_1' - g_2' + g_3' + g_4' - g_5' - g_6' + g_7' + g_8') - \frac{1}{N}(g_8g_5 + g_8'g_5' + g_8g_6 + g_8'g_6') - \frac{2}{N}(g_6g_5 + g_5'g_6')$$
(B.16)

Flow equations

$$\beta_{g_{7'}} = -g_{7'} - (4 - \frac{2}{N})g_{7'}^{2} + \frac{2}{N}g_{7'}(-g_{1} - g_{2} + g_{3} + g_{4} - g_{5} - g_{6} + g_{7} + g_{8} - g_{1'} - g_{2'} + g_{3'} + g_{4'} - g_{5'} - g_{6'} + g_{8'}) - \frac{1}{N}(g_{8}g_{5'} + g_{8'}g_{5} + g_{8'}g_{6} + g_{8}g_{6'}) - \frac{2}{N}(g_{6}g_{5'} + g_{5}g_{6'})$$
(B.17)

$$\beta_{g_8} = -g_8 - \frac{1}{N}(g_7g_5 + g_7'g_5' + g_7g_6 + g_7'g_6' - g_4g_1 - g_4'g_1' - g_4g_2 - g_4'g_2'),$$
(B.18)

$$\beta_{g_{8'}} = -g_{8'} - \frac{1}{N} (g_{7'}g_5 + g_7g_5' + g_7'g_6 + g_7g_6' - g_4'g_1 - g_4g_1' - g_4'g_2 - g_4g_2'),$$
(B.19)

at zero temperature. Here we considered couplings corresponding to intra-valley scattering.

Notice that even though we started with a model where only g_3 and g_4 are finite for spinless electrons, the subleading order corrections in 1/N generate all the other possible couplings allowed by symmetry. In the diagrammatic renormalization calculation the one loop particle-particle and some particle-hole diagrams generate new couplings when the subleading order corrections in 1/N are included.



Figure B.1: Feynman diagrams contributing to the leading order and the sub-leading order in 1/N in renormalization of couplings in the one-loop level. In the diagrams a solid line stands for the field with spin-up component and the dashed line corresponds to that with spin-down component. Diagram (1) contributes in both leading and sub-leading order, whereas the diagram (3) contributes only to the sub-leading order renormalization of the g_+ coupling. On the other hand diagram (2) and diagram (4) renormalize the g_- coupling both in leading and sub-leading order but only sub-leading order in 1/N respectively. A replica of the second diagram, where the propagators are built out of the spin-down fields also renormalizes the g_- coupling to both leading and sub-leading order in 1/N. Diagrams (5) and (6) renormalize g_- to the sub-leading order in 1/N. However these two contributions cancel each other if we consider the mixing of two couplings degenerate in bilinear space whereas they add and may generate new couplings if we consider couplings having different bilinear.

Appendix C

Susceptibilities of Dirac fermions in (2+1)-dimensions

In this appendix we answer the question as to which bilinear has the largest susceptibility in (2 + 1)- dimensions. To answer this question let us consider the free Lagrangian

$$L = \overline{\psi} \gamma^{\mu} \partial_{\mu} \psi \tag{C.1}$$

with a bilinear 'order parameter' $\overline{\psi} M \psi$

$$L = \overline{\psi} \partial \psi + i j \overline{\psi} M \psi, \tag{C.2}$$

where i, j are source fields. Integrating out the fermions gives

$$L = \frac{1}{2}j\chi j, \tag{C.3}$$

where χ is the required susceptibility given by

$$\chi(q) = -Tr \int d^D \vec{k} \quad \frac{ik_{\mu}\gamma_{\mu}}{k^2} \quad M \quad \frac{i(k_{\nu} + q_{\nu})\gamma_{\nu}}{(k+q)^2} \quad M.$$
(C.4)

Here our main concern is to find $\chi_0 = \chi(q = 0)$, given by

$$\chi_0 = \int \frac{d^D \vec{k}}{k^4} \quad k_\mu k_\nu \quad \{Tr(\gamma_\mu M \gamma_\nu M)\}.$$
(C.5)

For D = 3 one finds

$$\chi_0 = \int \frac{d^3k}{3k^2} \quad Tr(\gamma_\mu M \gamma_\mu M). \tag{C.6}$$

Hence our task is to find the M which gives the largest trace.

Let us now introduce a basis $\Gamma_{\alpha} \in$

$$\{I \quad \gamma_0 \quad \gamma_1 \quad \gamma_2 \quad \gamma_3$$
$$i\gamma_0\gamma_1 \quad i\gamma_0\gamma_2 \quad i\gamma_0\gamma_3 \quad i\gamma_1\gamma_2 \quad i\gamma_1\gamma_3 \quad i\gamma_2\gamma_3$$
$$i\gamma_0\gamma_1\gamma_2 \quad i\gamma_0\gamma_1\gamma_3 \quad i\gamma_0\gamma_2\gamma_3 \quad i\gamma_1\gamma_2\gamma_3$$
$$\gamma_0\gamma_1\gamma_2\gamma_3 = \gamma_5\}.$$

All the elements in this basis satisfy the following properties

$$\Gamma_{\alpha}^{\dagger} = \Gamma_{\alpha}, \quad \Gamma_{\alpha}^{2} = I. \tag{C.7}$$

Expanding M in this basis one gets

$$T = \sum_{\mu,a,b} C_a C_b \quad Tr(\gamma_{\mu} \Gamma_a \gamma_{\mu} \Gamma_b), \tag{C.8}$$

where, $T = Tr(\gamma_{\mu}M\gamma_{\mu}M)$ and $M = \sum_{a} C_{a}\Gamma_{a}$. Using the fact that the elements in Γ_{α} either commute or anti-commute with γ_{μ} one can decompose T as follows

$$T = \sum_{\mu} \sum_{b} C_b \left\{ \sum_{a}' C_a Tr(\Gamma_a \Gamma_b) - \sum_{a}'' C_a Tr(\Gamma_a \Gamma_b) \right\},$$
(C.9)

since $\gamma_{\mu}^{2} = I$ for all μ . In the above expression \sum_{a}' runs over Γ_{a} which commutes with γ_{μ} and \sum_{a}'' runs over Γ_{a} which anti-commute with γ_{μ} . Since

$$Tr\{\Gamma_a\Gamma_b\} = 4\delta_{a,b},\tag{C.10}$$

one gets

$$T = 4\sum_{\mu} \left(\sum_{a}' C_{a}^{2} - \sum_{a}'' C_{a}^{2} \right).$$
(C.11)

Therefore we get the bounds on T as

$$-4 \times 3 \leq T \leq 4 \times 3, \tag{C.12}$$

assuming $\sum_{a} C_{a}^{2} = 1$. Thus the trace optimized in two cases, either

$$\{M, \gamma_{\mu}\} = 0,$$
 (C.13)

for all μ , implying $M = \gamma_3, \gamma_5$, or

$$[M, \gamma_{\mu}] = 0, \tag{C.14}$$

for all μ , implying $M = I, i\gamma_3\gamma_5$. Hence from these solutions one immediately finds that the susceptibility of Dirac fermions in (2 + 1)-dimensions is maximized for $M = I, i\gamma_3, i\gamma_5$, and $i\gamma_3\gamma_5$, whereas it is minimum for $M = \gamma_3, \gamma_5$, and $\gamma_3\gamma_5$. Therefore the maximal susceptibility corresponds to the opening of the relativistic mass gap that either breaks the chiral symmetry $(\gamma_0, i\gamma_0\gamma_3, i\gamma_0\gamma_5)$ or doesn't break the chiral symmetry $(i\gamma_0\gamma_3\gamma_5)$.

On the other hand the susceptibility of the Dirac fermions is largest only for $M = \gamma_0, i\gamma_0\gamma_5$ for D = 3 + 1.

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