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Interaction effects in multilayer graphene

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Chapter 1

Introduction

Interaction among electrons usually does not drastically influence the ground-state properties of electronic systems. Actually, in the standard case, interacting electrons are well described by the so-called Fermi liquid theory which explains the reason why some properties of interacting fermionic systems are very similar to those of the ideal Fermi gas, where free particles are substituted by collective quasiparticles excitations. These quasi-particles have the same quantum numbers of the corresponding free particles, but with different, renormalized, masses.

There are other cases where, instead, such a mapping, which relies on the fact that the ground states of the free system and of the interacting one are adiabatically connected, cannot be applied. The system we are going to consider, for instance, exhibits an abruptly change of electronic properties upon turning on the interaction which allows the system to enter a symmetry broken gapped phase. Therefore, instead of getting a conducting phase from the ideal single-particle description, one observes an insulating phase. This system, we will focus on, is the multilayer graphene, which is a nanometric slab of graphite.

Several recent experiments, discussed in chapter 3, show that a sufficiently clean sample of multilayer graphene with even number of layers N develops a gapped insulating state ($N \leq 8$) at low temperatures, while systems with odd N retain a finite sizeable conductivity. Moreover, by increasing the number of even layers the system has higher and higher resistance at the band touching point, the so-called charge neutrality point. Time reversal symmetry and inversion invariance protect the band touching point from gap opening, this means that one of the two symmetries has to be broken in order for the gapped state to appear.

The commonly accepted explanation is that, in this state, adjacent layers are polarized with opposite charge, breaking inversion symmetry. The polarization gives rise to a mean-field potential that changes sign from one layer to the other. As we will see, such a potential opens a gap in even multilayers, while it does not do so for odd multilayers, in this way, giving account of the experimental findings. Despite its success, this phenomenological theory still lacks a microscopic derivation. The aim of this work is, therefore, that of addressing this important issue, within a quantum field theory (QFT) approach resorting to a functional integral formulation.

In chapter 4 we first derive an effective low-energy non-interacting Hamiltonian, projecting onto the low-energy bands. In chapter 5, then, we discuss the interacting term to be added to the free Hamiltonian in a suitable form which may include screening effects. The gapped ground state is derived in chapter 6, as a solution to the gap equation, obtained minimizing the action appearing in the functional integral. The estimates of the gap for different numbers of layers are compared with the experimental values, so as to check the validity of the model. Finally, in chapter 7 we discuss the most promising paths to pursue in order to improve and extend the present theoretical scheme.

Introduction

Chapter 2

Electronic structure of multilayer graphene

2.1 Single layer graphene (SLG)

A single graphene sheet is a hexagonal ("honeycomb") 2-dimensional lattice of carbon atoms [1], as shown in Fig.(2.1). The hexagonal lattice can be described as a triangular lattice with a two-atom basis, which we shall refer to as sublattice A and B. The lattice vectors are given by

$$\vec{a_1} = \frac{a}{2}(3,\sqrt{3}), \quad \vec{a_2} = \frac{a}{2}(3,-\sqrt{3}),$$
(2.1)

where the carbon-carbon distance is $a \sim 1.42$ Å. The reciprocal lattice vectors are instead given by

$$\vec{b_1} = \frac{2\pi}{3a}(1,\sqrt{3}), \quad \vec{b_2} = \frac{2\pi}{3a}(1,-\sqrt{3}).$$
 (2.2)

Notice that the Wigner-Seitz cell Γ of the reciprocal lattice is again hexagonal, and tilted by 90° with respect to the real space lattice. The carbon atoms are bound together by covalent σ -bonds of sp^2 hybrid orbitals, which accounts for the 120° angle between two bonds. In fact, the nearest-neighbours vectors are given by

$$\vec{\delta_1} = \frac{a}{2}(1,\sqrt{3}), \quad \vec{\delta_2} = \frac{a}{2}(1,-\sqrt{3}), \quad \vec{\delta_3} = -a(1,0).$$
 (2.3)

The electronic properties of graphene are mainly due to the electrons that do not participate to the covalent bonds, which are one per carbon atom. These spare electrons are somewhat free to roam around the lattice (compared to the covalent ones) and their physics is usually described by means of a tight binding scheme. The latter gives rise to a nearest neighbours hopping Hamiltonian of the form

$$H = t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{A,i,\sigma} c_{B,j,\sigma} + h.c.), \qquad (2.4)$$

where $t \sim 2.8 eV^1$, for example, $c_{A,i,\sigma}^{\dagger}$ is the creation operator on the *i* site of sublattice *A*, with spin σ . The energy spectrum is given by [1]

$$E_{\pm}(\vec{k}) = \pm t\sqrt{3 + f(\vec{k})},$$
 (2.5)

$$f(\vec{k}) = 2\cos(\sqrt{3}k_y a) + 4\cos(\frac{\sqrt{3}}{2}k_y a)\cos(\frac{3}{2}k_x a).$$
(2.6)

¹For our purposes the sign of t is irrelevant, since the Hamiltonian is particle-hole simmetric.



Figure 2.1: Real-space lattice and first Brillouin zone Γ .



Figure 2.2: Tight-binding Hamiltonian spectrum. Dirac points at Brillouin zone corners K, K' are visible.

The effect of including next-to-nearest-neighbours hopping is that of breaking particle hole symmetry, but since this is not crucial for our purposes we will not consider this effect. As shown in Fig.(2.2), there are two inequivalent Dirac points $\vec{K}, \vec{K'}$

$$\vec{K} = \frac{2\pi}{3a}(1, -\frac{1}{\sqrt{3}}), \quad \vec{K'} = \frac{2\pi}{3a}(1, \frac{1}{\sqrt{3}}), \tag{2.7}$$

at the corners of the first Brillouin zone, where the dispersion is approximately linear

$$E_{\pm}(\vec{k}) \sim \pm v\hbar |\vec{k}|. \tag{2.8}$$

The Fermi velocity is $v = \frac{3ta}{2\hbar} \sim 10^6 m/s$. Note that since there are two electrons per unit cell (one per atom in the basis), and electron spin degeneracy is 2, the lower band is completely filled, so that the Fermi level is exactly at E = 0. This is of fundamental importance, because the properties of an electron system are in exceedingly large measure dictated by dispersion at the Fermi level.

In the present work we shall resort to the approximation, valid for low excitation energy, that the system can be described by expanding the Hamiltonian for small momentum \vec{p} around Dirac points



Figure 2.3: Energetically favoured stacking configurations.

 $\vec{p} = \hbar(\vec{K} - \vec{k})$. This gives rise to the Hamiltonian²

$$H = \sum_{\vec{p},\sigma} \Psi^{\dagger}_{\sigma}(\vec{p}) H(\vec{p}) \Psi_{\sigma}(\vec{p})$$
(2.9)

where $H(\vec{p})$ is a matrix in the basis $(A_K, B_K, A_{K'}, B_{K'})$ and $\Psi_{\sigma}(\vec{p}) = (c_{A,K}, c_{B,K}, c_{A,K'}, c_{B,K'})_{\sigma}(\vec{p})$ is a vector of destruction operators, where spin and momentum indices have been gathered for convenience. The matrix is given by

$$H(\vec{p}) = \begin{pmatrix} 0 & v\pi^{\dagger} & 0 & 0 \\ v\pi & 0 & 0 & 0 \\ 0 & 0 & 0 & -v\pi \\ 0 & 0 & -v\pi^{\dagger} & 0 \end{pmatrix},$$
 (2.10)

where $\pi = p_x + ip_y$. In practice the system now has an extra degree of freedom due to the new "valley" index which can assume the values K, K'.

Let us point out that the Hamiltonian for a valley is the time reversed (or space inversed) version of the other, so that the total Hamiltonian is both time-reversal and space-inversion invariant, just like the original one. This implies that we need to break one of these symmetries in order to open a gap [4].

2.2 Multilayer graphene (NLG)

Let us now focus on multilayer graphene [10]. For simplicity we will consider only one valley, because the other one can be obtained by time-reversal ³. When graphene sheets are stacked one on top of each other, the system arranges itself so that energy is minimal. This usually happens for an interlayer distance of $d \sim 3.5$ Å, with one atom of the upper sheet placed over the center of each hexagonal conventional cell of the lower one, as shown in Fig.(2.4)⁴. Notice that these atoms all belong to the same sublattice, so that there are two possible choices.

Let us call α the position of the lower sheet (which is arbitrary), and β or γ the position of the upper one, depending on the previous choice, as shown in Fig.(2.3). For the purpose of the present work we shall consider only Bernal stacking, that is described in these scheme by the $\alpha\beta\alpha\beta\alpha...$ sequence ⁵. If we add only nearest-neighbour interlayer hopping terms t_{\perp} [14,15] we get the 2N by 2N Hamiltonian

²To be precise, the shown Hamiltonian arise if we choose as expansion points K', -K' instead of K, K'. Of course this is an equivalent choice, but has the advantage that under both time-reversal and spatial inversion $K' \to -K'$. Moreover, we need to do a unitary transformation to bring H in this form.

 $^{^{3}}$ Also multilayer graphene is time-reversal (and inversion) invariant, as it is described by a real hopping Hamiltonian on a inversion simmetric lattice. As time-reversal (and inversion) exchanges the two valleys, one has to be the reverse (inverse) of the other.

⁴We are not considering twisted stacking.

⁵As the atoms in the basis are equal actually this is the same as $\alpha\gamma\alpha\gamma\alpha\dots$. In other words, we can always rename sublattices so that the first two letters of the sequence are $\alpha\beta$.



Figure 2.4: Multilayer graphene lattice structure [6]. In our notation $\gamma_0 = t, \gamma_1 = t_{\perp}$, while the other hopping terms are neglected [14, 15]

matrix (of given spin component)

$$H(\vec{p}) = \begin{pmatrix} 0 & v\pi^{\dagger} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v\pi & 0 & t_{\perp} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t_{\perp} & 0 & v\pi^{\dagger} & 0 & t_{\perp} & 0 & 0 & 0 \\ 0 & 0 & v\pi & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t_{\perp} & 0 & v\pi^{\dagger} & 0 & 0 & 0 \\ 0 & 0 & t_{\perp} & 0 & v\pi & 0 & t_{\perp} & 0 & \ddots \\ 0 & 0 & 0 & 0 & 0 & v\pi & 0 & \ddots \\ 0 & 0 & 0 & 0 & 0 & v\pi & 0 & \ddots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \ddots & 0 \end{pmatrix},$$
(2.11)

in the basis $(A_1, B_1, ..., A_N, B_N)$, where the layer index has been introduced as subscript. In [10] a detailed description of the diagonalization of H can be found. We shall limit ourselves at reporting the results. For a N-multilayer, the energy is given by

$$E_{r,\vec{p}}^{\pm} = t_{\perp} \cos\left(\frac{r\pi}{N+1}\right) \pm \sqrt{v^2 |\vec{p}|^2 + t_{\perp}^2 \cos^2\left(\frac{r\pi}{N+1}\right)}$$
(2.12)



Figure 2.5: Example of odd and even multilayer spectrum. Computed with t = 3eV, $t_{\perp} = 0.1t$. Bands with same r share the same colour.

We can identify an effective mass

$$m_r = \frac{t_\perp}{v^2} \left| \cos\left(\frac{r\pi}{N+1}\right) \right| \tag{2.13}$$

so that if $m_r \neq 0$ the band is parabolic for small \vec{p} , the spectrum being given by

$$E_{r,\vec{p}}^{\pm} \sim \pm \frac{|\vec{p}|^2}{2m_r}.$$
 (2.14)

If $m_r = 0$, which happens only in odd multilayers with $r = \frac{N+1}{2}$, the dispersion is linear, giving rise to a Dirac band

$$E_{\vec{p}}^{\pm} \sim \pm v |\vec{p}| \tag{2.15}$$

Chapter 3

Experiments on suspended multilayer graphene

It is useful to have a brief overview of the experimental setting, in order to clarify which are the relevant quantities for this kind of systems, and how they are extracted from the experiments [14, 15].

3.1 Experimental setup

The experimental setup is the one of a field effect transistor (FET), as shown in Fig.(3.1). A slab of multilayer graphene acts as the body of the transistor, where the charge channel is located. Electrodes are attached to the ends of the sample in order to drive currents in the planar directions by applying a potential difference between them. Changing the potential of the back gate results in a shift of graphene Fermi energy. In this way, the density of charge carriers (holes in the valence band, electrons in the conduction band) can be, to some extent, modified.



Figure 3.1: Typical configurations of a graphene FET (GFET), showing also a top gate version (not used in the considered experiments). http://www.iue.tuwien.ac.at/phd/illarionov/dissch4.html

In this case [15] the substrate is heavily doped Si, which acts as the back gate, and is capped with 285nm thick insulating SiO_2 . Unfortunately, this surface can host charge impurities. Being so close to the material under examination, these impurities would induce a certain charge density in the sample. This implies that the Fermi level would be shifted from the charge neutral point (CNP), which in our case coincides with the band touching point. But since we are interested in studying the electronic properties of multilayer graphene near this precise point, we need the Fermi level be as close as possible to the CNP.

This can be obtained by suspending the slab over the substrate, in such a way that its bulk is far away from any charge impurity. In practice the device resembles a suspended bridge over a valley, as can be seen in Fig.(3.2), and hangs between the electrodes, which in turn lie on SiO_2 . By means of this stratagem (and by producing a sufficiently clean sample) it is possible to achieve charge densities below $10^{-10} cm^{-2}$, which allow the gapped state to emerge.



Figure 3.2: Suspended graphene device [13].

3.2 Gap detection through electron density

The main objective of the experiment [14] is that of identifying the gapped state and verify whether it develops out of a second order phase transition or not. In that case, it would be possible to measure a critical temperature T_c above which the order parameter, which is the gap Δ , is zero. Below T_c , instead, a certain law $\Delta = \Delta(T)$ would be obtained.

Let us consider for the moment the case of even multilayers, which only show quadratic bands (the conclusions are still valid for the odd case, as we will see). How does the presence of a gap influence the quantities that are accessible to experiments? Such quantities are in this case mainly related to transport, such as the square resistance R_{sq}^{1} . But transport quantities in electron systems are determined by the density of states ν_0 at the Fermi level. In turn, ν_0 is deeply affected by changes in the electronic structure, such as the opening of a gap, as shown in Fig.(3.3).

The gap suppresses the thermal electron density in the conduction band n_{th} , turning the material into an insulator. Therefore, by performing resistance measurements in a range of V_g it is possible to identify a sharp peak, if the temperature is low enough. Let us call the corresponding gate voltage V_{CNP} : when $V_g = V_{CNP}$ there is no induced electron density in the conduction band $(n \sim 0)$, so the CNP is obtained.

Unfortunately, it is not possible to derive T_c in this way, because the resistance grows without showing abrubt changes as T is lowered. Instead, the critical temperature can be identified by looking at n_{th} . As can be seen in Fig.(3.3), while n_{th} is expected to grow linearly above T_c (since $\nu_0 = \frac{m}{2\pi\hbar^2}$, where mis the effective mass, is constant for quadratic bands), below T_c it is suppressed. Then it would be possible to identify this point in a $n_{th}(T)$ plot.

¹The square resistance is defined as the resistance of a square, thin slab of material. Note that R_{sq} does not depend on the side of the square. It is measured in Ohms [Ω].



Figure 3.3: [14] (A,B,C) are, respectively, the low-energy bands, density of states and density of thermally excited electrons in the conduction band of bilayer graphene. (D,E,F) are the same quantities for gapped bilayer graphene, where the gap obeys mean-field dependance (inset of (F)). (H) shows resistance measurements of a bilayer. Even if a sharp peak is found at V_{CNP} for temperatures which are low enough, there are no abrupt changes of R depending on T, therefore it is not possible to identify T_c this way. (G) are the experimental values of n^* , fitted via the mean-field prediction shown in (F). A critical temperature is clearly identified as the one below which n^* is suppressed. In the inset of (G) we see the conductance measurements in log scale from which n^* is derived.

3.3 Measurement of the electron density

But how do we measure n_{th} ? First of all, we need to understand how n (conduction band induced density) can be derived from experimental data. This is obtained via the formula [3, 13, 15]

$$n = \alpha (V_g - V_{CNP}). \tag{3.1}$$

The α coefficient can be fixed using the quantum Hall effect (QHE). The sample is put in a strong magnetic field ~ 1*T* at low temperature ~ $10^{-1}K$. A voltage difference is held between two ends of the sample and both longitudinal σ_{xx} and transverse σ_{xy} conductivity are measured. If we plot these two quantities versus the filling factor $\nu = \frac{nh}{eB}$ we notice the presence of plateaux of σ_{xy} and sudden drops of σ_{xx} at certain integer values of ν , as shown in Fig.(3.4).

This fact can be understood as follows: in the presence of a magnetic field, the electrons organise themselves in Landau levels, which have a very large degeneracy, of order $\frac{eBA}{h}$. If B is large enough only a few of these levels are populated. The filling factor counts how many: in particular, band theory foresees that at $\nu = 2N$, where N is the number of layers, just one Landau level is filled. When ν hits one of these particular values, the Fermi level lies in a gap; we expect therefore the material to behave like an insulator, which accounts for the sudden drops in σ_{xx} . Moreover, it can be shown via topological arguments [7] that a material which is gapped in the bulk exhibits quantized values of σ_{xy} , accounting for the plateaux. What is relevant here is that the $\sigma(\nu)$ plots are universal with respect to B and n (i.e. V_g). In particular, the plateaux are given by $\sigma = \nu \frac{e^2}{h}$. Therefore, by collapsing the curves obtained using different values of V_g on top of one another, it is possible to obtain the α coefficient. Furthermore, the position of the first QHE plateau tells us how many layers compose the slab under examination, since the thickness is not a parameter under strict control during the fabrication of the sample.



Figure 3.4: [15] (A,B,C) are relative to a 4 terminal, 6 layer configuration, while (D,E,F) to a 2 terminal, 8 layer configuration. (A,D) show again the peak of resistance at V_{CNP} . (C,F) show QHE conductance, with the first plateau at $\nu = 2N$. (B) fan-diagram shows stationary points of longitudinal resistance (for fixed $\nu = 12$) characterised by constant $B(V_g)$ slope. This confirms the validity of Eq.(3.1). In (E) the fan-diagram is derived using $\frac{dG}{dV_a}$ since it is obtained in a 2 terminal configuration.

Let us now see how it is possible to measure n_{th} (B = 0). The experimenters undertook this approach: V_g is set at V_{CNP} $(n \sim 0)$ and conductance G is measured. Then V_g is varied until G starts to differ appreciably from its value at V_{CNP} . A logarithmic plot can be seen in Fig.(3.3). While n is small compared to n_{th} conductance is scarcely affected by changes in V_g . When $n \sim n_{th} G$ starts to grow. A threshold $n^*(T)$ is defined as the value of n such that G(n,t) = aG(0,T). It can be verified that the following analysis is not influenced by the arbitrariness of the choice of a^2 . Now it is possible to make a $n^*(T)$ plot and verify that it follows the behaviour found in Fig.(3.3).

Let us see how the theoretical $n_{th}(T)$ law is derived, as this is the main aim of the present work. That quantity is computed as follows:

$$n_{th}(T) = \int_0^\infty dE \ g(E,T)f(E,T)$$
 (3.2)

where $f(E,T) = \frac{1}{e^{\beta E}+1}$ is the Fermi-Dirac distribution and $g(E,T) = 4\nu_0 \frac{E}{\sqrt{E^2 - (\frac{\Delta(T)}{2})^2}}$ is the density of states. The $\Delta(T)$ law is obtained in a mean-field approximation, where electron-electron interaction gives rise to a staggered potential that changes sign from one layer to the other.³ It reads

$$\Delta(T) = \Delta_0 \tanh(1.74\sqrt{\frac{T_c}{T} - 1}), \quad \beta_c \Delta_0 = 1.76$$
(3.3)

The resulting n_{th} law's only free parameters are T_c and Δ_0 (the zero-temperature gap), which can be found by fitting the $n^*(T)$ curves with the theoretical prediction. The results of this analysis are summarized in Fig.(3.5).

As an important remark, let us point out that a similar analysis can be carried out for odd multilayers, too. This happens because the low-energy density of states of the additional Dirac band is negligible at the experimental temperatures. Therefore, n_{th} shows the same behaviour as in the even case, as

 $^{^{2}}a = 1.67$ is the value used in [14]. It is the one that gives $n^{*} = n_{th}$ for the bilayer.

³The details of the derivation have not been given by the authors of [14], by our present reckoning.



Figure 3.5: [14] (A) $n^*(T)$ for multilayers with N < 8 agrees with mean-field prediction. (B) The critical temperature (and zero-temperature gap) scales more or less linearly with respect to N. (C) $\Delta_0 \sim 1.76T_c$.

can be seen in Fig.(3.5). The main difference is that, due to the ungapped Dirac band, odd multilayers mantain finite resistivity at V_{CNP} .

Notice that, as it will be shown in this work, the staggered potential mean-field accounts for the facts that:

- all quadratic bands become gapped simultaneously, with the same gap;
- linear bands do not become gapped.

In fact, if the gap did not appear simultaneously in every quadratic band we should be able to see various critical temperatures in the n_{th} plots.

In conclusion, we can state that the experiment [14] found a second order phase transition to a brokensymmetry state for graphene multilayers with N < 8. The broken symmetry is spatial inversion, which is discrete, and therefore this finding does not conflict with the Mermin-Wagner theorem. In this state, quadratic bands become gapped simultaneously with the same gap amplitude, while linear bands do not. Critical temperature and zero-temperature gap are found to increase linearly with N. This is surprising, since the semimetallic behaviour of graphite $(N = \infty)$ implies the absence of a gap. Therefore we expect this relation to stop being valid at a certain N.

The purpose of all that follows will be to give as rigorous an explanation as possible for these facts, by deriving a staggered potential mean-field theory of multilayer graphene in the context of QFT.

Chapter 4

Low energy effective Hamiltonian

Let us briefly recall the results of chapter 2. The non-interacting, low energy Hamiltonian (for given spin and valley component) of Bernal stacked N-layer graphene is given by:

$$H(\vec{p}) = \begin{pmatrix} 0 & v\pi^{\dagger} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v\pi & 0 & t_{\perp} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t_{\perp} & 0 & v\pi^{\dagger} & 0 & t_{\perp} & 0 & 0 & 0 \\ 0 & 0 & v\pi & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t_{\perp} & 0 & v\pi^{\dagger} & 0 & 0 & 0 \\ 0 & 0 & t_{\perp} & 0 & v\pi & 0 & t_{\perp} & 0 & \ddots \\ 0 & 0 & 0 & 0 & 0 & v\pi^{\dagger} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & v\pi & 0 & \ddots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \ddots & 0 \end{pmatrix},$$
(4.1)

where $\pi = p_x + ip_y$. The Hilbert space \mathcal{H} basis is given by $(A_1, B_1, A_2, B_2, \ldots, A_N, B_N)$ (therefore $dim(\mathcal{H}) = 2N$), where X_i stands for the *i*-th layer's sublattice degree of freedom X. Only nearest neighbours are taken into account for both intralayer (*v* terms) and interlayer (t_{\perp} terms) tunneling.

4.1 Projection on low energy subspace

It is useful, for our purposes, to consider an effective Hamiltonian only tacking into account the lower lying energy bands, namely the ones that touch one another at $|\vec{p}| = 0$. This can be achieved via a projection operation.

The underlying idea is borrowed from perturbation theory: close to $|\vec{p}| = 0$ only interlayer t_{\perp} terms are relevant, while intralayer $\propto \pi$ are small. It is then possible to split up the Hilbert space in a high-energy subspace Q and low-energy one, \mathcal{P} .

Practically, the *n*-th basis vector belongs to the high-energy subspace if at least one entry in the *n*-th row (or column) of $H(\vec{p})$ is proportional to t_{\perp} , otherwise it belongs to the low-energy one. Of course we are interested in the projection of H on the low-energy subspace. According to perturbation theory, this can be achieved via

$$H_{eff} = H_{PP} - H_{PQ} H_{OQ}^{-1} H_{QP}.$$
(4.2)

A derivation of Eq.(4.2) can be found in Appendix A. If this procedure is applied to H we get $dim(\mathcal{P}) = dim(\mathcal{Q}) = N$

$$\mathcal{P} = \langle A_1, B_2, A_3, B_4, \dots \rangle, \mathcal{Q} = \langle B_1, A_2, B_3, A_4, \dots \rangle,$$

 $H_{PP}=0,$

$$H_{QQ} = t_{\perp} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & \ddots \\ 0 & 0 & 0 & \ddots & 0 \end{pmatrix},$$
$$H_{PQ} = \begin{pmatrix} v\pi^{\dagger} & 0 & 0 & 0 & 0 \\ 0 & v\pi & 0 & 0 & 0 \\ 0 & 0 & v\pi^{\dagger} & 0 & 0 \\ 0 & 0 & 0 & v\pi & 0 \\ 0 & 0 & v\pi^{\dagger} & 0 & 0 \\ 0 & 0 & v\pi^{\dagger} & 0 & 0 \\ 0 & 0 & v\pi^{\dagger} & 0 & 0 \\ 0 & 0 & v\pi^{\dagger} & 0 \\ 0 & 0 & 0 & v\pi^{\dagger} & 0 \\ 0 & 0 & 0 & 0 & \ddots \end{pmatrix}.$$

From now on we must discuss separately the even N layer case from the odd one. The reason for that is the fact that H_{QQ} is not invertible if N is odd, as it will be explained later on.

We could have foreseen that this procedure would not have succeeded in this case, as the resulting dimension of the low energy subspace $(dim(\mathcal{P}) = N)$ is different from the one we can infer by inspection of the spectrum (N + 1 low-lying bands), while in the even case it is correct (N low-lying bands).

4.1.1 Even N case

The inverse of H_{QQ} is given by

$$H_{QQ}^{-1} = t_{\perp}^{-1} \begin{pmatrix} 0 & 1 & 0 & -1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Please note that this matrix only features upper triangular elements in the odd rows (or even columns) and lower diagonal elements in the even rows (or odd columns).

As left (right) multiplication by a diagonal matrix barely rescales the rows (columns) of the correspondent diagonal factor, multiplying $H_{pq}H_{qq}^{-1}$ $(H_{qq}^{-1}H_{qp})$ just rescales upper triangular elements by $v\pi^{\dagger}$ and lower triangular elements by $v\pi$.

Therefore, the final H_{eff} in the even N layer is given by

$$H_{eff} = t_{\perp}^{-1} v^2 \begin{pmatrix} 0 & (\pi^{\dagger})^2 & 0 & -(\pi^{\dagger})^2 & 0 & (\pi^{\dagger})^2 & 0 \\ (\pi)^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & (\pi^{\dagger})^2 & 0 & -(\pi^{\dagger})^2 & 0 \\ -(\pi)^2 & 0 & (\pi)^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & (\pi^{\dagger})^2 & 0 \\ (\pi)^2 & 0 & -(\pi)^2 & 0 & (\pi)^2 & 0 & 0 \\ 0 & \ddots & 0 & \ddots & 0 & \ddots & 0 \end{pmatrix}$$
(4.3)

4.1.2 OddN case

After a closer inspection of H_{QQ} , one can see that its singularity is due to the presence of a 1dimensional kernel, generated by the vector

$$\vec{D} = \begin{pmatrix} 1 & 0 & -1 & 0 & 1 & \dots \end{pmatrix}. \tag{4.4}$$

Since $H_{QQ}\vec{D} = 0$, \vec{D} is actually a low-energy vector. As such, it should be put inside \mathcal{P} , recovering the dimensionality that can be inferred by looking at the original spectra.

The correct procedure in the odd N case then involves a change of basis with the following properties:

- one of the new basis vectors should be D;
- the new basis vectors should be orthonormal (unitarity).

Only after this preliminary step the procedure carried on for the even case can be properly utilized.

A possible choice for the new basis is the one obtained via orthonormalization of the set $(B_1, A_2, B_3, ..., D)$. This means that the new vectors $(D_1, D_2, D_3, ..., D)$ are iteratively obtained from the old ones as follows:

$$D'_{1} = B_{1} - D(D \cdot B_{1}) \qquad D_{1} = \frac{D'_{1}}{\sqrt{D'_{1} \cdot D'_{1}}}$$
$$D''_{2} = A_{2} - D(D \cdot A_{2}) \qquad D'_{2} = D''_{2} - D_{1}(D_{1} \cdot D''_{2}) \qquad D_{2} = \frac{D'_{2}}{\sqrt{D'_{2} \cdot D'_{2}}}$$

There could be a flaw in this procedure if the effective Hamiltonian depended on the particular change of basis we chose. Actually, this is not the case: let us apply to H_{eff} a unitary transformation which only acts on Ω (from which *D* has already been removed, so that we're only considering the ways of choosing the N-1 remaining orthonormal high-energy vectors).

$$\begin{pmatrix} \mathbb{I} & \mathbb{O} \\ \mathbb{O} & U^{\dagger} \end{pmatrix} \begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix} \begin{pmatrix} \mathbb{I} & \mathbb{O} \\ \mathbb{O} & U \end{pmatrix} = \begin{pmatrix} H_{PP} & H_{PQ}U \\ U^{\dagger}H_{QP} & U^{\dagger}H_{QQ}U \end{pmatrix}$$

If now we compute the transformed $(H')_{eff}$ we see that it is the same as the original one

$$(H')_{eff} = H_{PP} - H_{PQ}UU^{\dagger}H_{QQ}^{-1}UU^{\dagger}H_{QP} = H_{eff}.$$

This observation also allows us to not care about the particular change of basis in deriving the general form of H_{eff} .

If we carry on the outlined procedure using the proposed change of basis, we get the following for N = 3, 5, 7:

$$H' = A^{\dagger} H A$$

N = 3

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{-1}{\sqrt{2}} \end{pmatrix} \qquad H_{eff} = t_{\perp}^{-1} v^2 \begin{pmatrix} 0 & \frac{(\pi^{\dagger})^2}{2} & 0 & \frac{-t_{\perp}\pi^{\dagger}}{\sqrt{2}v} \\ \frac{(\pi)^2}{2} & 0 & \frac{(\pi)^2}{2} & 0 \\ 0 & \frac{(\pi^{\dagger})^2}{2} & 0 & \frac{t_{\perp}\pi^{\dagger}}{\sqrt{2}v} \\ \frac{-t_{\perp}\pi}{\sqrt{2}v} & 0 & \frac{t_{\perp}\pi}{\sqrt{2}v} & 0 \end{pmatrix}$$

N = 5

N = 7

Already from these first examples it is clear that the general form for the 2M - 1-layer H_{eff} is

$$H_{eff} = t_{\perp}^{-1} v^2 \begin{pmatrix} 0 & \frac{a_1(\pi^{\dagger})^2}{M} & 0 & -\frac{b_1(\pi^{\dagger})^2}{M} & \dots & \frac{z_1(\pi^{\dagger})^2}{M} & 0 & \frac{-t_{\perp}\pi^{\dagger}}{\sqrt{M}v} \\ \frac{a_1(\pi)^2}{M} & 0 & \frac{a_2(\pi)^2}{M} & \dots & -\frac{z_2(\pi)^2}{M} & 0 & \frac{z_1(\pi)^2}{M} & 0 \\ 0 & \frac{a_2(\pi^{\dagger})^2}{M} & 0 & \frac{a_{M-1}(\pi^{\dagger})^2}{M} & 0 & \frac{-z_2(\pi^{\dagger})^2}{M} & \vdots & \frac{t_{\perp}\pi^{\dagger}}{\sqrt{M}v} \\ \frac{-b_1(\pi)^2}{M} & \vdots & \frac{a_{M-1}(\pi)^2}{M} & 0 & \frac{a_{M-1}(\pi^{\dagger})^2}{M} & \vdots & \frac{a_2(\pi^{\dagger})^2}{M} & 0 \\ \vdots & \frac{-z_2(\pi^{\dagger})^2}{M} & 0 & \frac{a_{M-1}(\pi^{\dagger})^2}{M} & \vdots & \frac{a_2(\pi^{\dagger})^2}{M} & 0 & \frac{-t_{\perp}\pi^{\dagger}}{\sqrt{M}v} \\ \frac{z_1(\pi)^2}{M} & 0 & \frac{-z_2(\pi)^2}{M} & \dots & \frac{a_2(\pi)^2}{M} & 0 & \frac{a_1(\pi^{\dagger})^2}{M} & 0 \\ 0 & \frac{z_1(\pi^{\dagger})^2}{M} & \dots & \frac{-b_1(\pi^{\dagger})^2}{M} & 0 & \frac{a_1(\pi^{\dagger})^2}{M} & 0 & \frac{t_{\perp}\pi^{\dagger}}{\sqrt{M}v} \\ \frac{-t_{\perp}\pi}{\sqrt{M}v} & 0 & \frac{t_{\perp}\pi}{\sqrt{M}v} & 0 & \frac{-t_{\perp}\pi}{\sqrt{M}v} & 0 \end{pmatrix} \end{pmatrix}$$
(4.5)

where we stress that the submatrix corresponding to all vectors except D is Hermitian-symmetric with respect to the secondary diagonal.

This allows us to study the $a_1, \ldots, z_1, a_2, \ldots, z_2, \ldots, a_{M-1}$ coefficients only in one of the four triangular sectors which arise because of that symmetry (let's say the north one). Let's represent those coefficient in triangles according to their position in the matrix. The triangles represent, respectively,

1

1



the N = 3, 5, 7, 9, 11 cases. We can infer that the first row contains the numbers from 1 to M - 1 in reverse order, and odd columns are filled with that number. Every even row is filled with only one number, starting from 1 in the second row and then increasing.

4.2 Hamiltonian in block diagonal form

We will discuss the opportunity of casting the effective Hamiltonians we just obtained into a more readable form by means of a change of basis. In particular, the transformed Hamiltonians will be block diagonal, the blocks being given by bilayer or monolayer effective Hamiltonians. Each subsystem has the correct effective mass in order to yield the multilayer spectrum.

In [6] a new basis $\{\Phi\}$ for \mathcal{H} is described. Let us define the functions:

$$f_m(j) = \frac{2}{\sqrt{N+1}} \sin\left(\frac{\pi}{2}j\right) \cos\left(\frac{m\pi}{2(N+1)}j\right)$$
$$g_m(j) = \frac{2}{\sqrt{N+1}} \cos\left(\frac{\pi}{2}j\right) \sin\left(\frac{m\pi}{2(N+1)}j\right)$$

where j = 1, ..., N is the layer index and m is the subsystem index

$$m = \begin{cases} 1, 3, 5, \dots, N-1, & \text{if } N = even \\ 0, 2, 4, \dots, N-1, & \text{if } N = odd \end{cases}$$

Notice that $f_m(j) = 0$ if j = even, while $g_m(j) = 0$ if j = odd. The basis $\{\Phi\}$ is defined as follows:

$$\begin{aligned} |\phi_m^{(A,odd)}\rangle &= f_m(1)|A_1\rangle + f_m(3)|A_3\rangle + \dots \\ |\phi_m^{(B,odd)}\rangle &= f_m(1)|B_1\rangle + f_m(3)|B_3\rangle + \dots \\ |\phi_m^{(A,even)}\rangle &= g_m(2)|A_2\rangle + g_m(4)|A_4\rangle + \dots \\ |\phi_m^{(B,even)}\rangle &= g_m(2)|B_2\rangle + g_m(4)|B_4\rangle + \dots \end{aligned}$$

Let us call U the matrix of the change of basis, that is the one whose columns are the vectors belonging to $\{\Phi\}$ expressed in the old basis. Of course $U^{\dagger}U = UU^{\dagger} = \mathbb{I}$ (unitary). As described in [6] the transformed full Hamiltonian matrix $H' = U^{\dagger}HU$ is block diagonal. The blocks give a decomposition in subsystems, whose index is m. If $m \neq 0$ the block relative to $\{|\phi_m^{(A,odd)}\rangle, |\phi_m^{(B,odd)}\rangle, |\phi_m^{(B,even)}\rangle\}$

is given by

$$H_m(ec{p}) = egin{pmatrix} 0 & v\pi^\dagger & 0 & 0 \ v\pi & 0 & \lambda_m t_\perp & 0 \ 0 & \lambda_m t_\perp & 0 & v\pi^\dagger \ 0 & 0 & v\pi & 0 \end{pmatrix}$$

where $\lambda_m = 2 \cos\left(\frac{\pi}{2} - \frac{m\pi}{2(N+1)}\right)$. H_m is a bilayer Hamiltonian, with an effective mass

$$m_m = \frac{\lambda t_\perp}{2v^2} = \frac{t_\perp}{v^2} \cos\left(\frac{\pi}{2} - \frac{m\pi}{2(N+1)}\right)$$

It can be verified that if we set m = 2r - (N + 1) we recover the expression for m_r already found in Eq.(2.13). The case m = 0 only exists if N = odd, and has the peculiarity that $g_0(j) = 0$. Therefore, the corresponding block is a 2 by 2 matrix, relative to the $\{|\phi_0^{(A,odd)}\rangle, |\phi_0^{(B,odd)}\rangle\}$ subspace, and reads

$$H_{m=0}(\vec{p}) = \begin{pmatrix} 0 & v\pi^{\dagger} \\ v\pi & 0 \end{pmatrix}.$$

This is a monolayer Hamiltonian, with the usual Fermi velocity v.

Now, let us apply the procedure to extract the effective Hamiltonian to the block diagonal H'. As the procedure applies block by block, the bilayers are going to yield

$$H_{m,eff}(\vec{p}) = \begin{pmatrix} 0 & \frac{(\pi^{\dagger})^2}{2m_m} \\ \frac{(\pi)^2}{2m_m} & 0 \end{pmatrix},$$

while the monolayer block is left untouched. But what if we apply instead the change of basis U directly on an effective Hamiltonian H_{eff} ? We are going to see that, thanks to the peculiar properties of $\{\Phi\}$ the result is the same. In other words, the projection commutes with the change of basis.

The important property of U is that its action leaves the A_{odd} , B_{odd} , A_{even} , B_{even} subspaces unvaried. Therefore, it can be written as a tensor product of operators acting on the subspaces $U = U_{A,odd} \otimes U_{B,odd} \otimes U_{A,even} \otimes U_{B,even}$. Let us call L the projection operation that we used to extract the effective Hamiltonian $H_{eff} = L(H)$ from the full one H. We now prove that L commutes with the change of basis U. Let us recall that

$$\mathcal{P} = A_{odd} \oplus B_{even} \quad \mathcal{Q} = A_{even} \oplus B_{odd}.$$

then it is also true that

$$U = U_P \otimes U_Q = (U_{A,odd} \otimes U_{B,even}) \otimes (U_{A,even} \otimes U_{B,odd}).$$

If we apply the change of basis to the full Hamiltonian H

$$H' = \begin{pmatrix} U_P^{\dagger} & \mathbb{O} \\ \mathbb{O} & U_Q^{\dagger} \end{pmatrix} \begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix} \begin{pmatrix} U_P & \mathbb{O} \\ \mathbb{O} & U_Q \end{pmatrix} = \begin{pmatrix} U_P^{\dagger} H_{PP} U_P & U_P^{\dagger} H_{PQ} U_Q \\ U_Q^{\dagger} H_{QP} U_P & U_Q^{\dagger} H_{QQ} U_Q \end{pmatrix}$$

and subsequently apply the projection L

$$L(H') = U_P^{\dagger} H_{PP} U_P - (U_P^{\dagger} H_{PQ} U_Q) (U_Q^{\dagger} H_{QQ}^{-1} U_Q) (U_Q^{\dagger} H_{QP} U_P) = U_P^{\dagger} (H_{PP} - H_{PQ} H_{QQ}^{-1} H_{QP}) U_P = L(H)' \quad (4.6)$$

we get the desired result. This means that if we apply U_P to the even N-layer effective Hamiltonian $H_{eff} = L(H)$ we are going to obtain the projection of the block diagonal H'. We specified that N has to be even, because in the odd case we have to remember that before applying L we performed another change of basis. Nevertheless, a similar result holds, and the proof can be found in Appendix B.

In conclusion, we can state that if the change of basis is applied either after or before the projection, the resulting block-diagonal Hamiltonian is the same, and reads

where $m_r = t_{\perp} v^{-2} |\cos(\frac{r\pi}{N+1})|$, and the *SLG* block appears only if N = odd.

4.2.1 Staggered potential

As we shall see later, the mean-field approach we follow gives rise to a uniform potential that changes sign from one layer to the next. The quantity accounting for that will be a matrix $\tau_3 = diag(1, 1, -1, -1, ..., 1, 1, -1, -1)$ in the full basis $(A_1, B_1, A_2, B_2, ..., A_N, B_N)$.

It is useful to point out some properties of τ_3 . Firstly, since the transformation which brings the Hamiltonian in block-diagonal form does not mix different layers, the transformed $\tau'_3 = U^{\dagger} \tau_3 U$ is given by

 $\tau'_3 = diag(1, 1, -1, -1, ..., 1, 1, -1, -1, 1, 1)$ where last 2 by 2 block is relative to the SLG subsystem. This block is the identity because this subsystem is made up of odd layered vectors. Then, by projecting to the low energy subspace we get $L(\tau'_3) = diag(1, -1, ..., 1, -1, 1, 1)$, as half of the bilayers' basis vectors are thrown away, while the monolayer subspace is left as is.

4.3 Valley-spin simmetry

Up to now only one valley was kept into account in writing the multilayer Hamiltonian, that is, only momenta close to the Dirac point \vec{K} were considered.

For this reason we will refer to H_0 in Eq.(4.7) as $H_0^{(K)}$, and to the total Hamiltonian as H_0 from now on. If we include also the momenta that are close to K' we get

$$H_{0}(\vec{p}) = \begin{pmatrix} H_{0}^{(K)}(\vec{p}) & \mathbb{O} \\ \mathbb{O} & H_{0}^{(K')}(\vec{p}) \end{pmatrix} = \begin{pmatrix} H_{0}^{(K)}(\vec{p}) & \mathbb{O} \\ \mathbb{O} & T(H_{0}^{(K)}(\vec{p})) \end{pmatrix}$$
(4.8)

where T identifies the time-reversal operator. Its action on a single valley is $T(H_0^{(\alpha)}(\vec{p})) = H_0^{(\alpha)*}(\vec{-p})$, because time reversal is an anti-unitary operator that inverts momenta. If T operates on valley space it exchanges the valleys, so $H_0 = T(H_0)$ is time-reversal invariant, as should be.

It is possible to perform a unitary transformation U on H_0 so that it becomes manifestly invariant with respect to rotations in the valley-spin subspace. This transformation can be written as follows

$$U = \frac{1+\eta_3}{2} + \frac{1-\eta_3}{2}M \tag{4.9}$$

where η_i , σ_i stand for Pauli matrices for the valley and spin index, respectively. M is a matrix in layer/sublattice space, given by

$$M = \tau_1 \otimes \tau_1 \otimes \ldots \otimes \tau_2$$

where τ_i is a Pauli matrix relative to a bilayer (τ_1) or monolayer subsystem (τ_2) .

The action of U in each subsystem is transposition, but only in the K' subspace. Moreover, if the subsystem is SLG, the sign is changed. Therefore $U^{\dagger}H_0^{(K')}(\vec{p})U = (H_0^{(K')}(-\vec{p}))^T = (H_0^{(K')}(-\vec{p}))^* = T(H_0^{(K')}(\vec{p}))$, where last two equalities are obtained thanks to Hermitianity. It follows that

$$\tilde{H}_{0}(\vec{p}) = U^{\dagger} H_{0}(\vec{p}) U = \begin{pmatrix} H_{0}^{(K)}(\vec{p}) & \mathbb{O} \\ \mathbb{O} & T(T(H_{0}^{(K)}(\vec{p}))) \end{pmatrix} = \begin{pmatrix} H_{0}^{(K)}(\vec{p}) & \mathbb{O} \\ \mathbb{O} & H_{0}^{(K)}(\vec{p}) \end{pmatrix},$$

which is the desired result.

It is remarkable that in this case, the action of time-reversal (an anti-unitary operator) on H is reproduced by a unitary operator.

Let us conclude by looking at the action of the spin-valley transformation on the projected staggered potential matrix $L(\tau'_3)$. It can be easily seen that $U^{\dagger}L(\tau'_3)U = diag(-1, 1, ..., -1, 1, 1, 1)$ as the τ_1 2 by 2 matrices acting on BLG blocks exchange 1 with -1, while the τ_2 matrix acting on the SLG block (which is the identity) leaves it unvaried.

Chapter 5

Interaction Hamiltonian

Up to now we neglected the presence of electrostatic repulsion between electrons, focusing on the description of multilayer graphene from the point of view of band theory. Coulomb interaction between electrons can be introduced by adding a V term to the Hamiltonian $H = H_0 + V$. Following [8], V can be written as¹

$$V = \frac{1}{2L^2} \sum_{\vec{q}, ij} \rho_i(\vec{q}) V(q; z_i - z_j) \rho_j(-\vec{q}),$$
(5.1)

where i, j are layer indices and

$$V(q;z) = \int dxdy \ V(x,y,z)e^{-i(q_x x + q_y y)} = \frac{2\pi}{\kappa q}e^{-q|z|}$$
(5.2)

is the planar Fourier transform of the Coulomb potential, while

$$\rho_i(\vec{q}) = \sum_{\vec{k}\sigma\eta X_i} c^{\dagger}_{\sigma\eta X_i}(\vec{k} + \vec{q}) c_{\sigma\eta X_i}(\vec{k})$$
(5.3)

where X_i is the sublattice index for layer i, σ is the spin index and η the valley index. κ is the relative dielectric constant of the system.

5.1 Weak-coupling limit

Let us introduce the typical length scale of interactions, given by

$$a_0 = \frac{\hbar^2 \kappa}{M e^2}.\tag{5.4}$$

As we will see later, this is the RPA screening length for the multilayer. This means that, due to the presence of the other electrons, the electrostatic field due to an electron is exponentially suppressed on a distance of order a_0 . M is the sum of all bilayer effective masses

$$M = \sum_{r=1}^{\left\lfloor \frac{N}{2} \right\rfloor} m_r.$$
(5.5)

We shall assume $(N-1)d \ll a_0$ where $d \sim 3.5 \text{\AA}$ is the interlayer distance. In this way, for the purposes of interactions, it is as if the multilayer thickness were zero. As we will see, this weak-coupling approximation [11] is not adequate. In fact, as shown in the plot 5.1 the thickness to screening length ratio is far from being a small number.

¹The multilayer's planar directions are x, y while different planes are identified by their z position.



Figure 5.1: Multilayer thickness d(N-1) to screening length a_0 ratio. Weak coupling approximation $\frac{d(N-1)}{a_0} \ll 1$ is not adequate.

Nevertheless it is instructive to see where this line of reasoning is bringing us, and possibly amend this inconsistency later.

Let us cast V into matrix form:

$$V = \frac{1}{2L^2} \sum_{q,ij} \rho_i(\vec{q}) \frac{2\pi}{\kappa q} \begin{pmatrix} 1 & e^{-qd} & e^{-2qd} & \dots & e^{-(N-1)qd} \\ e^{-qd} & 1 & e^{-qd} & \dots & e^{-(N-2)qd} \\ & & \ddots & & \\ e^{-(N-1)qd} & \dots & e^{-2qd} & e^{-qd} & 1 \end{pmatrix}_{ij} \rho_j(-\vec{q}).$$
(5.6)

As $q \sim \frac{1}{a_0}$, the weak-coupling approximation yields

$$V = \frac{1}{2L^2} \sum_{q,ij} \rho_i(\vec{q}) \frac{2\pi}{\kappa q} \begin{pmatrix} 1 & 1 & \dots & 1\\ 1 & 1 & \dots & 1\\ & \ddots & \\ 1 & 1 & \dots & 1 \end{pmatrix}_{ij} \rho_j(-\vec{q}) = \frac{1}{2L^2} \sum_{q,ij} \frac{2\pi}{\kappa q} \rho_i(\vec{q}) \rho_j(-\vec{q}),$$
(5.7)

which is the result of keeping only the biggest eigenvalue of $V(q; z_i - z_j)$.

5.2 Projection to lower energy subspace

As we are considering only a certain subspace of \mathcal{H} in order to work with an effective low energy non-interacting Hamiltonian H_{eff} , we should do the same for the V term.

In order to do that we can exploit the fact that in the weak-coupling approximation, the interaction term is invariant with respect to unitary transformations in the layer/sublattice space. In fact, if $c_{\sigma\eta X_i}(\vec{p}) = \sum_{j,Y_j} U_{X_i,Y_j} d_{\sigma\eta Y_j}(\vec{p})$, then

$$\begin{split} \sum_{i} \rho_{i}(\vec{q}) &= \sum_{i} \sum_{p\sigma\eta X_{i}} c^{\dagger}_{\sigma\eta X_{i}}(\vec{p} + \vec{q}) c_{\sigma\eta X_{i}}(\vec{p}) = \\ &\sum_{i,j,k} \sum_{p\sigma\eta} \sum_{X_{i},Y_{j},Z_{k}} d^{\dagger}_{\sigma\eta Z_{k}}(\vec{p} + \vec{q}) U^{\dagger}_{Z_{k},X_{i}} U_{X_{i},Y_{j}} d_{\sigma Y_{j}}(\vec{p}) = \sum_{i} \sum_{p\sigma\eta X_{i}} d^{\dagger}_{\sigma\eta X_{i}}(\vec{p} + \vec{q}) d_{\sigma\eta X_{i}}(\vec{p}). \end{split}$$

Therefore, we can do any change of basis we like without complicating the interaction term, as would not be the case if we did not use the weak-coupling approximation. The same result holds for spin and valley unitary transformations.

In order to obtain H in the most suitable form, we can proceed this way: first we make the change of basis shown in section 4.2, that is the one to obtain H_0 in block diagonal form, and then project the

Hamiltonian to the low energy subspace \mathcal{P} . For the interacting term, this just consists in throwing away half of the basis' vectors for the bilayers, while the monolayer subsystem does not require further manipulations. In fact if $\mathcal{H}_{BLG} = \langle A_1, B_1, A_2, B_2 \rangle$ then $\mathcal{P}_{BLG} = \langle A_1, B_2 \rangle$. It is sufficient to consider only V_{PP} because $V_{PQ} = V_{QP} = 0$, as interaction cannot change electrons' X_i degree of freedom.

Finally we perform the valley/spin transformation described in section 4.3. Since the sublattice and layer degrees of freedom are not independent anymore, we can represent the projection by simply merging the i, X_i into one index i, together with σ and η . In fact, now neither H_0 nor V depend on spin and valley indices. This index runs i = 1, ..., 4N if N = even and i = 1, ..., 4(N + 1) if N = odd. The final form of the Hamiltonian is therefore

$$H = \sum_{i,j,\vec{p}} c_i^{\dagger}(\vec{p}) H_0(\vec{p})_{ij} c_j(\vec{p}) + \frac{1}{2L^2} \sum_{\vec{q},ij} \frac{2\pi}{\kappa q} \rho_i(\vec{q}) \rho_j(-\vec{q})$$
(5.8)

where $\rho_i(q)$ has been renamed to

$$\rho_i(\vec{q}) = \sum_{\vec{k}} \sum_{\sigma\eta} c^{\dagger}_{X_i \sigma\eta}(\vec{k} + \vec{q}) c_{X_i \sigma\eta}(\vec{k}).$$
(5.9)

5.3 RPA static screening

From now on, unless \hbar appears explicitly in a formula, it is assumed $\hbar = 1$. After all the described approximations have been done, we are left with the interaction term

$$V = \frac{1}{2L^2} \sum_{\vec{q}} \rho_{-\vec{q}} V(q) \rho_{\vec{q}}$$

where

$$\rho_{\vec{q}} = \sum_{i} \rho_i(\vec{q}), \quad V(q) = \frac{2\pi e^2}{\kappa q}.$$
(5.10)

It is possible to greatly simplify the problem by considering the static, long wavelength limit of RPA screening [11]. Let us recall [5] that RPA approximation consists in substituting the relative dielectric constant κ with the dielectric function $\kappa(q)$, given by

$$\kappa(q) = 1 - \frac{2\pi e^2}{\kappa^{(b)}q} \Pi(q),$$

where $q = (\omega_m, \vec{q}), \kappa^{(b)}$ is the background relative dielectric constant and the polarizability $\Pi(q)$ is computed as follows

$$\Pi(q) = \frac{g}{\beta L^2} \sum_{p} tr[G(p)G(p+q)]$$
(5.11)

where $p = (\omega_n, \vec{p}), g = 4$ is the degeneracy factor due to spin and valley indices, and G(p) is the free Green function

$$G(p) = (-i\omega_n + H_0(\vec{p}))^{-1}$$

Please note that if ω_n are fermionic Matsubara frequencies, then ω_m must be bosonic in order for G(p+q) to be non-zero.

In the static, long-wavelength limit $(\frac{\omega}{q} \to 0, q \to 0)$, if $\Pi(0, \vec{0})$ is non-zero, the effective interaction V becomes constant and will be called $\lambda = -\frac{1}{\Pi(0,\vec{0})}$ from now on. The resulting Hamiltonian is

$$H = \sum_{i,j,\vec{p}} c_i^{\dagger}(\vec{p}) H_0(\vec{p})_{ij} c_j(\vec{p}) + \frac{\lambda}{2L^2} \sum_{\vec{q},ij} \rho_i(\vec{q}) \rho_j(-\vec{q}).$$
(5.12)

It will prove useful to compute the polarizability for both bilayer and monolayer graphene. In fact, the general case has been reduced to a set of bilayers and monolayers via a change of basis.

5.3.1 Bilayer graphene

We recall that in this case the relevant Hamiltonian is given by

$$H_0 = \begin{pmatrix} 0 & \frac{(\pi^{\dagger})^2}{2m} \\ \frac{(\pi)^2}{2m} & 0 \end{pmatrix}.$$

It follows that

$$G(p) = \frac{1}{\omega_n^2 + \frac{|\vec{p}|^4}{4m^2}} \begin{pmatrix} i\omega_n & \frac{(\pi^\dagger)^2}{2m} \\ \frac{(\pi)^2}{2m} & i\omega_n \end{pmatrix}.$$

Let us compute the trace in Eq.(5.11):

$$\Pi(\omega_m, \vec{q}) = \frac{g}{\beta L^2} \sum_{\omega_n, \vec{p}} \frac{2((i\omega_n)(i\omega_{n+m}) + Re(\frac{\pi^2(\pi^{\dagger} + \sigma^{\dagger})^2}{4m^2}))}{(\omega_n^2 + \frac{|\vec{p}|^4}{4m^2})(\omega_{n+m}^2 + \frac{|\vec{p} + \vec{q}|^4}{4m^2})}$$

where $\sigma = q_x + iq_y$. It is possible to verify that

$$Re(\pi^{2}(\pi^{\dagger} + \sigma^{\dagger})^{2}) = |\vec{p}|^{2}|\vec{p} + \vec{q}|^{2} - 2|(\vec{p}) \wedge (\vec{p} + \vec{q})|^{2} = |\vec{p}|^{2}|\vec{p} + \vec{q}|^{2}\cos(2\theta),$$

 θ being the angle between \vec{p} and $\vec{p} + \vec{q}$. Therefore,

$$\Pi(\omega_m, \vec{q}) = \frac{g}{\beta L^2} \sum_{\omega_n, \vec{p}} \frac{2((i\omega_n)(i\omega_{n+m}) + \frac{|\vec{p}|^2}{2m} \frac{|\vec{p}+\vec{q}|^2}{2m} \cos(2\theta))}{(i\omega_n + \frac{|\vec{p}|^2}{2m})(i\omega_n - \frac{|\vec{p}|^2}{2m})(i\omega_{n+m} + \frac{|\vec{p}+\vec{q}|^2}{2m})(i\omega_{n+m} - \frac{|\vec{p}+\vec{q}|^2}{2m})}$$

Let us now evaluate the sum on Matsubara frequencies by means of the formula

$$\frac{1}{\beta} \sum_{\omega_n} f(i\omega_n) = \sum_k \operatorname{Res}_{z=z_k} [n(z)f(z)], \qquad (5.13)$$

1 → 2 1 → 1 → 2

where z_k are the poles of f(z). After some tedious but straightforward algebra² we are left with the result found in [5], namely

$$\Pi(\vec{q},\omega_m) = \frac{g}{L^2} \sum_{\vec{p},s,s'} \frac{n(\epsilon_s(\vec{p})) - n(\epsilon_{s'}(\vec{p}+\vec{q}))}{i\omega_m + \epsilon_s(\vec{p}) - \epsilon_{s'}(\vec{p}+\vec{q})} F_{ss'}(\vec{p},\vec{q})$$
(5.14)

where $s, s' = \pm 1$ are band indices,

$$F_{ss'}(\vec{p}, \vec{q}) = \frac{1 + ss'\cos(2\theta)}{2} \quad \epsilon_s(\vec{p}) = s\frac{|\vec{p}|^2}{2m}$$

Let us evaluate $\Pi(0, \vec{q})$, which is the relevant quantity in the static approximation. If we plug everything back into Eq.(5.14) and use a continuum limit for the momentum sum, we get the integral

$$\Pi(0,\vec{q}) = -\frac{2g}{(2\pi\hbar)^2} \int d^2\vec{p} \frac{\sin^2\theta}{\frac{|\vec{p}|^2}{2m} + \frac{|\vec{p}+\vec{q}|^2}{2m}}$$

We can make use of

$$\cos\theta = \frac{|\vec{p}| + |\vec{q}|\cos\phi}{|\vec{p} + \vec{q}|}$$

$$\Pi(\omega_m, \vec{q}) = \sum_{\omega_n, \vec{p}} \frac{2((i\omega_n)(i\omega_{n+m})(\sin^2\theta + \cos^2\theta) + \frac{|\vec{p}|^2}{2m} |\vec{p} + \vec{q}|^2}{(i\omega_n + \frac{|\vec{p}|^2}{2m})(i\omega_n - \frac{|\vec{p}|^2}{2m})(i\omega_{n+m} + \frac{|\vec{p} + \vec{q}|^2}{2m})(i\omega_{n+m} - \frac{|\vec{p} + \vec{q}|^2}{2m})}$$

²Computations are quite easy if we rewrite the polarizability this way:

which is obtained by expanding the product $\vec{p} \cdot (\vec{p} + \vec{q})$ in terms of θ , the angle between \vec{p} and $\vec{p} + \vec{q}$, and ϕ , the angle between \vec{p} and \vec{q} . This way the integral can be rewritten to yield

$$\Pi(0,\vec{q}) = -\frac{2g}{(2\pi\hbar)^2} \int_0^\infty dp \ p \int_0^{2\pi} d\phi \frac{|\vec{q}|^2 \sin^2 \phi}{|\vec{p} + \vec{q}|^2} \frac{1}{\frac{|\vec{p}|^2}{2m} + \frac{|\vec{p} + \vec{q}|^2}{2m}}$$

Then, it is possible with some algebra to arrive at

$$\Pi(0,\vec{q}) = -\frac{(2g)(2m)q^2}{(2\pi\hbar)^2} \int_0^\infty dp \; \frac{1}{p} \left[\frac{1}{p^2 + q^2} \int_0^{2\pi} d\phi \frac{\sin^2 \phi}{1 + B\cos \phi} - \frac{1}{2p^2 + q^2} \int_0^{2\pi} d\phi \frac{\sin^2 \phi}{1 + B'\cos \phi} \right] (5.15)$$
$$B = \frac{2pq}{p^2 + q^2} \quad B' = \frac{2pq}{2p^2 + q^2}.$$

Let us evaluate the $d\phi$ integral. By means of $z = e^{i\phi}$, it can be brought in the form of a line integral in the complex plane. The circuit is the unitary circle \mathcal{C}_1 .

$$\int_{0}^{2\pi} d\phi \frac{\sin^2 \phi}{1 + B \cos \phi} = \frac{i}{2B} \int_{\mathcal{C}_1} dz \ \frac{z^2 - 2 + z^{-2}}{z^2 + \frac{2}{B}z + 1}$$

In order to apply the residue formula, namely

$$\int_{\partial A} dz f(z) = 2\pi i \sum_{z_k \in A} \operatorname{Res}_{z = z_k} f(z), \qquad (5.16)$$

where z_k are the poles of f(z), we must first show the poles of the integrand explicitly.

$$\frac{i}{2B} \int_{\mathcal{C}_1} dz \, \frac{z^2 - 2}{(z - C)(z - D)} + \frac{A_1 z + A_2}{(z - C)(z - D)} + \frac{B_1}{z} + \frac{B_2}{z^2},$$
$$C = -\frac{1}{B} - \sqrt{\frac{1}{B^2} - 1}, \quad D = -\frac{1}{B} + \sqrt{\frac{1}{B^2} - 1},$$
$$A_1 = \frac{2}{B}, \quad A_2 = \frac{4}{B^2} - 1, \quad B_1 = -\frac{2}{B}, \quad B_2 = 1.$$

As 0 < B, B' < 1, we find that z = C is outside C_1 , while z = D and z = 0 are poles inside C_1 . It is easily shown that the double pole in z = 0 gives a null contribution:

$$\int_{\mathcal{C}_1} \frac{dz}{z^2} = i \int_0^{2\pi} d\phi e^{-i\phi} = 0.$$

Finally, by making use of the residue formula Eq.(5.16) we get the result

$$\frac{2\pi}{B}(\frac{1}{B} - \sqrt{\frac{1}{B^2} - 1}).$$

Once we plug this back in the original integral in Eq.(5.15) we get (after some manipulations)

$$-\nu_0 \int_0^\infty dp \frac{1}{p} (1+|1-\frac{q^2}{p^2}| - \sqrt{4+\frac{q^4}{p^4}})$$

where $\nu_0 = \frac{m}{2\pi\hbar^2}$ is the bilayer density of states for a single spin-valley species. Under $x = \frac{p}{q}$ the expression becomes manifestly constant with respect to q

$$-\nu_0 \int_0^\infty dx \frac{1}{x} (1+|1-\frac{1}{x^2}| - \sqrt{4+\frac{1}{x^4}})$$

It can be verified that the indefinite integral is given by

$$F(x) = -\sqrt{1 + \frac{1}{4x^4}} + \operatorname{arcsinh}(2x^2) - \begin{cases} \frac{1}{2x^2} + \log(x^2), & \text{if } x \ge 1\\ -\frac{1}{2x^2}, & \text{if } x < 1 \end{cases}$$

The final result is the one that can be found in [5], that is

$$\Pi(0, \vec{q}) = -g\nu_0 \log 4 \tag{5.17}$$

which in turn gives rise to $\lambda = \frac{1}{4\nu_0 \log 4}$, as found in [11].

5.3.2 Monolayer graphene

Let us start with the graphene Hamiltonian, namely

$$H_0 = \begin{pmatrix} 0 & v\pi^{\dagger} \\ v\pi & 0 \end{pmatrix}.$$

The corresponding free Green function is therefore

$$G(p) = \frac{1}{v^2 p^2 - (i\omega_n)^2} \begin{pmatrix} i\omega_n & v\pi^{\dagger} \\ v\pi & i\omega_n \end{pmatrix}.$$

Let us compute the trace in Eq.(5.11):

$$\Pi(\omega_m, \vec{q}) = \frac{g}{\beta L^2} \sum_{\omega_n, \vec{p}} \frac{2((i\omega_n)(i\omega_{n+m}) + v^2 \vec{p} \cdot (\vec{p} + \vec{q}))}{(i\omega_n - v|\vec{p}|)(i\omega_n + v|\vec{p}|)(i\omega_{n+m} + v|\vec{p} + \vec{q}|)(i\omega_{n+m} - v|\vec{p} + \vec{q}|)}$$

Once again, we evaluate the sum on Matsubara frequencies by means of Eq.(6.4). By defining $\theta = 2\xi$ the algebra is the same as in the bilayer case.

In fact, the result is still given by Eq.(5.14), but now

$$F_{ss'}(\vec{p},\vec{q}) = \frac{1 + ss'\cos(2\xi)}{2} \quad \epsilon_s(\vec{p}) = sv|\vec{p}|$$

This time we shall limit ourselves at showing the result of the needed computations, that is [5]

$$\Pi(0,\vec{q}) = g\nu_0^{SLG} \frac{\pi}{8} \tag{5.18}$$

where $\nu_0^{SLG} = \frac{q}{2\pi\hbar^2 v}$ is SLG density of states. Notice that in this case $\Pi(0, \vec{0}) = 0$.

5.3.3 Multilayer graphene

As H_0 is block-diagonal, so is G. Therefore, Eq.(5.11) can be written as sum of bilayers $G^{(r)}$ and monolayer G^{SLG} Green functions

$$\Pi(q) = \frac{g}{\beta L^2} \sum_{r,p} \left(tr[G^{(r)}(p)G^{(r)}(p+q)] + tr[G^{SLG}(p)G^{SLG}(p+q)] \right)$$
$$= -g \log 4 \sum_{r=1}^{\lfloor \frac{N}{2} \rfloor} \nu_0^{(r)} + \Pi^{SLG}(0, \vec{q}). \quad (5.19)$$

If now we take the static, long wavelength limit, we get that the SLG contribution disappears, leaving behind

$$\lambda = \frac{1}{g\nu_0^{NLG}\log 4} \tag{5.20}$$

where $\nu_0^{NLG} = \sum_{r=1}^{\lfloor \frac{N}{2} \rfloor} \nu_0^{(r)}$ is the multilayer total density of states (for a single species).

Chapter 6

Mean-field theory

We now proceed to compute the gap amplitude of the ground state, by applying the procedure described in [11] for bilayers to multilayers. The problem is tackled in the functional integral formalism.

Firstly, a Hubbard-Stratonovich transformation is performed on the partition function, which decouples the interaction term by adding a new field that encodes the physically relevant features of the theory. Then the original fields are integrated out, leaving behind an effective action for the new field. Finally, the gap equation is derived by finding the action's stationary points.

The equation is then solved by providing an ansatz for ground state, that is tailored to make the staggered potential we mentioned in chapter 3 appear in the mean-field Hamiltonian.

Let us point out that, while in [14,15] Δ stands for the full gap, we adopt the convention found in [11], where the energy gap is 2Δ .

6.1 Bilayer graphene

Let us first review how to extract a mean field theory for bilayer graphene in the presence of Coulomb interaction [11].

In particular we shall consider a theory in which Coulomb interaction is statically screened, as previously described in chapter 5.

The partition function can be expressed in the functional integral formalism with Euclidean time

$$Z = \int D\psi^{\dagger} D\psi \, exp(-\int dx \, \mathcal{L}[\psi^{\dagger}(x), \psi(x)])$$

where $x = (t, \vec{r}), dx = dt d^2 \vec{r}$. The ψ fields are fermionic (Grassmann) fields and the Lagrangian is given by

$$\begin{aligned} \mathcal{L} &= \psi^{\dagger}(\partial_t + H_0)\psi + \sum_{j,k=1,\dots,8} \frac{\lambda}{2} \psi_j^{\dagger} \psi_k^{\dagger} \psi_k \psi_j \\ &= \psi^{\dagger}(\partial_t + H_0)\psi - \frac{\lambda}{2} Tr(\rho^{\dagger}\rho) \end{aligned}$$

where j, k are combined layer/flavour¹ indices, H_0 is the non interacting Hamiltonian and $\rho_{ij} = \psi_i^{\dagger} \psi_j$. Note that $\rho^{\dagger} = \rho$, in fact

$$\rho_{ij}^{\dagger} = (\psi_j^{\dagger}\psi_i)^{\dagger} = \psi_i^{\dagger}\psi_j^2.$$

 $^{^1\}mathrm{As}\ H$ is isotropic in spin/valley space, we can refer to them collectively as flavour.

²Remember that for two complex Grassmann variables the following equality holds: $(\xi^{\dagger}\eta)^{\dagger} = \eta^{\dagger}\xi$

The λ coupling constant represents the statically screened Coulomb interaction, which in the RPA approximation takes the value $\lambda = \frac{1}{4\nu_0 \log 4}$ [5], where $\nu_0 = \frac{m}{2\pi}$ is the noninteracting single-species density of states.

It is possible to get rid of the quartic term in the fermionic field by performing a Hubbard-Stratonovich transformation in the exchange channel [2].

This implies the introduction of a decoupling field h(x) which is a Hermitian matrix in layer/flavour space. Let us first introduce the "fat-unity"

$$1 =: \int Dh \, exp(-\int dx \, \frac{1}{2\lambda} Tr(h^{\dagger}(x)h(x)))$$

where a normalization factor has been inglobed inside Dh. If we perform the integration variable change $h(x) \rightarrow h(x) + \lambda \rho(x)$

$$1 = \int Dh \, exp\left(\int dx \, -\frac{1}{2\lambda} Tr(h^{\dagger}h) - \frac{1}{2} Tr(h\rho^{\dagger} + \rho h^{\dagger}) - \frac{\lambda}{2} Tr(\rho^{\dagger}\rho)\right)$$

and we multiply by the partition function, the terms which are quadratic in ρ cancel out exactly, so that

$$1 \times Z = \int Dh D\psi^{\dagger} D\psi \, exp(\int dx \, -\psi^{\dagger} (\partial_t + H_0)\psi - Tr(h\rho) - \frac{1}{2\lambda}Tr(h^{\dagger}h)).$$

It is now possible to integrate the fermionic fields, leaving behind an effective theory for the decoupling field h

$$S[h(x)] = -\Im r \, \log(\partial_t + H_0 + h) + \int dx \, \frac{1}{2\lambda} Tr(h(x)^{\dagger} h(x))$$

where we have made use of the identity $log \mathcal{D}et = \Im r \ log$. $\Im r \ (or \ \mathcal{D}et)$ means trace (or determinant) in the space of all indices and coordinate space-time variable.

It is possible to obtain a gapped state by choosing $h = \Delta \tau_3 \otimes Q$ [11] where Δ is the (half) gap amplitude, τ_3 the Pauli matrix in layer space and Q an Hermitian matrix in flavour space. In order to see that, we need to extremize the action

$$S[\Delta(x), Q(x)] = -\Im r \, \log(\partial_t + H_0 + \Delta \tau_3 Q) + \int dx \, \frac{\Delta^2}{\lambda} \mathbf{tr}(Q^{\dagger}Q),$$

where tr stands for trace on flavour indices.

Let us see how it works in detail. First of all, the space-time trace can be expanded as follows:

$$= -\sum_{\mu} \int dx \ \phi_{\mu}^{\dagger}(x) Tr \ \log(\partial_t + H_0 + \Delta \tau_3 Q) \phi_{\mu}(x) + \int dx \ \frac{\Delta^2}{\lambda} \mathbf{tr}(Q^{\dagger}Q),$$

where ϕ_{μ} is an orthonormal basis for the Hilbert space of space-time functions, that is

$$\int dx \ \phi_{\mu}^{\dagger}(x)\phi_{\nu}(x) = \delta_{\mu\nu}, \quad \sum_{\mu} \phi_{\mu}(x) \int dx \ [\phi_{\mu}^{\dagger}(x) \cdot] = Id(\cdot)$$

Now we can compute the variation

$$0 = \delta S = -\sum_{\mu} \int dx \ \phi_{\mu}^{\dagger}(x) Tr[(\tau_{3}Q\delta\Delta)(\partial_{t} + H_{0} + \Delta\tau_{3}Q)^{-1}]\phi_{\mu}(x) + \int dx \ \frac{2\Delta \ \delta\Delta}{\lambda} \mathbf{tr}(Q^{2}) + \\ -\sum_{\mu} \int dx \ \phi_{\mu}^{\dagger}(x) Tr[(\Delta\tau_{3}\delta Q)(\partial_{t} + H_{0} + \Delta\tau_{3}Q)^{-1}]\phi_{\mu}(x) + \int dx \ \frac{2\Delta^{2}}{\lambda} \mathbf{tr}(\delta QQ),$$

here the cyclic property of traces has been exploited to change the order of terms. As the equality holds $\forall \delta \Delta, \delta Q$, then we have the two equations

$$A = \sum_{\mu} \phi_{\mu}^{\dagger}(x) Tr[(\tau_{3}Q)(\partial_{t} + H_{0} + \Delta\tau_{3}Q)^{-1}]\phi_{\mu}(x) - 2\frac{\Delta}{\lambda} \mathbf{tr}(Q^{2}) = 0,$$

$$B = \sum_{\mu} \phi_{\mu}^{\dagger}(x) tr[(\Delta \tau_3)(\partial_t + H_0 + \Delta \tau_3 Q)^{-1}] \phi_{\mu}(x) - 2\frac{\Delta^2}{\lambda} Q = 0.$$

where tr stands for trace only on the layerspace.

Actually the second equation implies the first one, as

$$\Delta A = \mathbf{tr}(QB).$$

Let us look for a solution of B = 0 in the form of a homogeneous mean-field (Δ, Q) . It is convenient to work in the plane waves basis, that is to choose $\mu = (\omega, \vec{p})$

$$\phi_{\mu}(x) = \frac{e^{i(-\omega t + \vec{p} \cdot \vec{r})}}{\sqrt{\beta L^2}} =: \frac{e^{ip \cdot x}}{\sqrt{\beta L^2}},$$

and to integrate $\int dx$. We thus obtain

$$\frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H_0(\vec{p}) + \Delta \tau_3 Q)^{-1}] = 2\frac{\Delta}{\lambda}Q.$$
(6.1)

One can recognize the imaginary time Green function $G(\omega_n, \vec{p}) = (-i\omega_n + H_0(\vec{p}) + \Delta \tau_3 Q)^{-1}$, therefore the ω sum can be restricted only to fermionic Matsubara frequencies $\omega_n = i\frac{\pi}{\beta}(2n+1)$ (as G comes from a fermionic field integral).

The mean-field Hamiltonian H corresponding to the Green function is

$$H = H_0 + \Delta \tau_3 Q = \begin{pmatrix} \Delta Q & \frac{(\pi^{\dagger})^2}{2m} \\ \frac{(\pi)^2}{2m} & -\Delta Q \end{pmatrix}$$

where different blocks in the matrix correspond to different values for layer indices.

In order to proceed with our discussion we must first solve the problem posed by H, namely finding its eigenvalues and eigenvectors.

As a first step, we can reduce the dimensionality of the problem by changing the basis vectors, so that Q is diagonal. As Q is Hermitian, this can be achieved via

$$V = \begin{pmatrix} U & \mathbb{O} \\ \mathbb{O} & U \end{pmatrix}$$

where U is the unitary matrix whose columns are Q's eigenvectors. In fact,

$$H' = V^{\dagger} H V = \begin{pmatrix} U^{\dagger} \Delta Q U & U^{\dagger} \frac{(\pi^{\dagger})^2}{2m} U \\ U^{\dagger} \frac{(\pi)^2}{2m} U & -U^{\dagger} \Delta Q U \end{pmatrix} = \begin{pmatrix} \Delta D & \frac{(\pi^{\dagger})^2}{2m} \\ \frac{(\pi)^2}{2m} & -\Delta D \end{pmatrix}$$

where $D = diag(q_1, ..., q_4)$. We can also permute the basis vectors, so that

$$H'' = \begin{pmatrix} H^{BLG}(q_1\Delta) & & \\ & \ddots & \\ & & H^{BLG}(q_4\Delta) \end{pmatrix}$$
$$H^{BLG}(\Delta) = \begin{pmatrix} \Delta & \frac{(\pi^{\dagger})^2}{2m} \\ \frac{(\pi)^2}{2m} & -\Delta \end{pmatrix}$$

The spectrum of $H^{BLG}(\Delta)$ is shown in Fig.(6.1). The mean-field potential opens an energy gap of size 2Δ .

By applying this series of transformations to both sides of Eq.(6.1), we obtain

$$\frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H^{BLG}(q_i\Delta))^{-1}] = 2\frac{q_i\Delta}{\lambda}.$$



Figure 6.1: Spectrum of a gapped bilayer.

These 4 equations are of the form $f(q_i\Delta) = 0$. We can just study the case $f(\Delta) = 0$ and then perform the substitution $\Delta \to q_i\Delta$.

Let us compute the Green function

$$G(\omega_n, \vec{p}) = (-i\omega_n + H^{BLG}(\Delta))^{-1}.$$
(6.2)

The inverse of this matrix is easily obtained, and yields

$$G(\omega_n, \vec{p}) = \frac{1}{\Delta^2 + \omega_n^2 + \frac{p^4}{4m^2}} \begin{pmatrix} \Delta + i\omega_n & \frac{(\pi^{\dagger})^2}{2m} \\ \frac{\pi^2}{2m} & -\Delta + i\omega_n \end{pmatrix}$$
(6.3)

We can finally compute the trace in Eq.(6.1), and obtain

$$\frac{1}{\beta V} \sum_{\omega_n, \vec{p}} \frac{1}{\sqrt{\Delta^2 + \frac{|\vec{p}|^4}{4m^2}}} \left(\frac{1}{i\omega_n + \sqrt{\Delta^2 + \frac{|\vec{p}|^4}{4m^2}}} - \frac{1}{i\omega_n - \sqrt{\Delta^2 + \frac{|\vec{p}|^4}{4m^2}}} \right) = \frac{2}{\lambda}$$

Let us take care of the sum on fermionic Matsubara frequencies. We use the identity [2]

$$\frac{1}{\beta} \sum_{\omega_n} f(i\omega_n) = \sum_k \operatorname{Res}_{z = z_k} \left[n(z)f(z) \right]$$
(6.4)

where z_k are the poles of f(z) and $n(z) = \frac{1}{e^{\beta z} + 1}$. We obtain

$$\frac{1}{V} \sum_{\vec{p}} \frac{1}{\sqrt{\Delta^2 + \frac{|\vec{p}|^4}{4m^2}}} \left(\frac{1}{e^{-\beta\sqrt{\Delta^2 + \frac{|\vec{p}|^4}{4m^2}}} + 1} - \frac{1}{e^{\beta\sqrt{\Delta^2 + \frac{|\vec{p}|^4}{4m^2}}}} \right) = \frac{2}{\lambda}.$$

In order to evaluate the momentum summation, let us use a continuum approximation

$$\frac{1}{L^2} \sum_{\vec{p}} = \frac{1}{(2\pi\hbar)^2} \int d^2 \vec{p} = \frac{1}{2\pi\hbar^2} \int dpp$$

where last passage is due to the integrand's isotropy. A change of variable $y = \frac{p^2}{2m}, dy = \frac{p}{m}dp$ is useful, too. After that we obtain

$$\nu_0 \int_0^{\Lambda} dy \frac{1}{\sqrt{\Delta^2 + y^2}} \left(\frac{1}{e^{-\beta\sqrt{\Delta^2 + y^2}} + 1} - \frac{1}{e^{\beta\sqrt{\Delta^2 + y^2}} + 1} \right) = \frac{2}{\lambda}$$
(6.5)

where Λ is the bandwidth of $H^{BLG}(\Delta)$ ($\Lambda \sim 0.4 eV$).

We are mainly interested in finding the gap energy at T = 0. Therefore, let us take the limit $\beta \to \infty$

$$\int_0^{\Lambda} dy \, \frac{1}{\sqrt{\Delta^2 + y^2}} = \operatorname{arcsinh}\left(\frac{\Lambda}{\Delta}\right) = \frac{2}{\lambda\nu_0}.$$

The integral is immediate and the formula becomes

$$|\Delta| = \frac{\Lambda}{\sinh\left(rac{2}{\lambda
u_0}
ight)}.$$

A good approximation is that of considering $\frac{\Delta}{\Lambda} \ll 1$ from which follows the result found in [11]³

$$|\Delta| = 2\Lambda e^{-\frac{2}{\lambda\nu_0}}.$$

Let us turn our attention to the other field, Q. It is a Hermitian matrix, and we used this fact to diagonalize it to $D = diag(q_1, ..., q_4)$.

After this step, the gap equation takes the form

$$F(|q_i\Delta|) = \frac{2}{\lambda} \quad \forall i$$

so, unless F were a non-injective function (which is not the case), we need $|q_i| = q \quad \forall i$ for all the equations to be satisfied with a single value of Δ .

This means that Q is proportional to a unitary matrix, its diagonalized form being equal to |q|diag(1,...,1,-1,...,-1). We will assume |q| = 1, just like was done in [11], because otherwise the physical meaning of Δ would not be anymore $\frac{1}{2}$ of the energy gap, as the fraction would change to $\frac{1}{2q_i}$.

6.1.1 Critical temperature

The critical temperature T_c of the second order phase transition is obtained as the temperature at which the gap closes $\Delta(T_c) = 0$. Therefore, from Eq.(6.5) we immediately obtain

$$\int_0^{\Lambda} dy \frac{1}{y} \left(\frac{1}{e^{-\beta_c y} + 1} - \frac{1}{e^{\beta_c y} + 1} \right) = \frac{2}{\lambda \nu_0}$$

that can be rewritten as

$$\int_0^{\Lambda} dy \frac{1}{y} \tanh(\frac{\beta_c y}{2}) \sim \operatorname{arcsinh}(\frac{\beta_c \Lambda}{2}) = \frac{2}{\lambda \nu_0}.$$

Finally we get that

$$k_B T_c = \frac{\Lambda}{2\sinh(\frac{2}{\lambda\nu_0})} \tag{6.6}$$

6.1.2 Finite temperature gap and critical exponent

Let us now derive the temperature dependence of the gap $\Delta = \Delta(T)$. This can be obtained via Eq.(6.5), equating the case $T = T_c$, $\Delta(T_c) = 0$ to the generic one $(T, \Delta(T))$

$$\int_0^{\Lambda} \frac{dy}{\sqrt{\Delta^2 + y^2}} \tanh(\frac{\beta\sqrt{\Delta^2 + y^2}}{2}) = \int_0^{\Lambda} \frac{dy}{y} \tanh(\frac{\beta_c y}{2}).$$

It is useful to rescale all the quantities by β_c :

$$z = y\beta_c, D = \Delta\beta_c, L = \Lambda\beta_c, B = \frac{\beta}{\beta_c},$$
(6.7)

³Actually the two results differ by a factor of 2.

so that we obtain

$$I(B,D) := \int_0^L \frac{dz}{\sqrt{D^2 + z^2}} \tanh(\frac{B\sqrt{D^2 + z^2}}{2}) - \int_0^L \frac{dz}{z} \tanh(\frac{z}{2}) = 0.$$
(6.8)

The level set I(B, D) = 0 can then be computed numerically. In Fig.(6.2) the result is shown alongside the fitting formula from [14], that is

$$\Delta(T) = \Delta_0 \tanh(1.74\sqrt{\frac{T_c}{T} - 1}), \beta_c \Delta_0 = 1.76$$
(6.9)



Figure 6.2: $\Delta(T)$ in units of $k_B T_c$. Both numerical solution of Eq.(6.8) and fitting formula by [14] are shown.

Even if the $\Delta(T)$ law we have just found is identical to the one used in [14], we remark that our convention is that Δ is half the gap, while in [14] Δ is the full gap. Therefore the two formulas differ by a factor 2 that has still to be explained.

Although the critical exponent could be easily inferred from Eq.(6.9), we shall nevertheless derive it analytically from Eq.(6.8). Let us then consider the limit $D \sim 0, B = 1 + b, b \gtrsim 0$. Upon first order expansion of I(b, D) we obtain

$$D^{2} \int_{0}^{L} \frac{dz}{z} \left[-\frac{1}{2z^{2}} \left(\frac{1}{e^{-z}+1} - \frac{1}{e^{z}+1} \right) + \frac{1}{2z} \left(\frac{e^{-z}}{(e^{-z}+1)^{2}} + \frac{e^{z}}{(e^{z}+1)^{2}} \right) \right] + b \int_{0}^{L} dz \left[\frac{e^{-z}}{(e^{-z}+1)^{2}} + \frac{e^{z}}{(e^{z}+1)^{2}} \right] = 0$$

Now, as $b \sim \frac{T_c - T}{T_c}$, we get the critical exponent

$$\Delta \propto \left(\frac{T_c - T}{T_c}\right)^{\frac{1}{2}}.$$
(6.10)

6.2 Even N multilayer

Let us generalize the procedure in the case of even N-layer graphene with Bernal stacking. In order to get the correct Lagrangian, we just need to substitute the bilayer free Hamiltonian H_0 with

$$H_{0}(\vec{p}) = \begin{pmatrix} 0 & \frac{(\pi)^{2}}{2m_{1}} & 0 & 0 & 0 & 0 & 0 \\ \frac{(\pi)^{2}}{2m_{1}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{(\pi^{\dagger})^{2}}{2m_{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{(\pi^{\dagger})^{2}}{2m_{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{(\pi^{\dagger})^{2}}{2m_{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{(\pi^{\dagger})^{2}}{2m_{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{(\pi^{\dagger})^{2}}{2m_{2}} \\ \end{pmatrix},$$
(6.11)

that is the effective low-energy Hamiltonian of the considered system.

In this case H_0 is a N by N matrix, therefore the combined layer and flavor indices j, k run from 1 to 4N.

$$\mathcal{L} = \psi^{\dagger}(\partial_t + H_0)\psi + \sum_{j,k=1,\dots,4N} \frac{\lambda}{2} \psi_j^{\dagger} \psi_k^{\dagger} \psi_k \psi_j$$

The same computations made before bring the action in the usual form,

$$S[h(x)] = -\Im r \log(\partial_t + H_0 + h) + \int dx \ \frac{1}{2\lambda} Tr(h(x)^{\dagger} h(x))$$

where h is now a Hermitian 4N by 4N matrix.

We now have to make an ansatz for the structure of h, in such a way that a gapped solution be obtained. A successful choice turns out to be $h = \Delta \tau_3 \otimes Q$, with $\tau_3 = diag(1, -1, 1, -1, ..., 1, -1)$ (with a slight abuse of notation). τ_3 is a N by N matrix in layer space, that represents the layer-staggered potential, as described in subsection 4.2.1⁴. Q is a 4 by 4 Hermitian matrix in flavor space and Δ is a real scalar quantity.

The resulting action is given by

$$S[\Delta(x), Q(x)] = -\Im r \, \log(\partial_t + H_0 + \Delta \tau_3 Q) + \int dx \, \frac{N\Delta^2}{2\lambda} \mathbf{tr}(Q^{\dagger}Q),$$

The same computations shown above are needed to find the extremal points of the action, and lead to

$$\frac{1}{\beta V} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H_0(\vec{p}) + \Delta\tau_3 Q)^{-1}] = N \frac{\Delta}{\lambda} Q.$$
(6.12)

Let us study the new mean-field Hamiltonian H, given by

$$H = H_0 + \Delta \tau_3 Q = H_0(\vec{p}) = \begin{pmatrix} \Delta Q & \frac{(\pi^{\dagger})^2}{2m_1} & 0 & 0 & 0 & 0 & 0 \\ \frac{(\pi)^2}{2m_1} & -\Delta Q & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Delta Q & \frac{(\pi^{\dagger})^2}{2m_2} & 0 & 0 & 0 \\ 0 & 0 & \frac{(\pi)^2}{2m_2} & -\Delta Q & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Delta Q & \frac{(\pi^{\dagger})^2}{2m_2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{(\pi)^2}{2m_2} & -\Delta Q \end{pmatrix}$$

The Q terms can still be diagonalized via a $V = \mathbb{I} \otimes U$ unitary transformation that acts only on the flavor subspace. Also, the same reordering considered before can be applied and yield

We can now apply these transformations to both sides of Eq.(6.12) and obtain

$$\frac{1}{\beta V} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H^{NLG}(q_i\Delta))^{-1}] = N \frac{q_i\Delta}{\lambda}.$$

⁴Actually, by following the notation in subsection 4.2.1, we are using $L(\tau'_3)$, because we are working with the transformed and projected H_0 .

Mean-field theory

Of course we can again study only the case $q_i = 1$.

By writing explicitly the sum over effective masses, we can reduce the problem to a sum of BLG subsystems

$$\frac{1}{\beta V} \sum_{r=1}^{\frac{N}{2}} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H^{BLG}(\Delta, m_r))^{-1}] = N\frac{\Delta}{\lambda}.$$

The same steps outlined for the bilayer case can be carried on here, in order to get

$$\sum_{r=1}^{\frac{N}{2}} \nu_0^{(r)} \operatorname{arcsinh}\left(\frac{\Lambda}{|\Delta|}\right) = \frac{N}{\lambda}$$

where Λ is again the free Hamiltonian's bandwidth.

It follows that

$$|\Delta| = \frac{\Lambda}{\sinh\left(\frac{N}{A_N}\left(\frac{2\pi}{\lambda t_{\perp}v^{-2}}\right)\right)}$$

where

$$A_N = \sum_{r=1}^{\left\lfloor \frac{N}{2} \right\rfloor} \cos\left(\frac{r\pi}{N+1}\right)$$

Now, if we substitute in the last equation the result found in chapter 5, that is

$$\frac{2\pi}{\lambda} = 2\pi g \log 4 \sum_{r}^{\frac{N}{2}} \nu_0^{(r)} = g \log 4t_{\perp} v^{-2} A_N,$$

we find

$$|\Delta| = \frac{\Lambda}{\sinh(gN\log 4)}.\tag{6.13}$$

If we want to compare the results for different N, we must keep in mind that the Hamiltonian's bandwidth decreases for increasing N, as we deduce from Eq.(2.12). Let us choose $\Lambda \sim 0.1 eV$, so that the cut-off is smaller than the bottom of the lowest high-energy band up to $N \sim 8$. The results are shown in Fig.(6.3). The gap is suppressed exponentially with N, contrary to the experimental findings, which instead show a linear behaviour (Fig.(3.5)). Moreover, the experimental gap is orders of magnitude larger.



Figure 6.3: Log-scale plot of $\Delta(N)$ for even N, $\Lambda \sim 0.1 eV$. The gap is exponentially suppressed with growing N.

As far as the critical temperature is concerned, we point out that Eq.(6.8) is still valid, so by replacing Δ_0 with the one we just found we already know all the relevant quantities for the phase transition.

6.3 Odd N multilayer

Let us now consider the case of odd N-layer graphene with Bernal stacking. The relevant free Hamiltonian H_0 is in this case a N + 1 by N + 1 matrix given by

(_t)2

The interacting Lagrangian is therefore

$$\mathcal{L} = \psi^{\dagger}(\partial_t + H_0)\psi + \sum_{j,k=1,\dots,4(N+1)} \frac{\lambda}{2} \psi_j^{\dagger} \psi_k^{\dagger} \psi_k \psi_j$$

By means of the usual Hubbard-Stratonovich transformation we can obtain the action

$$S[h(x)] = -\Im r \log(\partial_t + H_0 + h) + \int dx \ \frac{1}{2\lambda} Tr(h(x)^{\dagger} h(x))$$

where h is now a Hermitian 4(N+1) by 4(N+1) matrix.

As far as the structure of $h = \Delta \tau_3 Q$ is concerned, we recall from subsection 4.2.1 that the layerstaggered potential matrix, once the usual transformations have been done is $\tau_3 = diag(1, -1, ..., 1, -1, 1, 1)^5$ τ_3 is a N+1 by N+1 matrix in layer space, Q is a 4 by 4 Hermitian matrix in flavour space and Δ is a real scalar quantity.

The resulting action is given by

$$S[\Delta(x), Q(x)] = -\Im r \, \log(\partial_t + H_0 + \Delta \tau_3 Q) + \int dx \, \frac{(N+1)\Delta^2}{2\lambda} \mathbf{tr}(Q^{\dagger}Q),$$

The same computations shown above are needed to find the extremal points of the action, and lead to

$$\frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H_0(\vec{p}) + \Delta \tau_3 Q)^{-1}] = (N+1)\frac{\Delta}{\lambda}Q.$$
(6.15)

Let us now analyze the mean-field Hamiltonian $H = H_0 + \Delta \tau_3 Q$. As usual, we can diagonalize Q via a unitary transformation and reduce to a block diagonal matrix in flavor space, where the blocks are $H^{NLG} = H_0 + \Delta \tau_3 q_i$, being q_i the eigenvalues of Q.

⁵Again, with some abuse of notation we actually mean $L(\tau'_3)$.

The result is

$$\frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} tr[\tau_3(-i\omega_n + H^{NLG}(q_i\Delta))^{-1}] = (N+1)\frac{q_i\Delta}{\lambda}.$$

It is now clear that if we compute the trace in terms of the single subsystems, we get

$$\frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} \left[\sum_{r=1}^{\frac{N-1}{2}} tr[\tau_3(-i\omega_n + H^{BLG}(\Delta, m_r))^{-1}] + tr[(-i\omega_n + H^{SLG}(\Delta, v))^{-1}] \right] = (N+1)\frac{\Delta}{\lambda}, \quad (6.17)$$

where

$$H^{SLG}(\Delta, v) = \begin{pmatrix} \Delta & v\pi^{\dagger} \\ v\pi & \Delta \end{pmatrix}$$

The spectrum of $H_{SLG}(\Delta, v)$ is shown in Fig.(6.4). While the order parameter Δ opens a gap in a bilayer subsystem, in the case of a monolayer subsystem it merely shifts in energy the Dirac point.



Figure 6.4: Spectrum of a shifted monolayer.

Now, as the addend due to bilayer blocks was already discussed, we shall focus on the monolayer term. It can be rewritten as

$$\frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} tr[\frac{1}{v^2 p^2 - (\Delta - i\omega_n)^2} \begin{pmatrix} i\omega_n - \Delta & v\pi^{\dagger} \\ v\pi & i\omega_n - \Delta \end{pmatrix}]$$
$$= \frac{1}{\beta L^2} \sum_{\omega_n, \vec{p}} \frac{2(\Delta - i\omega_n)}{(i\omega_n - (\Delta + vp))(i\omega_n - (\Delta - vp))}$$

We can compute the sum on Matsubara frequencies by means of 6.4. The result is

$$= -\frac{1}{L^2} \sum_{\vec{p}} [n(\Delta + vp) + n(\Delta - vp)].$$

As usual, we evaluate the momentum sum via an integral, and consider the $T \to 0$ limit, in which $n(x) \to \theta(x)$. Here θ is the Heaviside step function.

$$= -\frac{1}{2\pi\hbar^2} \int_0^P dp p[\theta(-(\Delta + vp)) + \theta(-(\Delta - vp))]$$

where P is a momentum cutoff. The integral can be easily computed, in order to yield

$$=\frac{1}{4\pi\hbar^2 v^2}(\Delta^2 - \Lambda^2).$$

where $\Lambda = vP$. Let us go back to Eq.(6.17) and plug back last result, together with the known bilayers' term

$$\sum_{r=1}^{\frac{N-1}{2}} \nu_0^{(r)} \log\left(\frac{\Lambda}{|\Delta|}\right) + \frac{1}{4\pi\hbar^2 v^2} \frac{\Delta^2 - \Lambda^2}{\Delta} = \frac{N+1}{\lambda}$$

where the same Λ is used for every band.

Since the SLG term is $\sim \nu_0^{SLG} \frac{\Lambda}{\Delta}$ and $\nu_0^{SLG} \ll \sum_r \nu_0^{(r)6}$ one could be tempted to dismiss such term as negligible. Actually, the fact that the SLG subsystem shows a linear behaviour $\propto \frac{\Lambda}{\Delta}$ instead of a logarithmic one $\propto \log(\frac{\Lambda}{\Delta})$ may counterbalance the smaller density of states, if the cutoff Λ is large enough. Therefore we are keeping the full formula.

Now, if we substitute the values for λ and $\nu_0^{(r)}$ we found in chapter 5, after some algebra we finally get to the equation

$$\frac{\Lambda}{|\Delta|} exp\left(\frac{1}{2t_{\perp}A_N} \frac{\Delta^2 - \Lambda^2}{\Delta}\right) - exp((N+1)g\log(4)) = 0$$
(6.18)

Let us look at Eq.(6.18) for a moment: as $\frac{\Delta}{\Lambda} \sim 0$, $\Lambda \sim t_{\perp}$ and $A \sim 1$ we have

$$\frac{\Lambda}{|\Delta|} exp\left(\frac{-\Lambda}{\Delta}\right) - exp((N+1)g\log(4)) \sim 0$$

where the second addend is in fact quite a large number. This equation cannot be solved unless $\Delta < 0$.

We can find the solutions of Eq.(6.18) numerically. For a fixed value of $\Lambda \sim 0.1 eV$ and $t_{\perp} = 0.39 eV$ we get Fig.(6.5), where an approximate law $\frac{\Delta}{\Lambda} \sim -0.091 N^{-2}$ is also shown. As shown in Fig.(6.5) the gap



Figure 6.5: $\Delta(N)$ for odd N multilayer, $\Lambda = 0.1 eV$. The gap is suppressed in a power law fashion $\frac{\Delta}{\Lambda} \sim -0.091 N^{-2}$.

is still suppressed with growing N (in contrast with experimental data), but now the suppression is less drastic, as it follows a power law. Moreover, the gap amplitude is closer in value to the experimental one than it was in the even case.

6.4 Discussion of the results

If we were to draw some conclusions from our analysis, we would have to admit that the gap estimates do not reproduce the experimental data. In fact our predictions show neither the correct order of magnitude of the gap, nor the linear behavior $\Delta \propto N$. While there is indeed a better agreement in the odd case, we must remark that this depends heavily on the choice of the cut-off Λ .

⁶At 100K, $\frac{\nu_0^{SLG}}{\nu_c^{BLG}} < 10^{-1}$, and the experimental temperatures are usually well below that.

⁷If Δ could assume any value, then it could be solved also for $\Delta > 0$, but this case is unphysical, as experimentally $\frac{\Delta}{\Lambda} \sim 10^{-2}$.

We should now ask why the proposed scheme does not work. As far as the linear behavior $\Delta \propto N$ is concerned, let us remark that it would be obtained for $N \leq 8$ if λ were constant. Of course we are not concerning about the fact that the order of magnitude is wrong. If we plot $\Delta(N)$ using a fixed value for λ , we get Fig.(6.6)



Figure 6.6: Half gap Δ taking $\lambda = \lambda_{BLG} = \frac{1}{4 \log(4)\nu_0}$. For $N \leq 8$ a linear behaviour is found.

Is there a good argument to justify an interaction constant which does not depend on N? The weakcoupling approximation we made in chapter 5 assumes that the electrons in every layer contribute to the Coulomb screening of all the others equally. But, clearly, only the electrons within a distance of order a_0 (screening length) from a layer can actually participate to the screening of its electrons. Therefore, if $a_0 < d(N-1)$ some layers will not participate to the screening of the layer under examination.

It follows that the weak-coupling approximation overestimates the screening, leading to a $\lambda \propto \frac{1}{\nu_0^{NLG}}$ which is smaller than due, and decreases with the number of layers. Since $\Delta \propto exp(-\frac{N}{\lambda\nu_0^{NLG}})$, this leads to the suppression of the gap.

What we expect to happen is instead that, as N increases, and more electrons are available for the screening, a_0 (and λ) decreases, preventing some layers to participate in the screening of a given one. But this has the opposite effect of increasing a_0 (and λ). The "equilibrium" value for a_0 and λ , is the one for which the screening is computed only keeping into account the layers within a_0 . If this value is $a_0 < d(N-1)$ then we will soon reach a point at which adding layers is irrelevant for the bulk screening because they are too far away to contribute. Therefore λ should at that point become constant, which is what is needed to explain the experimental data.

Chapter 7

Conclusions and future perspectives

We generalized the quantum field theory approach developed for a bilayer to treat graphene samples made of several layers. We found that our low-energy theory tailored for such multilayer graphene supports a symmetry broken gapped state, as expected from the experiments.

However, the gap amplitude observed in the experiments [14,15] are not well reproduced by our model. Our gap is both far too small and has the wrong functional dependence on the number of layers N. Indeed, while the experiments show an almost linear dependence, $\Delta \propto N$, our model predicts a gap which is suppressed either exponentially or with a power law by increasing N, when static screening effects are included. On the contrary, if we discard the screening effects, the linear dependence is also theoretically recovered.

We explained this discrepancy as a consequence of the weak-coupling approximation, which is, in this case, equivalent to approximating the system as if it had no thickness for the purposes of interaction. This implies that screening effects are overestimated in our description, which leads to the gap suppression. The starting point to derive a successful model is, therefore, reconsidering the weak-coupling approximation, either resorting to a better approximation scheme or keeping the interaction term in its full complexity. It could be useful, also, considering the screening effects in a dynamical manner, as done in Ref. [12]. In this way an UV cut-off can emerge from the theory without arbitrarily including it by hand. Moreover, the dynamical screening may increase the energy gap, providing a better agreement with the experimental data.

In conclusion, we believe that, including the layer distances in the effective model and treating the screening dynamically, we could reach a better and faithful understanding of the interaction driven insulating state observed experimentally.

So far, our investigation concerned the insulating state characterizing the bulk. An interesting open question, worth being addressed in this context but concerning edge states, is the possible emergence of a quantum anomalous Hall effect. Since the action describing the effective low-energy theory is invariant under SU(4) transformations in the spin-valley subspace, all the several ground states connected via such transformations are degenerate at the mean-field level. Gaussian quantum fluctuations might lift this degeneracy, identifying the true ground state. In Ref. [11] the authors argued that the true ground state of the bilayer obtained in this way is a quantum anomalous Hall state, namely a state of matter where spontaneous breaking of time-reversal symmetry produces an integer quantum Hall effect in the absence of any external magnetic field. The question we may raise is whether such a behavior can appear also for a generic multilayer and which is its dependence on the number of layers.

Appendix A

Derivation of projection operation

Let us derive the formula

$$H_{eff} = H_{PP} - H_{PQ}H_{QQ}^{-1}H_{QP}$$

which we used to obtain an effective Hamiltonian matrix for the low-lying bands. The proof follows [9] closely. Let us define the Green function G

$$G = \begin{pmatrix} G_{PP} & G_{PQ} \\ G_{QP} & G_{QQ} \end{pmatrix} = \begin{pmatrix} G_{PP}^{(0)-1} & H_{PQ} \\ H_{QP} & G_{QQ}^{(0)-1} \end{pmatrix}^{-1} = (H - \epsilon)^{-1}$$

where $G_{\alpha\alpha}^{(0)} = (H_{\alpha\alpha} - \epsilon)^{-1}$. Let us compute the inverse matrix

$$\begin{pmatrix} G_{PP}^{(0)-1} & H_{PQ} \\ H_{QP} & G_{QQ}^{(0)-1} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbb{I} & G_{PP}^{(0)} H_{PQ} \\ G_{QQ}^{(0)} H_{QP} & \mathbb{I} \end{pmatrix}^{-1} \begin{pmatrix} G_{PP}^{(0)} & 0 \\ 0 & G_{QQ}^{(0)} \end{pmatrix}.$$

In order to find the first columns of the inverse matrix appearing at right hand side, we have to solve the problem:

$$\begin{pmatrix} \mathbb{I} & A \\ B & \mathbb{I} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} \mathbb{I} \\ 0 \end{pmatrix}$$

It can be verified that

$$\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} \mathbb{I} \\ -B \end{pmatrix} (\mathbb{I} - AB)^{-1}$$

solves the problem. V_1 is therefore the first entrance of the inverse matrix:

$$G_{PP} = V_1 G_{PP}^{(0)} = (\mathbb{I} - AB)^{-1} G_{PP}^{(0)} = (1 - G_{PP}^{(0)} H_{PQ} G_{QQ}^{(0)} H_{QP})^{-1} G_{PP}^{(0)}$$

After inverting both sides and substituting the expressions for $G^{(0)}$ we get

$$G_{PP}^{-1} = (H_{PP} - \epsilon) - H_{PQ}(H_{QQ} - \epsilon)^{-1}H_{QP}$$

which gives the result, once evaluated for $\epsilon = 0$.

Appendix B

Odd N effective Hamiltonian and block diagonal form

Let us show that also in the odd N case the order in which the projection L to the low-energy subspace and the transformation U that brings the Hamiltonian in block diagonal form are applied is not important, the result being the same.

In the odd N case we performed an extra passage (in comparison with the even case) during the derivation of the effective Hamiltonian H_{eff} , as we needed to isolate the one dimensional kernel of H_{QQ} from the other basis vectors.

This extra passage consisted in a change of basis V_Q in the Q subspace, where D, the generator of the kernel, was one of the new basis vectors.

It turns out that also U_Q maps the canonical basis into a new one featuring D. But then, as we already pointed out in Eq.(4.6), we could use U_Q instead of V_Q and getthe same effective Hamiltonian.

Therefore, if we also apply U_P to the full Hamiltonian, we get the block diagonal form described in [6], with $\frac{N-1}{2}$ bilayer blocks and 1 single layer block, corresponding to the linear band.

The low energy effective Hamiltonian corresponds to the usual projection on bilayer blocks, leaving the monolayer block unvaried, as it does not contain big quantities with regards to the perturbative expansion described in chapter 4.

If instead we apply U_P after the projection, we get the same result because of Eq.(4.6).

In other words,

$$\begin{split} U_{P}^{\dagger}H_{eff}U_{P} &= U_{P}^{\dagger}L(V_{Q}^{\dagger}HV_{Q})U_{P} = U_{P}^{\dagger}L(U_{Q}^{\dagger}HU_{Q})U_{P} = \\ & L(U_{P}^{\dagger}U_{Q}^{\dagger}HU_{Q}U_{P}) = L(diag(H_{1},...,H_{\frac{N-1}{2}},H_{0}^{SLG}(v))) = \\ & diag(L(H_{1}),...,L(H_{\frac{N-1}{2}}),L(H_{0}^{SLG}(v))) = diag(H_{0}^{BLG}(m_{1}),...,H_{0}^{BLG}(m_{\frac{N-1}{2}}),H_{0}^{SLG}(v)). \end{split}$$

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