Variational approach to the excitonic phase transition in graphene

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We analyze the Coulomb interacting problem in undoped graphene layers by using an excitonic variational ansatz. By minimizing the energy, we derive a gap equation which reproduces and extends known results. We show that a full treatment of the exchange term, which includes the renormalization of the Fermi velocity, tends to suppress the phase transition by increasing the critical coupling at which the excitonic instability takes place.

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Introduction. The role of Coulomb interactions in the low-energy regime of undoped graphene layers has arisen great interest and still remains somewhat controversial. This is rooted to the poor screening properties of graphene, a peculiarity that can be traced back to the linear density of states of the low-energy theory, which vanishes at the Dirac point. An early weak-coupling analysis of the problem, based on the Renormalization Group (RG) method, showed that the Coulomb interaction is marginally irrelevant, flowing to a non-interacting fixed point. This picture can be rigorously justified at all couplings in the limit of a large number of electron flavors. In that scenario, undoped graphene layers would behave mostly as a non-interacting system of electrons, with minor traces of interactions reflected in the lifetime of quasiparticles and in a logarithmic renormalization of the Fermi velocity. Remarkably, this picture seems to match reasonably well with current experimental data.

The relative strength of the Coulomb interaction measured, as compared with the kinetic energy of the electrons, is ruled by the dimensionless coupling constant $g_0 \equiv e^2/\epsilon v_F$, where $e$ is the electron charge, $v_F$ the Fermi velocity, and $\epsilon$ the dielectric constant of the medium in which graphene is embedded. We use the subscript 0 to denote unscreened values of the coupling, see below. For samples in vacuum, $e^2 \simeq 14.4$ eV Å, and $v_F \simeq 6.3$ eV Å, so that $g_0 \simeq 2.3$. Density Functional Theory\textsuperscript{2} give a value for the screened coupling in the range $g \sim 0.5 - 2$. This puts graphene in the intermediate coupling regime, and hence the validity of the weak-coupling analysis relies on the absence of a strong coupling fixed point in the RG transformation. Indications of such a fixed point have been found by extending the weak-coupling RG to higher orders in the coupling constant expansion. The experimental data would still be compatible with this strong-coupling scenario if current setups had graphene sufficiently isolated from the environment and could operate with perfectly neutral samples.

The possibility of phases beyond the reach of perturbative or weak coupling renormalization group methods in undoped graphene has been explored in the literature by using different approaches. The main candidate for a strong coupling phase is an excitonic condensate, in which electron and holes bind together opening up a gap in the density of states and rendering the system insulating. The mechanism responsible for this phase would be the gain in exchange energy arising from the long range Coulomb interaction. A gap equation for this transition has been derived within the Dyson-Schwinger formalism\textsuperscript{10} and different solutions of this equation yield (unscreened) critical couplings for the phase transition around an unscreened coupling $g_{0c} \sim 1 - 2$. This scheme is equivalent to the summation of a class of diagrams, and can be considered an extension of weak coupling approaches. Monte Carlo calculations in the lattice have been carried out to analyze this problem, finding an insulating phase above $g_{0c} \simeq 1.11$ and $g_{0c} \simeq 1.66$, respectively. A phase transition beyond a certain coupling can also be found for short range interactions in the half filled honeycomb lattice\textsuperscript{13} although the critical coupling takes the model beyond the regime where the approximation of the electronic bands by the Dirac equation is valid. Finally, the study of the two-body problem in graphene, with Coulomb interactions, leads to a remarkable instability of the wave-function for a critical coupling $g_{0c} = 1.16$ that might underlie the eventual formation of excitons.

In this paper we investigate the possibility of an excitonic strong coupling phase in undoped graphene by using a variational ansatz. The method used here can be extended in a straightforward way to finite temperatures or to finite carrier concentrations. We derive a gap equation similar to that obtained in the previous literature\textsuperscript{10,12} but with the inclusion of a the renormalization of the Fermi velocity. By analyzing numerically and analytically the resulting gap equation, we find that the latter produces a suppression of the phase transition by increasing the critical coupling.

The model and variational ansatz. As we have mentioned, we will address the problem of an undoped graphene sample with Coulomb interactions in the low-energy regime, where the electron motion is described by the Dirac equation. The Hamiltonian for this problem reads:

$$
\mathcal{H} = \sum_{k_s} skn_{k_s} + \frac{1}{2} \sum_{q} V_q n_{q} n_{-q}
$$

(1)
where $s = \pm$ refers to the upper and lower cones, respectively. In our model, the spin and valley degrees of freedom are considered only as extra degeneracies in the number of fermions. The Coulomb potential is given by $V_q = 2\pi g/q$, where $g$ is the dimensionless coupling constant introduced above. We assume that $g$ includes contributions from static screening. In the RPA approximation, transitions between the valence and conduction bands lead to a momentum independent dielectric constant, which can be incorporated in a straightforward into this formalism. Alternatively, one can view this approach as the leading approximation in the limit $N \to \infty$, where $N$ is the number of fermion flavors.

Our goal is to analyze the ground state of this Hamiltonian by using a variational ansatz which includes the possibility of pairing between electron and holes. Such an ansatz was proposed to study excitons formation in semiconductors and is reminiscent of the ansatz used in the BCS theory of superconductivity:

$$\Psi = \Pi_k(v_k^+ + v_k^c |D)$$

(2)

The ansatz contains a coherent superposition of states with a different number of electron-hole pairs. Here $|D\rangle$ stands for the filled Dirac sea, and $u_k$ and $v_k$ are variational parameters to be determined by minimizing the ground state energy. Without loss of generality, they are taken real. Notice that they are not independent, since the normalization of the wave function imposes the constraint:

$$u_k^2 + v_k^2 = 1$$

(3)

**Derivation of the gap equation.** Following the lines of a typical variational calculation, the energy of the ansatz is evaluated by projecting the Hamiltonian into this state. It has two contributions, the Hartree and the exchange one, as shown in Fig. 1. The Hartree contribution is zero, by virtue of the normal ordering of the Hamiltonian with respect to the Dirac sea, which is physically related to the neutrality of charge of the global system. The dominant contribution comes from the exchange energy, which includes terms with a momentum transfer of $q = k' - k$. The projected Hamiltonian reads then:

$$\langle \Psi | : H : \Psi \rangle = \sum_k k(v_k^2 - u_k^2)$$

$$-\frac{1}{2} \sum_{k,k'} V_{|k' - k|} |2u_k v_{k'} v_{k'}^* + v_k^* v_{k'} v_{k'}^*\rangle$$

$$+ \cos^2\left(\frac{\theta_{k'} - \theta_k}{2}\right)(u_k^2 v_{k'}^2 + v_k^* v_{k'} v_{k'}^*)$$

$$+ \sin^2\left(\frac{\theta_{k'} - \theta_k}{2}\right)(u_k^2 v_{k'}^2 + v_k^* v_{k'} v_{k'}^*)$$

(4)

where we have used the normal-ordered Hamiltonian in order to carry out the calculation. The extreme condition must be imposed respecting the normalization constraint. The result gives the following equation:

$$\left[k + \sum_{k'} V_{|k' - k|} \cos(\theta_{k'} - \theta_k)(u_{k'}^2 - v_{k'}^2)\right] u_k v_k$$

$$= (u_k^2 - v_k^2) \sum_{k'} V_{|k' - k|} u_{k'} v_{k'}$$

(5)

This equation can be simplified by introducing the following parameters:

$$\xi_k = k + \sum_{k'} V_{|k' - k|} \cos(\theta_{k'} - \theta_k)(u_{k'}^2 - v_{k'}^2)$$

(6)

$$\Delta_k = 2 \sum_{k'} V_{|k' - k|} u_{k'} v_{k'}$$

(7)

$$E_k^2 = \xi_k^2 + \Delta_k^2$$

(8)

The first equation is the self-energy insertion to the electron propagator, which adds to the linear term coming from the non-interacting dispersion relation and represents a renormalization of the Fermi velocity. The second equation introduces $\Delta_k$, which can be identified with the gap that arises in the electronic spectrum when excitons are formed. This is clearly expressed in the third equation, which gives the dispersion relation of Bogoliubov quasiparticles in the excitonic condensate.

In terms of these new parameters, the solution to the variational problem reads:

$$u_k v_k = \frac{\Delta_k}{2E_k}$$

$$v_k^* = \frac{1 - \xi_k/E_k}{2}$$

(10)

$$u_k^2 = \frac{1 + \xi_k/E_k}{2}$$

(11)

By plugging these expressions into the equation for the gap, Eq. (7), we get a self-consistent integral equation, namely:

$$\Delta_k = \sum_{k'} V_{|k' - k|} \frac{\Delta_{k'}}{E_{k'}}$$

(12)
As we have already mentioned, a similar gap equation has been already found by using the Schwinger-Dyson formalism.\textsuperscript{10}

Further insight can be obtained by carrying out the angular integral while keeping the lowest order terms in a Legendre polynomial expansion of the Coulomb interaction $V(|k^* - k|)$. This yields a simplified integral equation in the continuum limit of the problem:

$$\Delta_k = g \int_0^\Lambda dk' k' \Delta_{k'} \frac{\mathcal{K}(k,k')}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}},$$

where we have introduced the following kernel:

$$\mathcal{K}(k,k') = \frac{1}{k} \theta(k - k') + \frac{1}{k'} \theta(k' - k).$$

The main feature of this gap equation, as compared with previous approaches, is the inclusion of the exchange correction to the free electron dispersion relation, Eq. (5).

**Analysis of the gap equation.** In order to extract information from the gap equation, we make the following assumption\textsuperscript{10,19} the dominant contribution to the gap equation corresponds to the region $k \gg \Delta^*$, where $\Delta^* \equiv \Delta_{\Delta^*}$ (with $v_F \equiv 1$). This allows us to make $E_q \simeq \xi_q$ and write $\Delta^*$ as the lower limit of the integral:

$$\Delta_k \simeq g \int_0^\Lambda dk' k' \Delta_{k'} \frac{\mathcal{K}(k,k')}{\xi_{k'}}.$$

By using the same type of reasoning, an expression for the $\xi_k$ can be derived, which only retains the leading, most divergent terms (and valid for $\xi_k > \Delta^*$):

$$\xi_k = k + g^2 k \log \left( \frac{\Lambda}{k} \right)$$

As mentioned above, this is actually the renormalization of the Fermi velocity that arises from a RG analysis\textsuperscript{1} which has been so far neglected in the literature on the excitonic instability. The condition $g(k) > 1/4$ for all values of $k$, leads to the requirement $\Delta^* > \Delta_{\text{min}} = \Lambda^{-8(1-1/4g)}$. We find that a nonzero, real solution of Eq. (22) (with $n = 1$) satisfying $\Delta^* > \Delta_{\text{min}}$, exists for $g$ greater than a critical value $g_c \simeq 0.5$, which marks the onset of the excitonic instability.

**Numerical solution.** We further check the previous analysis by numerically solving Eq. (17) with the boundary conditions (19)-(20). The results are shown in Fig. 2. We find solutions for $g \geq g_c \simeq 0.59$, in reasonable agreement with the adiabatic approximation. The asymptotic limit $\Delta_k \sim 1/\sqrt{k}$ [see Eq. (21)] is only clearly visible for $g \sim g_c$ and $k \ll \Lambda$. A detailed analysis of the region where $(g - g_c) \to 0^+$ suggests that $\Delta^* \propto (g - g_c)$, see Fig. 3. For comparison, we also show the numerical results obtained by neglecting the renormalization of the Fermi velocity. They reproduce correctly the main features found in analytical studies, namely, $g_c = 1/4$ and $\Delta^* \sim e^{-A/\sqrt{9-\pi^2}}$, where $A$ is a constant.\textsuperscript{10,12}

**Conclusions.** We have analyzed the problem of Coulomb interactions in undoped graphene by using a variational ansatz that includes the possibility of exciton formation. Our approach can be readily extended to other two- and three-dimensional materials, as well as to finite temperatures and carrier concentrations.\textsuperscript{23} It allows us to calculate the total free energy, which can be compared to that of other broken symmetry phases.

Our variational analysis reproduces the main features of the excitonic transition in graphene.\textsuperscript{24} In addition, we find that a renormalization of the Fermi velocity is a natural by-product of the variational treatment. The resulting change in one particle energies leads to a cancellation of the leading divergences with trigger the excitonic
transition. A similar effect is observed in the analysis of the excitonic transition due to short range interactions in graphene bilayers\textsuperscript{21,22}. Our variational analysis leads to a critical coupling \( g_c \simeq 0.59 \), which is about a factor two larger than the critical coupling obtained neglecting the Fermi velocity renormalization, \( g_c = 1/4 \text{.} \textsuperscript{10,12,23,24} \) The renormalization of \( g \) to two loops gives a transition at \( g_c \simeq 0.83 \text{.} ^{2} \)

In suspended graphene, we can assume that the effective value of \( g \) is modified solely by internal screening\textsuperscript{21,10} so that \( g = g_0/(1 + N \pi g_0/8) \), where \( N = 4 \) is the number of electron flavors, and \( g_0 = e^2/v_F \) is the bare coupling constant. Then, an upper bound of \( g \) is \( g_{\text{max}} = \lim_{e^2/v_F \to \infty} g(e^2/v_F) = 2/\pi \simeq 0.64 \), which lies slightly above the value of \( g_c \) obtained with our variational ansatz. For the realistic value of \( g_0 = 2.3 \) we obtain \( g = 0.50 \), which is below the critical value \( g_c \simeq 0.59 \) which we have found by solving Eq. \textsuperscript{\textit{17}} numerically\textsuperscript{22}.

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\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{fig2.png}
\caption{(Color online). Left: Dependence of \( \Delta^* \) on \( g \) obtained by numerically integrating Eq. \textsuperscript{\textit{17}} with the boundary conditions in Eqs. \textsuperscript{\textit{19}}\textsuperscript{\textendash}20. Right: Dependence of \( \Delta_k \) on \( k \) for \( g = 0.6, 0.65, 0.7, 0.75 \) and 0.8 (from top to bottom). The thick black line shows the position of the maxima of \( \Delta_k \), which give the value of \( \Delta^* \), see Eq. \textsuperscript{\textit{19}}.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{fig3.png}
\caption{(Color online). Details of the dependence of \( \Delta^* \) on \( g \) near the transition. The inset on the right graph shows the results from numerically solving Eq. \textsuperscript{\textit{17}} without velocity renormalization [i.e. assuming \( g(k) = g \) in Eq. \textsuperscript{\textit{18}}].}
\end{figure}

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\bibitem{25} Montecarlo results suggest a critical coupling in the range of expected values in suspended samples, which is smaller than the value predicted by our variational ansatz. The origin of this discrepancy is unclear. It could arise from differences in the regularization of the short range part of the interaction, or in the treatment of screening at high frequencies.
\end{thebibliography}