Critical Behavior in Graphene with Coulomb Interactions

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We demonstrate that in the presence of Coulomb interactions, electrons in graphene behave like a critical system, supporting power law correlations with interaction-dependent exponents. An asymptotic analysis shows that the origin of this behavior lies in particle-hole scattering, for which the Coulomb interaction induces anomalously close approaches. With increasing interaction strength the relevant power law changes from real to complex, leading to an unusual instability characterized by a complex-valued susceptibility in the thermodynamic limit. Measurable quantities, as well as the connection to classical two dimensional systems, are discussed.

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Graphene continues to fascinate physicists with its many unique properties \cite{1,2}. The low energy physics of electrons in graphene may be described by a Dirac Hamiltonian, analogous to the theory of massless neutrinos, with the two components of the electron wavefunctions representing amplitudes on the two sublattices that make up the graphene lattice. One class of problems yet to be understood in a fuller description involves the effect of the Coulomb interaction. Its strength may be characterized by an effective fine structure constant $\beta = e^2/\epsilon v_F$, where $v_F$ is the electron speed near the Dirac point and $\epsilon$ is a dielectric constant due to a substrate. For suspended graphene, $\beta$ is estimated to be of order 2. Naively, then, Coulomb interactions are relatively strong in graphene, so that one may expect to see its effects in a clean enough sample. This is the subject of our study.

In the presence of Coulomb interactions, the Hamiltonian of this system, remarkably, has no natural length scale: the $1/r$ interaction has precisely the same operator dimension as the (Dirac) kinetic energy. This suggests that the system behaves as if it is at a critical point, even though no parameters need be tuned to attain this situation. In what follows, we demonstrate that a dramatic effect of Coulomb interactions is that they induce power law correlations, a hallmark property of critical systems. The underlying cause of this originates in short distance physics – an anomalously large probability for close approaches of particle-hole pairs – but consequences are manifested at long distances because of the absence of a length scale in the Hamiltonian. The power law correlations in this system are reminiscent of the behavior of a variety of classical two-dimensional systems \cite{3}, and like those, when the coupling constant is sufficiently large we find indications of an unusual phase transition, characterized in the thermodynamic limit by a susceptibility that goes from real to complex rather than diverging. We speculate that resulting state may represent a precursor to the formation of a (gapped) exciton condensate \cite{4,5}.

The many-body physics we describe below is present in a simpler form for non-interacting Dirac electrons scattering from a Coulomb potential $V(r) = -Ze^2/r$ \cite{6,7,12}. For small $r$, the wavefunctions vanish as $\psi_m(r) \sim r^{(m+1/2)^2-2\beta^2-1/2}$. In contrast, for impurity potentials which do not diverge so strongly at $r = 0$, the power law is fixed by the “centrifugal barrier” associated with a given angular momentum channel $m$, and does not depend on the potential itself. The fact that the exponent becomes a continuously varying function of $\beta$ is unusual: the $1/r$ attraction allows an anomalous penetration of the centrifugal barrier. Moreover, for $2\beta \geq m$, the exponent becomes complex, and one must introduce a short distance cutoff to obtain sensible wavefunctions. This “Coulomb implosion” phenomenon is accompanied by the appearance of a screening cloud $\rho(r) \sim 1/r^2$ around the impurity which is not present for smaller $\beta$.

General particle-hole channel propagators support analogous behavior, generating power law behavior in certain correlation functions. We show in particular that the sublattice-antisymmetric susceptibility does this, so that critical-like behavior is manifested in the response to potentials which are not symmetric for the two sublattices. Moreover we find a divergence when $\beta$ exceeds $\beta_c$, when the centrifugal barrier in particle-hole scattering is overcome and the power changes from real to complex, a many-body manifestation of Coulomb implosion.

Analysis in Momentum Representation – To motivate our approach, we begin by analyzing the noninteracting problem in the presence of a Coulomb impurity as a scattering problem, using a standard momentum representation. The Hamiltonian is $H_0 \psi = [\epsilon - V(\rho)]\psi$, where $H_0 = \hbar v_F \vec{\sigma} \cdot \hat{p}$ is the kinetic energy for one of the two valleys, with $\vec{\sigma}$ the Pauli matrices acting on the space of the two sublattices, $\hat{p}$ the momentum operator, and $V(\rho)$ the Coulomb impurity potential. This is a low-energy effective Hamiltonian valid at distances large compared to the lattice scale; we ignore the small separation between different sublattice points of the same lattice site. In clean noninteracting graphene there is negligible inter-valley scattering. This remains approximately true here.
as well because the valleys are separated by a large momentum, and the Coulomb interaction vanishes for large momenta. We only consider one spin species. The standard (Lippman-Schwinger) equation for scattering states \[ \psi^{(+)}(\vec{p}) = \psi^{(0)}(\vec{p}) - G^{(0)}(\vec{p}) \sum_{\mu} e^{-imn^\mu} \psi^{(+)}(\vec{p}', \mu), \]

where \( G^{(0)} \) is the unperturbed (matrix) Green’s function and \( \psi^{(0)} \) is an eigenstate for \( V = 0 \). Eq. 1 is conveniently recast in terms of angular components, for which we define \( \psi_{m}(\vec{p}) = f_{m}^{(2)} \frac{d\theta}{2\pi} e^{-im\theta_{p}} \psi(\vec{p}), \) and decompose the Coulomb interaction in the form \( V(\vec{p}' - \vec{p}) = \sum_{n} e^{-im(\theta_{p}' - \theta_{p})} f_{n}(\vec{p}' / \vec{p}) / \vec{p}, \) where

\[
f_{m}(x) = \int_{0}^{2\pi} \frac{d\theta}{2\pi} e^{-im \theta} \frac{1}{\sqrt{1 + x^2 - 2x \cos(\theta)}}. \tag{2}
\]

In terms of these quantities one arrives at a set of equations coupling \( \psi^{(+)}_{1,m} \) and \( \psi^{(+)}_{2,m+1} \); where \( 1, 2 \) are sublattice indices. To search for power law behavior in \( \psi^{(+)}(\vec{p}) \) at large momentum \( p \), we adopt the ansatz

\[
\psi_{m}(\vec{p}) = c_{m,m} / p^{s} \text{ for } p \to \infty. \text{ To lowest order in } 1/p, \text{ non-vanishing solutions are supported when}
\]

\[
1 - (Z \beta)^{2} I_{m}(s) I_{m+1}(s) = 0, \tag{3}
\]

where \( I_{m}(s) = \int_{0}^{\infty} x^{1-s} f_{m}(x) dx. \) Note that \( I_{m}(s) \) diverges for real \( s \) when \( s = 1 - |m| \) and \( s = 2 + |m| \), and has a positive minimum value at \( s = 3/2 \). From these properties, one may see that Eq. 3 has solutions with real \( s \) when \( Z \beta \) is below a critical \( (Z \beta)_{c} \); above this \( s \) becomes complex. In particular, for \( m = 0 \), \( (Z \beta)_{c} = 1/2 \). This is Coulomb implosion expressed in momentum-space, which may be readily translated into a many-body context.

**Power Law Behavior for Interacting Dirac Electrons** – The same analysis for a single particle-hole pair (the analog of the Cooper problem in superconductivity) reveals a short-distance power law changing from real to complex in the particle-hole channel as \( \beta \) is increased. While a generic four point vertex includes the non-analytic behavior, the nonanalyticity cancels in the density-density response \[ \chi^{M}_{\alpha\beta}(\vec{k}, \vec{q}) = \frac{d\vec{q'} \cdot U(|\vec{q'}|) \chi^{M}_{\alpha\beta}(\vec{k} - \vec{q'}, \vec{q}) \chi^{M}_{\alpha\beta}(\vec{k} - \vec{q'}, \vec{q}), \]

where \( U(|\vec{q'}|) = 2\pi \epsilon^{2} / |\vec{q'}|, \) and

\[
\tilde{\chi}^{M}_{\alpha\beta}(\vec{k}, \vec{q}) = \chi^{M}_{\alpha\beta}(\vec{k}, \vec{q}) \gamma_{\alpha\beta}(\vec{k}, \vec{q}), \tag{8}
\]

Note that on the right-hand side of this expression, momenta are 3-vectors \( (q_{0} = 0) \), whereas elsewhere only the spatial components of the momenta remain. Defining \( \tilde{\chi}^{M}_{\alpha\beta}(\vec{k}, \vec{q}) = \chi^{M}_{\alpha\beta}(\vec{k}, \vec{q}) \gamma_{\alpha\beta}(\vec{k}, \vec{q}), \) one finds

\[
\tilde{\chi}^{M}_{\alpha\beta}(\vec{k}, \vec{q}) = \tilde{K}_{\alpha\beta\gamma}(\vec{k}, \vec{q}) \tilde{\chi}^{M}_{\gamma\beta}(\vec{k}, \vec{q}) \tag{8}
\]

This quantity is related to the susceptibility by

\[
M(\vec{q}) = \int \frac{d^{2}k}{(2\pi)^{2}} \sigma_{\alpha\alpha} \tilde{\chi}^{M}_{\alpha\alpha}(\vec{k}, \vec{q}). \tag{9}
\]

Henceforth we focus on the long wavelength limit (small \( q \), so for the moment we drop all terms of \( O(q^{2}) \) and

\[ FIG. 1: (Color online) (a) Diagrammatical equation for the 3-leg vertex \( \tilde{\Gamma}_{\beta\gamma}(\vec{k}, \vec{q}) \) with \( \sigma^{+} \) as the zeroth order vertex (the shaded cross in the figure). (b) Diagram for \( M(\vec{q}) \). \]
higher. Using a circular moment expansion, one finds
\[
\tilde{\chi}^{M(0)}(\vec{k}, \vec{q}) = \tilde{K}^{(0)}_{\alpha \beta}(\vec{k}, \vec{q}) \sigma^\alpha_{\beta}\]
\[
+ \tilde{K}^{(0)}_{\alpha \beta}(\vec{k}, \vec{q}) \int_{k_0}^{\Lambda} k' dk' f_0(\frac{k'}{k}) \tilde{\chi}^{M(0)}_{\beta}(\vec{k}', \vec{q}).
\] (10)

Here we used the superscript \((0)\) to denote the circular component \(m = 0\), and the underlined indices are not summed over. In this equation we have introduced explicit ultraviolet \((\Lambda \sim 2\pi/a, a = \text{lattice spacing})\) and infrared \((k_0 \sim 2\pi/L, L = \text{linear size of system})\) cutoffs.

Defining \(\tilde{\chi}^{M(0)}(k, \vec{q}) \equiv \sigma^\alpha_{\beta} \tilde{\chi}^{M(0)}(\vec{k}, \vec{q})\), in the limit \(q \to 0\) the solution to Eq. (10) may be written in the form \(\tilde{\chi}^{M(0)}(k, 0) = \frac{1}{\nu F(k)}\), where \(F\) obeys the integral equation
\[
F(\frac{k}{\Lambda}) = 1 + \frac{\beta}{2k} \int_{k_0}^{\Lambda} dk' f_0(\frac{k'}{k}) F(\frac{k'}{\Lambda}).
\] (11)

Note that \(F\) depends on the ratio \(k/\Lambda\), a reflection of the fact that the original Hamiltonian has no intrinsic length scale, so (in the limit \(k_0 \to 0\)) it can enter only in this ratio. For \(k/\Lambda \ll 1\), one easily confirms that Eq. (11) is solved by a power law \(F(\frac{k}{\Lambda}) \sim (\Lambda/k)^s\), with \(s\) going from real to complex above some critical \(\beta\).

To confirm this, we solved Eq. (11) numerically. For small \(\beta\), the solution is indeed a power law, provided \(k \gg k_0\) [see Fig. 2(a) inset]. For large enough \(\beta\), the solution is consistent with a power law of complex exponent, such that \(F\) becomes oscillatory with a power law envelope [Fig. 2(a)]. Moreover, \(M(\vec{q} \to 0) = \int \frac{d^2k}{(2\pi)^2} \tilde{\chi}^{M}(k, \vec{q} \to 0)\) has a series of divergences [Fig. 2(b)]. The positions and weights of these poles depend on \(k_0\). We return to this important point momentarily.

For small but nonzero \(q\), it is interesting to compute the correction \(\Delta M(q) = M(q) - M(0)\). The equation for the corresponding \(\Delta F\) has a form very similar to Eq. (11), with only the \("1\) replaced by an inhomogeneous term, which is proportional to \(q^2/k^2\) for \(k \gg q\). The \(\Delta M(\vec{q})\) resulting from this then vanishes with an exponent that varies with \(\beta\). The inset of Fig. 3 illustrates a typical result for \(\beta\) not too large; the exponent as a function of \(\beta\) is illustrated in Fig. 3. One physical consequence of this is that the difference in charge between sublattices for an impurity placed asymmetrically with respect to the sublattices will fall off with a \(\beta\)-dependent power law at large distances, behavior which may be observable with a local scanning probe. We note that \(\Delta M(q)\) has singularities at the same values of \(\beta\) as \(M(0)\), as should be expected from the form of Eq. (11).

Figs. 2 and 3 are the central results of our work. They demonstrate that in the ladder approximation for the many-body problem of interacting electrons in undoped graphene: (i) For \(\beta < \beta_c\) generic particle-hole correlators decay with a power law at long distances, with an exponent varying continuously with \(\beta\). The weak-coupling many-body ground state thus displays a basic property of a critical phase. The power law behavior is directly visible in the sublattice-antisymmetric density correlator. (ii) For \(\beta > \beta_c\) the exponent becomes complex, as in the noninteracting Coulomb implosion problem. In the interacting many-body case, the susceptibility \(M(q)\) of Eq. (5) diverges for \(k_0 > 0\). This strongly suggests a quantum phase transition to broken symmetry state with staggered charge order \([4,5]\). However, the presence of many such divergences as a function of \(\beta\) suggests there are different ways to break the symmetry. (iii) The singularities vanish in the thermodynamic limit, with the poles merging into a continuous function. The separation between them vanishes only logarithmically as \(k_0 \to 0\), as we demonstrate below, resulting in a branch point at \(\beta_c\). We interpret this latter non-analytic behavior as the signal of a phase transition. Since it is a result of the merging poles, a natural interpretation is that the instability is into a state involving fluctuations among different realizations of a chiral order parameter which, if static, would produce a gapped exciton phase \([4,5]\). We speculate that with further increase in \(\beta\), one of these orderings could
be favored over the others, resulting in a true condensed phase.

Analytical Results for Model Kernel — A fuller understanding of Eq. (11) may be obtained by adopting a model kernel,

\[ \tilde{f}_0(x) = \theta(1-x) + \frac{1}{x} \theta(x-1). \]  

(12)

This has the same behavior as the real kernel at large and small \( x \), and is simple enough to allow analytic solutions. We have verified numerically that the results for \( F \) and \( M \) are qualitatively very similar to those obtained with the correct \( f_0 \). With this kernel, Eq. (11) has general solutions of the form

\[ F(\tilde{k}) = A_+ \tilde{k}^{\lambda_+} + A_- \tilde{k}^{\lambda_-}, \]  

(13)

with \( \tilde{k} = k/\Lambda \), \( \lambda_\pm = \frac{\mp \theta \beta - 1}{2} \), and \( \gamma = \sqrt{1 - 2\beta} \). The coefficients \( A_\pm \) are determined by substituting Eq. (13) back into the integral equation. This results in power law behavior for \( k \gg \tilde{k}_0 \), with exponent \( \lambda_+ \), which goes from real to complex when \( \beta \) exceeds 1/2. Moreover, \( M(q \to 0) \) may be evaluated, yielding

\[ M(0) = \frac{\Lambda}{v_F} \frac{2 - 2\tilde{k}_0^\gamma}{1 + \gamma - \beta + \tilde{k}_0^\gamma(-1 + \gamma + \beta)}. \]  

(14)

This has poles for \( \beta > 1/2 \) when

\[ \sqrt{2\beta + 1} \ln \tilde{k}_0 = 2 \arctan \left( \frac{\sqrt{2\beta + 1}}{1 - \beta} \right) + 2\pi n, \]  

(15)

with integer \( n \) and \( 0 < \arctan(x) < \pi \). Note that the distance between poles vanishes logarithmically as \( \tilde{k}_0 \to 0 \), as discussed above. Furthermore, for \( \beta > 1/2 \), \( \tilde{k}_0^\gamma \) becomes ill-defined unless an infinitesimal imaginary part is introduced in \( \beta \), so that \( \beta = 1/2 \) becomes a branch point for \( M(0) \). We interpret this as the signal of a phase transition in the thermodynamic limit, since \( M(0) \) need not be real and positive beyond this point.

In this work we have examined the problem of interacting electrons in undoped graphene in the ladder approximation. For \( \beta < \beta_c \) the ground state has \( \beta \)-dependent power law correlations in the antisymmetric-sublattice density response. We note that in light of the logarithmic growth of \( v_F \), one may expect logarithmic corrections to this power, which may be difficult to detect for finite size systems. For \( \beta > \beta_c \), there is a nonstandard phase transition in which susceptibilities become divergent only for a finite size system. The continuously varying exponent (in the ladder approximation) and the instability when it reaches a critical value are reminiscent of the behavior of two-dimensional classical XY models. A central feature of our analysis is that, due to the absence of an intrinsic length scale, short distance power laws from anomalous penetration of a centrifugal barrier by the Coulomb interaction have an impact on the long-distance decay of correlators. Corresponding behavior occurs for non-interacting Dirac electrons near a Coulomb impurity. This analogy has been noted recently in a different way.

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