I. INTRODUCTION

Two-dimensional crystals of Carbon atoms (graphene) are recently discovered. Graphene, a single, one-atom thick sheet of carbon atoms arranged in a honeycomb lattice. High quality graphene single crystals some thousands of µm² in size are sufficient for most fundamental physics studies. There are significant efforts to grow graphene epitaxially by thermal decomposition of SiC, or by vapor deposition of hydrocarbons on catalytic metallic surfaces which could later be etched away leaving graphene on an insulating substrate.

This stable crystal has attracted considerable attention because of its unusual effective many-body properties, quasi-particle properties and its Landau Fermi liquid picture and the effect of electron-electron interactions to plasmon behavior and angle resolved photoemission spectroscopy (ARPES). There are significant efforts to control the impurities and defects and minimum conductivity at the Dirac point. Initially, it was believed that this universality is a native property, but recent experimental and theoretical reports indicate that the transport properties are very sensitive to impurities and defects and minimum conductivity is not universal.

Conventional two-dimensional electron gas (2DEG) has been a fertile source of surprising new physics for more than four decades. Although the exploration of graphene is still at an early stage, it is already clear that the strong field properties of Dirac electrons in graphene are different from and as rich as those of a semiconductor heterojunction 2DEG. The Fermi liquid phenomenology of Dirac electrons in graphene and conventional 2DEG have the same structure, since both systems are isotropic and have a single circular Fermi surface. The strength of interaction effects in a conventional 2DEG increases with decreasing carrier density. At low densities, the quasiparticle weight Z is small, the velocity is suppressed, the charge compressibility changes sign from positive to negative, and the spin-susceptibility is strongly enhanced. These effects emerge from an interplay between exchange interactions and quantum fluctuations of charge and spin in the 2DEG.

In the Dirac electrons in graphene, it was shown that interaction effects also become noticeable with decreasing density, although more slowly, that the quasiparticle weight Z tends to larger values, that the velocity is enhanced rather than suppressed, and that the influence of interactions on the compressibility and the spin-susceptibility changes sign. These qualitative differences are due to exchange interactions between electrons near the Fermi surface and electrons in the negative energy sea and to interband contributions to Dirac electrons from charge and spin fluctuations.

Compressibility measurements of conventional 2DEG have been carried out and it is found qualitatively that Coulomb interactions affect the compressibility at sufficiently low electron density or strong coupling constant region. Recently, the local compressibility of graphene has been measured using a scannable single electron transistor and it is argued that the measured compressibility is well described by the kinetic energy contribution and it is suggested that exchange and correlation effects have canceling contributions. From the theoretical point of view, the compressibility was first calculated by Peres et al. considering the exchange contribution to the non-interacting doped or undoped graphene flake. A related quantity ∂μ/∂n (where μ is the chemical potential and n is the electron density) is recently considered by Hwang et al. within the same approximation. Going beyond the exchange contribution, the correlation effects were taken into account by Barlas et al. based on an evaluation of graphene’s exchange and random phase approximation (RPA) correlation energies. Moreover, Sheehy and Schmalian by exploiting the proximity to relativistic electron quantum critical point, derived explicit expressions for the temperature and density dependence of...
the compressibility properties of graphene. All these theoretical efforts have been carried out for clean systems. Since disorder is unavoidable in any material, there has been great interest in trying to understand how disorder affects the physics of electrons in material science specially here in graphene and its transport properties.

Our aim in this work is to study the ground-state properties in the presence of electron-impurity and electron-electron interactions. For this purpose, we use the self-consistent theory of Götz et al. to calculate the scattering rate, ground-state energy and the compressibility of the system at the level of RPA including disorder effects. Our calculation is in the same spirit of our earlier work on conventional 2DEG. We note that recent work of Adam et al. also use a self-consistent approach where the impurity scattering by the charge carriers is treated self-consistently in the RPA and the static conductivity is calculated in the Boltzmann kinetic theory. Thus, the main difference between the present work and that of Adam et al. is that we are interested in a thermodynamic quantity (compressibility) whereas the latter is aimed at calculating a transport property (conductivity). We also remark that direct solution of Dirac equation for Dirac-like electrons incorporating the charge impurities has been discussed by Novikov and the validity of the Born approximation is seriously questioned. Similar work has been carried out by Pereira et al. in which they studied the problem of a Coulomb charge and calculated the local density of state and local charge by solving the Dirac equation. They found new characteristics of bound states and strong renormalization of the van Hove singularities in the lattice description that are beyond the Dirac equation.

In this work, we consider the charged impurity and the surface-roughness potentials which are established experimentally to be important. It has been demonstrated that a short-range scattering potential is irrelevant for electronic properties of graphene. We have used the same method to investigate some properties of the conventional 2DEG. In this paper, we point out the differences between the graphene and conventional 2DEG due to disorder effects. The scattering rate behavior within our self-consistent theory shows that impurity scattering cannot localize the carriers in graphene. The effect of disorder on spin susceptibility is similar to that on compressibility and accordingly we will not show any result for spin susceptibility.

The rest of this paper is organized as follows. In Sec. II, we introduce the models for self-consistent calculation of impurities effect. We then outline the calculation of compressibility. Section III contains our numerical calculations of ground state properties and comparison of models with recent experimental measurements. We conclude in Sec. IV with a brief summary.

II. THEORETICAL MODEL

We consider a system of 2D Dirac-like electrons interacting via the Coulomb potential $e^2/er$ and its Fourier transform $v_q = 2\pi e^2/(eq)$ where $e$ is the background dielectric constant. The Dirac electron gas Hamiltonian on a graphene sheet is given by

$$\hat{H} = v \sum_{\mathbf{k},\alpha} \psi_{\mathbf{k},\alpha}^\dagger \left[ \tau^3 \otimes \sigma \cdot \mathbf{k} \right] \psi_{\mathbf{k},\alpha} + \frac{1}{2A} \sum_{\mathbf{q} \neq 0} v_q (\hat{n}_{\mathbf{q}} \hat{a}_{-\mathbf{q}} - \hat{N})$$

(1)

where $v = 3t_0/2$ is the Fermi velocity, $t$ is the tight-binding hopping integral, $a$ is the spacing of the honeycomb lattice, $A$ is the sample area and $\hat{N}$ is the total number operator. Here $\tau^3$ is a Pauli matrix that acts on $K$ and $K'$ two-degenerate valleys at which $\pi$ and $\pi^*$ bands touch and $\sigma^1$ and $\sigma^2$ are Pauli matrices that act on graphene’s pseudospin degrees of freedom.

A central quantity in the theoretical formulation of the many-body effects in Dirac fermions is the dynamical polarizability tensor $\chi^{(0)}(\mathbf{q}, i\Omega, \mu \neq 0)$ where $\mu$ is chemical potential. This is defined through the one-body noninteracting Green’s functions. The density-density response function $\chi^{(0)}(\mathbf{q}, \Omega, \mu)$ of the doped two-dimensional Dirac electron model was first considered by Shung as a step toward a theory of collective excitations in graphite. The Dirac electron $\chi^{(0)}(\mathbf{q}, \Omega, \mu)$ expression has been considered recently by us and others. Implementing the Green’s function $G^{(0)}(\mathbf{k}, \omega, \mu)$ in the calculation a closed form expression for $\chi^{(0)}(\mathbf{q}, i\Omega, \mu \neq 0)$ is found. To describe the properties of Dirac electrons we define a dimensionless coupling constant $\alpha_{gr} = g_e^2/v \epsilon h$ where $g = g_e g_s = 4$ is the valley and spin degeneracy.

The effect of disorder is to dampen the charge-density fluctuations and results to modify the dynamical polarizability tensor. Within the relaxation time approximation the modified $\chi^{(0)}(\mathbf{q}, i\Omega, \mu, \Gamma)$ is given by

$$\chi^{(0)}(\mathbf{q}, i\Omega, \mu, \Gamma) = \frac{\chi^{(0)}(\mathbf{q}, i\Omega + i\Gamma, \mu)}{1 - \frac{\Gamma}{\Gamma + \Gamma} \frac{\chi^{(0)}(\mathbf{q}, i\Omega + i\Gamma, \mu)}{\chi^{(0)}(\mathbf{q})}},$$

(2)

in which the strength of damping is represented by $\Gamma$. To include the many-body effects, we consider the density-density correlation function within the RPA,

$$\chi_{\rho\rho}(\mathbf{q}, i\Omega, \mu, \Gamma) = \frac{\chi^{(0)}(\mathbf{q}, i\Omega, \mu, \Gamma)}{1 - v_q \chi^{(0)}(\mathbf{q}, i\Omega, \mu, \Gamma)}.$$

(3)

As the short-range disorder is shown to have negligible effect in the transport properties of graphene, we consider long-ranged charged impurity scattering and surface roughness as the main sources of disorder. The latter mechanism also known as ripples comes either from thermal fluctuations or interaction with the substrate. The disorder averaged surface roughness (ripples) potential (SRP) is modeled as

$$\langle |U_{surf}(q)|^2 \rangle = \pi \Delta^2 \hbar^2 (2\pi e^2 n/e)^2 e^{-\sigma^2 \Delta^2 / 4},$$

(4)
where \( h \) and \( \Delta \) are parameters describing fluctuations in the height and width, respectively. We can use the experimental results of Meyer et al., who estimate \( \Delta \sim 10 \) nm and \( h \sim 0.5 \) nm. It is important to point out that there are other models to take into account the surface-roughness potential. The effect of bending of the graphene sheet has been studied by Kim and Castro Neto. This model has two main effects, firstly the decrease of the distance between carbon atoms and secondly a rotation of the \( p_z \) orbitals. Due to bending the electrons are subject to a potential which depends on the structure of the graphene sheet. Another possible model is described by Katsnelson and Geim, considering the change in in-plane displacements and out-of-plane displacements due to the local curvature of a graphene sheet. Consequently, the change of the atomic displacements results to change in nearest-neighbour hopping parameters which is equivalent to the appearance of a random gauge field described by a vector potential. These different models need to be implemented in our scheme and to be checked numerically to assess their validity in comparison to the available measurements.

The charged disorder potential (CDP) is taken to be

\[
|U_{\text{imp}}(q)|^2 = n_i e^2 e^{-2qd},
\]

in which \( n_i \) is the density of impurities and \( d \) is the setback distance from the graphene sheet.

We use the mode-coupling approximation introduced by Götze to express the total scattering rate in terms of the screened disorder potentials

\[
i\Gamma = \frac{v_F k_F}{2\hbar n A} \sum_q \left[ \langle |U_{\text{imp}}(q)|^2 \rangle \right] \frac{\varphi_0(q, i\Gamma)}{\varepsilon^2(q)} + \frac{\langle |U_{\text{surf}}(q)|^2 \rangle}{\varepsilon^2(q)} \frac{\varphi_0(q, i\Gamma)}{1 + i\Gamma \varphi_0(q, i\Gamma) / \chi^0(q)},
\]

where \( \varepsilon(q) = 1 - \varphi_0(q, i\Gamma) / \chi^0(q) \) is the static screening function and \( \varphi_0(q, i\Gamma) / \chi^0(q) \) is the relaxation function for electrons scattering from disorder.

Since the scattering rate \( \Gamma \) depends on the relaxation function \( \varphi_0(q, i\Gamma) \), which itself is determined by the disorder included response function, the above equation needs to be solved self-consistently to yield eventually the scattering rate as a function of the coupling constant. Note that at the present level of approximation (i.e., RPA) the static dielectric function \( \varepsilon(q) \) does not depend on \( \Gamma \). In the conventional 2DEG correlation effects beyond the RPA (through the local-field factor) render \( \varepsilon(q) \) also \( \Gamma \) dependent.

The ground state energy is calculated using the coupling constant integration technique, which has the contributions \( E_{\text{tot}} = E_{\text{kin}} + E_x + E_c \).

The first-order “exchange” contribution per particle is given by

\[
\varepsilon_x = \frac{E_x}{N} = \frac{1}{2} \int \frac{d^2 q}{(2\pi)^2} v_q
\]

To evaluate the correlation energy in the RPA, we follow a standard strategy for uniform continuum models.

\[
\varepsilon_{\text{RPA}}^c = \frac{E_c}{N} \int \frac{d^2 q}{(2\pi)^2} \int_0^{+\infty} d\Omega \left\{ v_q \chi^{(0)}(q, i\Omega, \mu, \Gamma) - 1 \right\}.
\]

Since \( \chi^{(0)}(q, \Omega, \mu, \Gamma) \) is linearly proportional to \( q \) at large \( q \) and decrease only like \( \omega^{-1} \) at large \( \omega \), accordingly the exchange and correlation energy built by Eqs. (7) and (8) is divergent. In order to improve convergence, it is convenient at this point to add and subtract \( \chi^{(0)}(q, i\Omega, \mu = 0, 2\Gamma) \) inside the frequency integral and regularize the exchange and correlation energy. Therefore, these ultraviolet divergences can be cured calculating

\[
\delta\varepsilon_x = -\frac{1}{2\pi n} \int \frac{d^2 q}{(2\pi)^2} v_q \int_0^{+\infty} d\Omega \delta\chi^{(0)}(q, i\Omega, \mu, \Gamma)
\]

and

\[
\delta\varepsilon_{\text{RPA}}^c = \frac{1}{2\pi n} \int \frac{d^2 q}{(2\pi)^2} \int_0^{+\infty} d\Omega \left\{ v_q \delta\chi^{(0)}(q, i\Omega, \mu, \Gamma) - 1 \right\}.
\]

where \( \delta\chi^{(0)} \) is the difference between the doped (\( \mu \neq 0 \)) and undoped (\( \mu = 0 \)) polarizability functions. With this regularization the \( q \) integrals have logarithmic ultraviolet divergences, we can introduce an ultraviolet cutoff for
the wave vector integrals $k_c = \Lambda k_F$ which is the order of
the inverse lattice spacing and $\Lambda$ is dimensionless quan-tity. Fermi momentum is related to density as given by
$k_F = (4\pi n/g)^{1/2}$. Once the ground state is obtained the
compressibility $\kappa$ can easily be calculated from
\[ \kappa^{-1} = n^2 \frac{\partial^2 (n\delta\varepsilon_{\text{tot}})}{\partial n^2}, \]
where the total ground-state energy is given by $\delta\varepsilon_{\text{tot}} = \delta\varepsilon_{\text{kin}} + \delta\varepsilon_x + \delta\varepsilon_{\text{RPA}}$. Here the zeroth-order kinetic contribution to the ground-state energy is $\delta\varepsilon_{\text{kin}} = \frac{\hbar^2}{2m}$. We con-sider the dimensionless ratio $\kappa / \kappa_0$ where $\kappa_0 = 2/(n\varepsilon_F)$ is the compressibility of the noninteracting system.

\[ \textbf{FIG. 2:} (Color online) (a): The correlation energy $\delta\varepsilon_c$ as a function of the coupling constant $\alpha_{gr}$ for cut-off value $\Lambda = k_c/k_F = 50$. (b): The exchange energy $\delta\varepsilon_x$ as a function of the coupling constant $\alpha_{gr}$ for cut-off value $\Lambda = 50$. Results of fixed $\Gamma$ values are compared to those calculated within the mode-coupling approximation.\]

\[ \text{III. NUMERICAL RESULTS} \]

In this section we present our calculations for ground
state properties of graphene in present of impurities that
we model them as mentioned above. The inverse com-presibility $1/(n^2\kappa)$ is calculated by using the theoretical
models described above and compare them with the re-
cent experimental measurements. In all numerical calcu-
lations we consider $d = 0.5$ nm. Electron density is taken to be $1 \times 10^{12}$ cm$^{-2}$ for Figs. 1-3.

Increasing disorder (increasing $n_i$ or decreasing $d$ for charge-disorder potential or increasing $h$ for surface roughness potential) decrease the $\chi^{(0)}(q, \Omega, \mu, \Gamma)$ as the scattering rate $\Gamma$ gets bigger. Thus, decreasing $\chi^{(0)}(q, \Omega, \mu, \Gamma)$ (or increasing correlation effects) results in a stronger disorder potential. Despite $\Gamma$ increases with increasing $\alpha_{gr}$, apparently it turns to a saturation limit and does not diverge. This behavior is quite different than what is seen in conventional 2DEG when the many-body effects influence the scattering rate through the local-field factor. In the conventional 2DEG sys-
tem, at a critical level of disorder this nonlinear feedback causes $\Gamma$ to increase rapidly and diverge, which is taken as an indication for the localization of carriers. However, in graphene, our calculations show that the $\Gamma$ does not diverge therefore impurities cannot localize carriers and we have a weakly localized system in the presence of impu-
rities compatible with experimental observations. We can understand the saturated behavior of $\Gamma$ qualitatively as follows. In the context of conventional 2DEG, Mott argument says that the mean-free path $l$ in a metal could not be shorter than the wavelength $\lambda$. Since $l$ is propor-
tional to the inverse of $\Gamma$, for large values of $\Gamma$ obtained in 2DEG, the electron mean-free path decreases and be-
comes less than or equal to $\lambda$. At this point we should have a metal-insulator phase transition. In the context of graphene, on the other hand, Mott’s argument is similar to that light does not notice any roughness (one source of scattering) on a scale shorter than its wavelength. Conse-
quently there is a lower limit for the electron’s mean-free path in graphene and it turns out that we would have a maximum (saturation) value for $\Gamma$.

The issue of localization in graphene has recently at-
ttracted some attention and the chiral nature of elec-
tron behavior has been discussed in the literature. Suzuura and Ando claimed that the quantum correction to the conductivity in graphene can differ from what is observed in normal 2DEG due to the nature of elas-
tic scattering in graphene possibly changing the sign of
the localization correction and turn weak localization into weak antilocalization for the region when intervalley scat-
tering time is much larger than the phase coherence time.

Further consideration of the behavior of the quantum cor-
rection to the conductivity in graphene conclude that this behavior is entirely suppressed due to time-reversal symmetry breaking of electronic states around each de-
egenerate valley.

We have found through our calculations that $\Gamma$ in-
creases with increasing $n_i / n$ as a function of $\alpha_{gr}$. Fig-
ure 1 shows $\Gamma$ for various scattering mechanisms. As it is clear, CDP is the dominant mechanism for $\Gamma$ in our
model. The effect of SRP is mostly negligible, except at large values of the coupling constant. This finding is to be contrasted with the the statement of Martin et al. that both substrate induced structural distortions (SRP) and chemical doping (CDP) are conceivable sources of
density fluctuations. We stress that our model calculations indicate that at realistic coupling constant values (c.f. Fig. 1) only the charged impurity scattering dominates.

![Graph showing the inverse compressibility as a function of impurity density](image1)

**FIG. 3:** (Color online) The compressibility $\kappa/\kappa_0$ scaled by that of a noninteracting clean system as a function of the coupling constant $\alpha_{gr}$ for cut-off value $\Lambda = 50$.

![Graph showing the inverse compressibility as a function of electron density](image2)

**FIG. 4:** (Color online) The inverse compressibility $[n^2\kappa]^{-1} = \partial \mu / \partial n$ (in units of meV $10^{-10}$ cm$^2$) as a function of the electron density (in units of $10^{12}$ cm$^{-2}$). The filled squares are the experimental data by Martin et al.$^{18}$.

We have calculated the exchange and correlation energies as a function of $\alpha_{gr}$ in the presence of disorder. It is found that the disorder effects become more appreciable at large coupling constants, within the mode coupling approximation. The exchange energy is positive because our regularization procedure implicitly selects the chemical potential of undoped graphene as the zero of energy; doping either occupies quasiparticle states with positive energies or empties quasiparticles with negative energies. Figure 2(a) shows the correlation energy $\delta \varepsilon_c$ as a function of $\alpha_{gr}$. It appears that the disorder effects become more appreciable at large coupling constant. Note that $\delta \varepsilon_c$ has the same density dependence as $\delta \varepsilon_x$ apart from the weak dependence on $\Lambda$. In contrast to the exchange energy, Figure 2(b), the correlation energy is negative. Figure 3 shows the charge compressibility, $\kappa/\kappa_0$ scaled by its non-interacting contribution as a function of $\alpha_{gr}$ for various models of $\Gamma$. The behavior of $\kappa$ shows some novel physics, which is qualitatively different from the physics known in the conventional 2DEG. Exchange makes a positive contribution to the inverse compressibility and thus tends to reduce (rather than enhance) the compressibility. On the other hand, correlations make a negative contribution to the inverse compressibility and thus tends to enhance $\kappa$. In the conventional 2DEG both contributions tend to enhance the compressibility. In the case of graphene instead, apparently exchange and correlation compete with each other in determining the compressibility of the system. It is interesting to note that similar physics is true also in the spin susceptibility.

In Fig. 4 we compare our theoretical predictions for the inverse compressibility of doped graphene with the experimental results of Martin et al.$^{18}$. For definiteness we take $\Lambda = k_e/k_F$ to be such that $\pi(\Lambda k_F)^2 = (2\pi)^2/\mathcal{A}_0$, where $\mathcal{A}_0 = 3\sqrt{3}a_0^2/2$ is the area of the unit cell in the honeycomb lattice, with $a_0 \approx 1.42$ Å the carbon-carbon distance. With this choice $\Lambda \approx (gn^{-1}\sqrt{3/9.09})^{1/2} \times 10^2$, where $n$ is the electron density in units of $10^{12}$ cm$^{-2}$. Martin et al.$^{18}$ fitted the experimental inverse compressibility, $(n^2\kappa)^{-1}$ to the kinetic term using a single parameter Fermi velocity which is larger than the bare Fermi velocity. Note that the kinetic term in graphene has the same density dependence as the leading exchange and correlations terms.

As it is clear in Fig. 4 the inverse compressibility of noninteracting system is below the experimental data. By increasing the interaction effects, i.e., increasing the coupling constant strength, $\alpha_{gr}$ our theoretical results move up. Unfortunately, in the experimental sample, the value of $\alpha_{gr}$ is not specified and we considered it to be $\approx 1$. Therefore, including the exchange-correlation effects in our RPA theory, gives results very close to experimental data. Furthermore, the results of incorporating impurity density, $n_i = 10^{10}$ cm$^{-2}$ in the system and solving the self-consistent equations to obtain the scattering rate value, yield very good agreement with the measured values in the large and middle electron density regions. We have examined the inverse compressibility by the kinetic term contribution only including a fitting value for Fermi velocity and our numerical results are well described by a fitting velocity about $1.28 v_F$. We would stress here that this fitting velocity is different from the renormalized velocity defined within the Landau-Fermi liquid theory in graphene.

In a recent calculation of $\partial \mu / \partial n$ within the Hartree-Fock approximation in graphene where $\mu$ is the chemical potential and $n$ is the electron density Hwang et al.$^{20}$ stated that correlation and disorder effects would only introduce small corrections. This is not, in general, true since it has been shown by Barlas et al.$^{4}$ that the correlation effects are essential in the ground-state properties.
Although these effects are not significant in very weak interaction strength regime and high electron density, including many-body exchange-correlation effects together with disorder effect are necessary to get agreement with quantities measured in experiments of Martin et al. It would be useful to carry out further experimental work at larger interaction strengths to assess the role played by correlation effects.

IV. CONCLUSION

We have studied the ground state thermodynamic properties of a graphene sheet within the random phase approximation incorporating the impurities in the system. Our approach is based on a self-consistent calculation between impurity effect and many-body electron-electron interaction. We have used a model surface roughness potential together with the charged disorder potential in the system. Our calculations of inverse compressibility compared with recent experimental results of Martin et al. demonstrate the importance of including correlation effects together with disorder effects correctly in the thermodynamic quantities.

We remark that in a very small density region, the system is highly inhomogeneous where experimental data tends to a constant and the effect of the impurities are very essential. A model going beyond the RPA is necessary to account for increasing correlation effects at low density. To describe the experimental data in this region more sophisticated theoretical methods which incorporate inhomogeneities are needed. One approach would be the density-functional theory where Dirac electrons in the presence of impurities are considered.

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$$(d\rho/dt)_{coll} = -\gamma(\rho - \rho_0) - \gamma(\rho - \rho_v)$$.

We assume that $\rho_0 = \rho_v$. 

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