Quantum Bohm correction to polarization spectrum of graphene

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In this paper, by using a quantum hydrodynamic plasma model which incorporates the important quantum statistical pressure and electron diffraction force, we present the corrected plasmon dispersion relation for graphene which includes a $k^4$ quantum term arising from the collective electron density wave interference effects. This correction may well describe the shortening of the previous results based on the classical hydrodynamics and confirms that the quantum hydrodynamic model may be as effective as the random phase approximation in successful description of the collective density excitations in quantum plasmas. It is clearly observed that the quantum correction due to the collective interaction of electron waves gives rise to significant contribution in the dispersion behavior of the collective plasmon density waves in a wide range of wavelength, as a fundamental property of the monolayer atom-thick graphene. It is revealed that the plasmon density-perturbation linear phase-speed in graphene possesses some universal minimum characteristic value, in the absence of an external magnetic field. It is further remarked that such correction also has important effect on the dielectric function, hence on the impurity screening, in graphene. © 2013 AIP Publishing LLC.

I. INTRODUCTION

Graphene, despite the emergence in recent few years, has become one of the most amazing and technologically appealing fields of scientific research which has captured enormous amount of attention among researchers of diverse fields. The ideal atom-thick honeycomb monolayer lattice of carbon atoms has brought into existence many exciting features absent in ordinary materials, including a celebrated 2010 Nobel Prize for its experimental discoverers, Geim and Novoselov. The dense monolayer honeycomb arrangement of carbon atoms, with photon-like massless energy relation, has made it possible for the charge carriers in graphene to mimic both relativistic and quantum effects at the same time, making also possible to observe the relativistic quantum electrodynamical effects within the laboratory, which until now have been expected to occur in the core of super-dense astrophysical compact objects such as white dwarf stars. The existence of such earthly remarkable effects is due to the photon-like linear energy dispersion character of the low-energy electron hopping excitations between the so called Dirac points of the graphene lattice. Recent investigations reveal that graphene nonlinearly responds to a wide range of electromagnetic spectrum in the terahertz frequency range. Furthermore, the dynamic frequency-dependent conductivity of graphene with strong nonlinear characteristics predicts its very promising applications in developments of future advanced terahertz source and detector technologies (terahertz gap technology). Particularly, the discovery of frequency multiplication property of graphene has many applications in fabrication of the low-power terahertz electromagnetic radiation and detection devices. It has been found that graphene, usually considered as a gapless semiconductor, shows a profoundly different behavior from semiconductors, regarding the plasmon excitation resonances. Recent investigations reveal the possibility of propagation of the strongly localized electromagnetic surface transverse electric and magnetic plasmons as well as electromagnetic and electrostatic solitary excitations in graphene.

On the other hand, graphene may provide us with important information on the matter under extreme external pressure. In the core of a gravitationally compressed massive compact star the plasma matter undergoes a critical change in the equation of state (EoS) due to the change in degeneracy state the so called relativistic degeneracy state, where the relativistic and quantum statistical effects become equally important. In the ultra-relativistic degeneracy limit this effect leads to the well known supernova phenomenon, which is expected to happen in some rare astrophysical occasions due to the existence of over critical dense regions in the stellar core. In the ultra-relativistic degeneracy limit the free electrons achieve the photon-like energy dispersion, just like the low energy exciting Dirac electrons in graphene. The extreme-relativistic state of matter is well-known for the Chandrasekhar mass limit on white dwarfs and causes the ultimate faith of compact objects in the main sequence stars. Therefore, it is remarkable that the newly discovered graphene can provide us with a unique opportunity for inspection of the fundamental physics of matter under extreme conditions in order to explore the relativistic quantum effects on earth. More recently, there has been an experimental support for the atomic collapse with ultra-relativistic electrons in a heavy-ion doped graphene. Such effect has also been predicted to occur in superdense plasma of white dwarf cores due to the prevalence of the extreme-relativistic degeneracy effects, the core crystallization, and collapse.
The quantum hydrodynamics (QHD) model, since the first developments\textsuperscript{25–32} several decades ago, has become one of the most convenient and useful methods in description of collective modes in quantum plasmas. A great deal of research appeared in recent years, inspecting the quantum plasma effects within the framework of QHD and quantum magnetohydrodynamic (QMHD) models, including the electron spin polarization and exchange-correlation effects. Recent development of effective hydrodynamic models incorporating the electron recoil, spin magnetization, and relativistic effects\textsuperscript{33–43} has turned the hydrodynamics approach into a direct method of evaluation of the collective modes in wide variety of plasmas. The most important component of a QHD, which causes different dispersion effects in a quantum plasma compared to that of a classical counterpart, is the degeneracy pressure.\textsuperscript{44} However, the second order effects, such as the quantum electron diffraction and spin magnetization effects, has been shown to lead to observable effects\textsuperscript{34–48} on ion acoustic and magnetosonic wave propagations and instabilities in quantum plasmas. Recently, different hydrodynamic models\textsuperscript{41,42,49,50} has been developed which incorporates the effects caused by relativistic quantum electrons in plasmas. Particularly, the application of the classical relativistic hydrodynamic model for graphene has been shown to be successful in description of the unexpected minimum conductivity of this material.\textsuperscript{51} In our study we will shown to be successful in description of the unexpected minimum conductivity of this material. In our study we will...
positive background ion number-density, respectively, with \( q = -e \) being the electron charge state. It is clearly noted that in the electron-momentum equation the terms appearing in the right hand side are the Lorentz, degeneracy pressure, collective induced electrostatic, and the quantum Bohm forces, respectively. The major difference of the current hydrodynamics model with that of Ref. 55 is that we included the quantum diffusion effect represented by the Bohm quantum correction which attributes to the quantum wave-interference of electronic density. As will be apparent soon, this component contributes a significant correction to the spectrum of collective polarization in graphene.

In order to calculate the important quantum degeneracy pressure for fermions in the electron fluid, i.e., \( P_{\text{deg}} \), we assume that the plasma is in complete degeneracy state. This of-course is true if \( \lambda_{D} \ll a \) where \( \lambda_{D} = h/\sqrt{2\pi n_{0}k_{B}T_{p}} \) is the de Broglie thermal wavelength (with \( h \), \( k_{B} \), and \( T_{p} \) being the scaled Plank constant, the Boltzmann constant and the particle temperature, respectively). It can be observed that for the two and three dimensional electron gases the degeneracy condition occurs for \( n_{0} \gg 10^{11} \text{ cm}^{-2} \) and \( n_{0} \gg 10^{16} \text{ cm}^{-3} \) at room temperature, quite satisfied for the monolayer two-dimensional graphene with the typical electron density of \( n_{0} \approx 10^{13} \text{ cm}^{-2} \). Hence, a well-defined Fermi wavevector, \( k_{F} \), exists assuming the above number-density criteria, with \( n_{0} = \int_{k_{F}}^{\infty} dk/k/(2\pi)^{3} \), where \( \eta \) is the system dimensionality. Moreover, using the thermodynamical identity, \( P = n(\partial e/\partial n) - e \), with \( e = \int_{k_{F}}^{\infty} E(k) dk \), and \( E(k) \) being the corresponding energy dispersion relation, one is able to easily obtain the following pressure components of the Fermi and Dirac electron plasmas in different dimensionality

\[
P_{2D} = \frac{\sqrt{2\pi}}{3} \hbar v_{F} n^{3/2}, \quad P_{3D} = \frac{(3\pi^{2})^{2/3}}{12\pi^{2}} \hbar v_{F} n^{4/3},
\]

\[
P_{2F} = \frac{\pi h^{2} n^{2}}{2m_{e}}, \quad P_{3F} = \frac{(3\pi^{2})^{2/3}h^{2} n^{3/3}}{5m_{e}}.
\]

It is particularly interesting to note that, like for photons, for the Dirac electron fluids the relation \( P = e/\eta \) holds, in general. In what follows we will use the model equations (Eq. (1)), which include all quantum features such as the collective Bohm and the statistical quantum degeneracy pressure component given by Eq. (2), in order to calculate the corresponding dispersion relation and plasmon excitations mode dispersion of graphene.

### III. THE DIELECTRIC FUNCTION AND QHD PLASMON SPECTRUM

To make use of simplicity and without loss of generality, we assume a linear density wave propagating in \( x \)-direction which happens to be the electrostatic field vector \( E \). This means that \( B = \{0, 0, B_{0}\} \), \( k = \{k, 0, 0\} \) and \( E = \{E_{x}, 0, 0\} \), hence, \( \mathbf{J} \times \mathbf{B} = \{J_{y}, -J_{x}, 0\} \). Also, the collective induced electrostatic potential can be written as

\[
\varphi_{\text{ind}}(r) = \int \frac{\delta n(r')}{r-r'} d^{3}r',
\]

where the \( \delta n(r) \) is the local variations in the electron number-density. Therefore, the QHD equations in reduced coordinate, \( (x,t) \), can be written as follows:

\[
e \frac{\partial n}{\partial t} = \frac{\partial I_{s}}{\partial x} = 0,
\]

\[
m_{e} \frac{dJ_{s}}{dt} = -eJ_{s}B_{0} + e \frac{\partial P_{\text{deg}}}{\partial x} - e^{2} n \frac{\partial}{\partial x} \left( \frac{\partial n}{x-x'} dx' \right)
\]

\[
- e n \hbar^{2} \frac{\partial}{\partial x} \left[ \frac{1}{\sqrt{n}} \frac{\partial n}{\partial x'} \right].
\]

### (4)

Also, the collective induced electrostatic, and the quantum Bohm correction which attributes to the quantum wave-interference of electronic density. As will be apparent soon, this component contributes a significant correction to the spectrum of collective polarization in graphene.

\[
m_{e} \frac{dJ_{s}}{dt} = eJ_{s}B_{0},
\]

\[
\frac{\partial E_{s}}{\partial x} = -4\pi e \delta n.
\]

Assuming a general plane-wave solutions of the form, \( n = n_{0} + n_{1} \exp(ikx-i\omega t) \), \( E_{x} = E_{1} \exp(ikx-i\omega t) \) and \( J_{(x,y)} = J_{(1,x,y)} \exp(ikx-i\omega t) \) and ignoring the nonlinear terms, we arrive at the linear equations

\[
kJ_{1x} + e \omega n_{1} = 0,
\]

\[
im \omega J_{1y} + eB_{0} J_{1x} = 0,
\]

\[
\frac{ie kE_{x}}{2} n_{1} + k^{n_{0} e^{2}} E_{1x} + \frac{ie h^{2} k^{3}}{4m_{e}} n_{1} + im \omega J_{1x} = 0\]

\[
- eB_{0} J_{1y} = 0,
\]

where we have used the 2D Fourier transform of the Coulomb force, \( \nabla \phi(x) \) to obtain \( \nabla_{k} \phi(k) = 2\pi k^{2} e^{2} n_{1}/k \) with \( 4\pi e n_{1} = k E_{1x} \), which is obtained by Fourier transforming the Poisson’s relation in Eq. (4). Solving the linearized equations (Eq. (5)), we arrive at the conductivity components for the two-dimensional magnetized graphene as

\[
\begin{pmatrix}
J_{1x} \\
J_{1y}
\end{pmatrix} =
\begin{bmatrix}
\sigma_{xx} & \sigma_{xy} \\
\sigma_{yx} & \sigma_{yy}
\end{bmatrix}
\begin{pmatrix}
E_{1x} \\
0
\end{pmatrix},
\]

with \( \sigma_{xx} \) and \( \sigma_{yy} \) being the diagonal and off-diagonal conductivity components, respectively, given as below

\[
\sigma_{xx} = - \frac{2e^{2} n_{0} E_{x}}{4B_{0} e^{2} + h^{2} k^{4} v_{F}^{4}}
\]

\[
\sigma_{xy} = \frac{2e^{2} B_{0} n_{0} v_{F}^{2}}{4B_{0} e^{2} + h^{2} k^{4} v_{F}^{4}}
\]

Using the relations \( D_{xx} = 1 + 4\pi i \sigma_{xx}/\omega \) and \( D_{xy} = 1 + 4\pi i \sigma_{xy}/\omega \), we may derive the dielectric function \( D_{xx} \) with the wavenumber \( k_{F} \) normalized by \( k_{F} = \sqrt{2n_{0}} \) and the frequency \( \omega \) by \( \omega_{F} = k_{F} v_{F} \) as

\[
D_{xx} = 1 + \frac{\alpha k}{\Omega^{2} + k^{2}/2 + k^{4}/4 - \omega^{2}}, \quad \Omega = \frac{\omega}{\omega_{F}},
\]

with \( \omega_{F} = eB_{0}/m_{e} \) and \( \alpha = e^{2}/\hbar v_{F} \) being the electron cyclotron frequency and the fine-structure constant for graphene, respectively. The dielectric function (Eq. (8)) includes the quantum Bohm correction which is reflected in the term...
The extended dispersion relation is obtained as 
\[ \omega = \sqrt{\Omega^2 + 2k + k^2/2 + k^4/4}, \]
which reduces to the dispersion relation reported in Ref. 55 when \( k^4 \) term corresponding to higher-order quantum correction is ignored. The above quantum corrected dispersion of graphene up to the \( k^2 \)-order is completely consistent with the \( k \rightarrow 0 \) limit dispersion given by Eq. (7) in Ref. 58 which has been obtained using the RPA method, while, the \( q^2 \) dispersion component given in Eq. (5.66) of Ref. 59 obtained also via the RPA approach gives rise to a negative sign for the second-order, \( k^2 \), correction term which is inconsistent with that of our and Ref. 58. However, unlike the previous works, Refs. 52, 55, 58, and 59, in this research we find an analytic closed form of the graphene dispersion up to the fourth order in wavenumber. Also, it should be noted that the \( k^4 \) contribution is positive in dispersion consistent with original findings of Klimontovich and Silin and Bohm and Pines for quantum plasmas.

The potential around a static test charge may be easily obtained from the unmagnetized static dielectric function \( D_{xx} = D_{xx}(\Omega = 0, \omega = 0) \) as
\[ \phi(r) = \frac{Q}{\pi} \left[ \int_0^\infty \exp(ikr \cos \theta) dk \right], \]
where \( Q \) is the screened charge state. It is easily confirmed that it is not possible to obtain an analytical solution for the screened potential and it might be evaluated numerically which is beyond the purpose of the current research.

**IV. RESULTS AND DISCUSSION**

In Fig. 1 we have shown the dispersion curve for graphene and its variation with respect to the change in the applied perpendicular magnetic field strength. The dashed curve in Fig. 1(a) represents the classical hydrodynamic dispersion relation, given in Ref. 55, and the solid line represents the quadratic form (up to order \( k^2 \)) quantum corrected dispersion spectrum. Figure 1(a) clearly shows a significant contribution of the quantum Bohm correction on the plasmon dispersion spectrum. It is observed that while the classical and quantum corrected dispersions match at the long wavelength limit, the quantum corrected curve rapidly departs from that of the classical one as the wavenumber is increased. Roldán et al. have correctly attributed the shortcoming of classical hydrodynamic dispersion and its deviations from that of the RPA, to the ignorance of the important Bohm collective electron diffraction effect in classical hydrodynamic treatment, which is explicitly hidden in the RPA method. Although the \( k^4 \) correction leads to larger corrections than is observed from RPA, shown in Fig. 1 of Ref. 55, however, it should be noted that the RPA dispersion spectrum presented in Fig. 1 of Ref. 55 comes from \( k^2 \) expansion of RPA approach, and for a detailed comparison one needs to take into account the \( k^4 \) term from RPA dispersion expansion.

Therefore, it is concluded that the quantum corrected hydrodynamic model can effectively describe the plasmon dispersion spectrum in degenerate plasmas, since it takes into account the full picture of collective electron-wave interference via the quantum Bohm potential. On the other hand, there may be other minor corrections coming from the electron spin interaction effects such as the electron exchange and correlations or the magnetic polarizations to be considered in a full quantum treatment. Such minor corrections, with contributions proportional to \( k \)-order, can be a future project by easily replacing a generalized effective quantum potential in the conventional QHD model. On the other hand, Fig. 1(b) shows the effect of the normalized cyclotron frequency, \( \Omega = \omega_c/\omega_F \), on the dispersion spectrum.

![Quantum-corrected plasmon spectrum of graphene](image)

**FIG. 1.** The dispersion curves for the polarization spectrum of graphene (a) with and without the quantum Bohm correction and (b) opening of the energy-gap in the spectrum due to the application of a uniform magnetic field perpendicular to the graphene plane. The increase in the thickness of curves reflects the increase in the varied parameter in Fig. 1(b).
of plasmon excitations in graphene. It is shown that the application of the magnetic field opens an energy gap the width of which is linearly proportional to the magnetic field strength, $B_0$ and inversely proportional to the electron number-density, $n_0$. It is however remarked that the magnetic field effect on the plasmon spectrum of graphene becomes exceedingly ineffective as the wavelength is lowered.

The variation of plasmon phase-speed, $v_p = \partial \omega / \partial k$ (normalized to the Fermi-speed, $v_F$), is shown in Fig. 2. Presence of a distinct minimum value is remarked for Fig. 2(a) without the external magnetic field for the quantum corrected plasmon phase-speed. It is interesting to note that, the observed minimum for the phase-speed value is $v_p \approx 1.19v_F$ occurring at $k \approx 0.778k_F$ which is a universal value for graphene and is independent of the career number-density and dependent only on the electron Fermi-speed $v_F \approx c/300$ in graphene. The career number-density itself is known to be a strong function of the temperature and the doping character.

FIG. 2. The variation of the plasmon phase-speed, with (solid curve) and without (dashed curve) the Bohm correction, with respect to wavenumber showing a distinct minimum value in the absence of external magnetic field and (b) in presence of the magnetic field with different field parameters. The increase in the thickness of curves reflects the increase in the varied parameter in Fig. 2(b).

FIG. 3. (a) The effect of the Bohm correction on the inverse of the transverse dielectric function of graphene and (b) the effect of magnetic field parameter on the dielectric function. The horizontal $k$-values are normalized to the Fermi wavenumber, $k_F = \sqrt{2\pi n_0}$. The increase in the thickness of curves reflects the increase in the varied parameter in Fig. 3(b).
or impurity contamination. Therefore, it is observed that, the position and value of the minimum plasmon-wave phase-speed is a universal feature of graphene. However, as it is observed from Fig. 2(b) the phase-speed profile is significantly affected by the magnitude of an external magnetic field. It is observed that, the increase in the external magnetic field strength slightly lowers the minimum phase-speed value and the corresponding wavenumber. It is also revealed that the $k \rightarrow 0$ limit of the phase-speed, unlike the case of un magnetized graphene which diverges at the long-wavelength limit, approaches the value $v_{p}(k \rightarrow 0) = \Omega / 2\Omega$. It is also found that in the low-wavelength limit the phase-speed approaches the value of $\partial v_{p} / \partial k(k \rightarrow \infty) = 1$, regardless of the value of the scaled cyclotron frequency, $\Omega$.

It is clearly remarked that the existence of the minimum value in the phase-speed (the change in plasmon spectrum curvature) is a direct consequence of the quantum electron non-locality effect due to the so-called Bohm quantum potential. This has been previously attributed to the cross-over from the square-root dispersion law of Dirac fermions to the behavior of the conventional 2D electron gas, as the energy is increased. In Fig. 3 we depicted the significant effects of quantum Bohm correction and external magnetic field parameter on the dielectric function of graphene. It is clearly noted that the impurity screening is related to the dielectric function via Eq. (9), hence, is critically affected by the quantum correction and field parameter too. From Figs. 3(a) and 3(b) it is observed that while the quantum correction affects the inverse dielectric function for a wide range at low-wavelength regime, the presence of a uniform external magnetic field affects the inverse dielectric function in high wavelength regime. Although, it is not possible to find an analytic expression for the screening potential in graphene, however, it is clearly remarked that, the quantum Bohm and magnetic field effects can both have significant effects on the screening feature of graphene. Quantum correction has been shown to lead to completely different screening features in quantum plasma and to a Lennard-Jones-like attraction among the constituent ions.

V. SUMMARY

In this paper we used the proper QHD model, which incorporates the essential quantum features such as the statistical pressure and the collective wave interference effects for the electrons in a plasma, to obtain a quantum corrected dispersion spectrum of monolayer graphene up to the quadratic term in the wavevector. It was shown that inclusion of such term has a significant effect on both the dispersion of low-wavelength plasmon (the electron density perturbations) and the screening of a stationary charge in graphene. It was concluded that the QHD model, which captures the essential collective quantum picture of a degenerate electron fluid, can properly account for a more detailed structure of the polarization spectrum of graphene for a wide range of the electron plasmon excitation frequency range. The QHD model applied in this paper may be extended to include other electron interaction features such as the spin polarization and exchange-correlation effects, which is our future project.

61D. Bohm, Phys. Rev. 85, 166 (1952).