Aspects of the theory of graphene

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Following a brief review of the device-friendly features of graphene, recent work on its Green's functions with and without a normal magnetic field are discussed, for an infinite graphene sheet and also for a quantum dot, with analyses of the Landau-quantized energy spectra of the sheet and dot. The random phase approximation dielectric response of graphene is reviewed and discussed in connection with the van der Waals interactions of a graphene sheet with atoms/molecules and with a second graphene sheet in a double layer. Energy-loss spectroscopy for a graphene sheet subject to both parallel and perpendicular particle probes of its dynamic, non-local response properties are also treated. Furthermore, we discuss recent work on the coupling of a graphene plasmon and a surface plasmon, yielding a collective plasma mode that is linear in wavenumber. Finally, we discuss the unusual aspects of graphene conduction and recent work on diffusive charge transport in graphene, in both the DC and AC regimes.

Keywords: graphene; transport; dielectric properties

1. Introduction

Owing to its remarkable properties and its strong potential to provide the material basis for a new generation of electronic devices, graphene has been the subject of massive research throughout the world since the first experiments in 2004 (Das Sarma et al. 2007a; Geim & Novoselov 2007; Castro Neto et al. 2009; Geim 2009). It is one of the most heavily researched materials ever (Barth & Marx 2008). Graphene is a single-atom-thick two-dimensional planar layer of carbon atoms in a hexagonal honeycombed array composed of two superposed triangular sub-lattices. The band structure of graphene involves two nodal zero-gap (‘Dirac’) points (\(K, K'\)) in the first Brillouin zone at which the conduction and valence bands touch. In the vicinity of these points, the low-energy electron/hole energy dispersion relation is proportional to momentum, rather than its square. This is analogous to the energy dispersion relation of massless relativistic electrons, so the electrons/holes of graphene are described as ‘Dirac fermions’ having no mass.

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One contribution of 12 to a Theme Issue ‘Electronic and photonic properties of graphene layers and carbon nanoribbons’.
The exceptional properties of graphene as a ‘device-friendly’ material include high mobility reaching up to \(200000 \text{cm}^2 \text{Vs}^{-1}\), over two orders of magnitude higher than that of silicon-based materials, over 20 times that of GaAs and over twice that of InSb. Furthermore, graphene supports a high-electron density, about \(10^{13} \text{cm}^{-2}\) in a single sub-band. It has a long mean-free-path, \(l \sim 400 \text{nm}\) at room temperature, which is promising for ballistic devices based on graphene. There is also a quantum Hall effect at room temperature\(^1\), and graphene is stable to high temperatures of approximately 3000 K. It also has great strength. Finally, graphene has a planar form, suggesting that some variant of the well-developed top-down complementary metal oxide semiconductor (CMOS) compatible process flow may be developed for fabrication of graphene-based devices. This promises a substantial advantage over carbon nanotubes, which are difficult to integrate into electronic devices and are difficult to produce in consistent sizes and electronic properties.

Some graphene-based device fabrication has already been carried out. In particular, a field-effect transistor was constructed by Walt de Heer’s group Georgia Tech Research News (http://gtresearchnews.gatech.edu/circuitry-based-on-graphite-may-provide-a-foundation-for-devices-that-handle-electrons-as-waves) and it has also been addressed by Lemme (2007). Most recently, Xiangfeng Duan of the California Nanosystems Institute at UCLA reported the development of the fastest transistor to date, which has the potential to operate in the terahertz range (Liao et al. 2010). Furthermore, Schedin et al. (2007) reported that graphene-based chemical sensors can detect minute concentrations (1 ppb) of various active gases, even to discern individual events when a molecule attaches to the sensor’s surface (in this, the high sensitivity is a consequence of the high two-dimensional surface/volume ratio, which maximizes the role of adsorbed molecules as donors/acceptors, coupled with the high conductivity of graphene and low noise). The advantageous properties of graphene in regard to long spin lifetime, low spin-orbit coupling and high conductivity have facilitated the fabrication of a simple spin valve (Hill et al. 2006) employing it to provide a spin transport medium between ferromagnetic electrodes. Scott Bunch et al. (2007) employed a graphene sheet (in contact with a gold electrode) to construct an electromechanical resonator actuated electrostatically, with the sheet suspended over a trench in an SiO\(_2\) substrate. The activation mechanisms involve a radio frequency gate voltage superposed on a DC voltage applied to the graphene sheet; also, optical actuation using a laser focused on the sheet has been used. Furthermore, a quantum interference device using a ring-shaped graphene structure was built to manipulate electron wave interference effects. As graphene research is only about 6 years old, this is just the beginning. Other possible uses of graphene are touched upon in recent articles by Geim (2009).

This presentation does not purport to be a thorough review of graphene phenomenology or its theory. It addresses selected topics of interest and importance, providing detailed background of particular instances in the hope that it may be of some pedagogical value.

\(^1\)In addition to its other exceptional properties, it has just been reported that graphene under appropriate mechanical strain influences the spectrum of particle states as if they were in a gigantic pseudo-magnetic field of 300 T (Levy et al. 2010).
2. Graphene Hamiltonian, Green's function for a graphene sheet and quantum dot with and without a magnetic field

(a) Hamiltonian and Green’s function in the absence of a magnetic field

The fundamental low-energy graphene electron/hole dispersion relation proportional to momentum, \( \vec{p} = (p_x, p_y) \), which likens graphene carriers to massless relativistic Dirac fermions, is embodied in the Hamiltonian written in ‘pseudo-spin’ notation (\( \vec{\sigma} = [\sigma_x, \sigma_y] \) are Pauli matrices), which distinguishes the two triangular sub-lattices of the honeycomb lattice on which a graphene quasi-particle can be located,

\[
\hat{h}_1 = \gamma \vec{p} \cdot \vec{\sigma} = \gamma \begin{pmatrix} 0 & p_x - \text{sgn}(s) i p_y \\ p_x + \text{sgn}(s) i p_y & 0 \end{pmatrix}, \tag{2.1}
\]

where the two zero-gap ‘Dirac’ points correspond to

\[
\text{sgn}(s) = \begin{cases} 1 & s = K \\ -1 & s = K' \end{cases}
\]

and \( \gamma \) is given in terms of graphene band-structure parameters as \( \gamma = 3 \sqrt{\ell} / 2 \) (\( \sqrt{\ell} \) is the hopping parameter in the tight-binding approximation and \( \ell \) is the lattice spacing): \( \gamma \) plays the role of a constant Fermi velocity independent of density. This Hamiltonian is responsible for features in graphene that are analogous to relativistic phenomena such as Klein tunnelling, ‘zitterbewegung’ and others. As in the study of massless relativistic neutrino fermions, pseudo-helicity, the component of pseudo-spin in the momentum direction, commutes with \( \hat{h}_1 \) and its eigenvectors can be used as a basis in which \( \hat{h}_1 \) is diagonal. Introducing the transformation from pseudo-spin basis to pseudo-helicity basis,

\[
U_p^{(s)} = \frac{1}{\gamma p} \begin{pmatrix} p_x - \text{sgn}(s) i p_y & p_x + \text{sgn}(s) i p_y \\ \gamma p & \gamma p \end{pmatrix}, \tag{2.3}
\]

\( \hat{h}_1 \) can be diagonalized as

\[
\hat{h}_1 = [U_p^{(s)}]^+ \hat{h}_1 U_p^{(s)} = \text{diag}[\epsilon_1(p), \epsilon_2(p)], \tag{2.4}
\]

where

\[
\epsilon_{\mu} = (-1)^{\mu+1} \gamma p. \tag{2.5}
\]

Of course, the propagation of electrons/holes in graphene is described by its Green’s function. As the Hamiltonian in pseudo-spin representation, \( \hat{h}_1 \), is a 2 \( \times \) 2 matrix and the corresponding Green functions (in the absence, and in the presence, of a magnetic field) are also 2 \( \times \) 2 matrices. The retarded Green function matrix, \( \hat{G}_0 \), is defined by the following equation (\( \hat{I} \) is the unit 2 \( \times \) 2 pseudo-spin matrix; no magnetic field; \( h \rightarrow 1 \)):

\[
\left( i \hat{I} \frac{\partial}{\partial t} - \hat{h}_1 \right) \hat{G}_0(p, t) = \hat{I} \delta(t - t'). \tag{2.6}
\]
In position–frequency representation, this reads as \((px \rightarrow X = x - x'; py \rightarrow Y = y - y'; \mathbf{R} = (X, Y); s \equiv \nu = \pm 1\) for \(K, K'; \gamma = \gamma; T = t - t' \rightarrow \omega\) under Fourier transformation)

\[
\left[ \hat{I} \omega - \gamma \sigma_x \frac{1}{i} \frac{\partial}{\partial X} - \gamma \sigma_y \frac{1}{i} \frac{\partial}{\partial Y} \right] \hat{G}_0(\mathbf{R}, \omega) = \hat{I} \delta(X) \delta(Y).
\] (2.7)

The individual elements satisfy

\[
\omega G_{011} - \left[ \gamma \frac{1}{i} \frac{\partial}{\partial X} - \gamma \nu \frac{\partial}{\partial Y} \right] G_{021} = \delta(X) \delta(Y)
\] (2.8)

and

\[
\omega G_{021} = \left[ \gamma \frac{1}{i} \frac{\partial}{\partial X} + \gamma \nu \frac{\partial}{\partial Y} \right] G_{011},
\] (2.9)

with similar equations for \(G_{022}\) and \(G_{012}\). The results for the retarded Green function elements in pseudo-spin/momentum representation in the absence of a magnetic field are

\[
G_{011}(p, \omega) = G_{022}(p, \omega) = \frac{\omega}{(\omega^2 - \gamma^2 p^2)}
\] (2.10)

and

\[
G_{012}(p, \omega) = G_{021}^*(p, \omega) = \frac{\gamma(px - ipy)}{(\omega^2 - \gamma^2 p^2)},
\] (2.11)

from which the \(2 \times 2\) spectral weight matrix, \(\hat{A}(p, \omega)\), may be obtained using

\[
\hat{A}(p, \omega) = -2\text{Im}[\hat{G}_0(p, \omega)].
\] (2.12)

(b) Graphene Green’s function in a quantizing magnetic field

To incorporate the magnetic field, \(\mathbf{B}\), (taken normal to the graphene plane), we make the usual replacement \(p \rightarrow p - eA\), where \(A = \frac{1}{2} \mathbf{B} \times \mathbf{r}\) for a uniform, constant magnetic field. The requirement of gauge invariance leads to (Horing 1965)

\[
\hat{G}'(\mathbf{r}, \mathbf{r}'; t, t') = C(\mathbf{r}, \mathbf{r}') \hat{G}'(\mathbf{r} - \mathbf{r}'; t - t'),
\] (2.13)

where the factor \(\hat{G}'(\mathbf{r} - \mathbf{r}'; t - t')\) is spatially translationally invariant and gauge invariant, satisfying the equation (Horing & Liu 2009) \((\mathbf{R} = \mathbf{r} - \mathbf{r}', T = t - t', \hbar \rightarrow 1)\)

\[
\left( \frac{i}{\hbar T} - \gamma \sigma_\nu \cdot \left[ \frac{1}{i} \frac{\partial}{\partial \mathbf{R}} - \frac{e}{2} \mathbf{B} \times \mathbf{R} \right] \right) \hat{G}'(\mathbf{R}, T) = \hat{I} \delta^{(2)}(\mathbf{R}) \delta(T),
\] (2.14)
while the factor $C(r, r')$ embodies all non-spatially translationally invariant structure and all gauge dependence as

$$C(r, r') = \exp \left[ \frac{ie}{2\hbar c} \mathbf{r} \cdot \mathbf{B} \times \mathbf{r}' - \phi(r) + \phi(r') \right], \quad (2.15)$$

where $\phi(r)$ is an arbitrary gauge function.

The role of Landau quantization in graphene electron dynamics is embedded in the solution of equation (2.14) for $\mathbf{G}'(\mathbf{R}, T)$, which may be written in $\omega$-frequency representation as (define $\gamma_\nu = \gamma \text{sign}(\nu)$; also $\hbar \to 1$ and $c \to 1$)

$$[\omega - \gamma_\sigma \Pi_{XY} - \gamma_\varphi \sigma_y \Pi_{YX}] \mathbf{G}'(\mathbf{R}, \omega) = i \delta(X) \delta(Y), \quad (2.16)$$

where we have defined

$$\Pi_{XY} = \frac{1}{i} \frac{\partial}{\partial X} + \frac{eB}{2} Y \quad \text{and} \quad \Pi_{YX} = \frac{1}{i} \frac{\partial}{\partial Y} - \frac{eB}{2} X. \quad (2.17)$$

The elements of the matrix equation, equation (2.16), yield equations for $G'_{11}$ and $G'_{21}$ as (similar results obtained for $G'_{22}$ and $G'_{12}$)

$$\left[ \omega + \frac{\gamma_\gamma}{\omega} (eB) \right] G'_{11}(X, Y; \omega) + \frac{\gamma^2}{\omega} \left\{ \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} - \left( \frac{eB}{2} \right)^2 [X^2 + Y^2] \right\} G'_{11}(X, Y; \omega) = \delta(X) \delta(Y) \quad (2.18)$$

and

$$\omega G'_{21} = [\gamma \Pi_{XY} + i \gamma_\varphi \Pi_{YX}] G'_{11}. \quad (2.19)$$

Defining the operator

$$L_Z = \frac{1}{i} \left( X \frac{\partial}{\partial Y} - Y \frac{\partial}{\partial X} \right) = L_z + L_y', \quad (2.20)$$

where $L_z$ is the angular momentum operator, we note that $L_Z \mathbf{G}'(\mathbf{R}, T) = 0$ (Horing 1965; Horing & Liu 2009).

Therefore, equation (2.18) may be written in the form

$$\mathbf{\Omega} G'_{11}(\mathbf{R}, \mathbf{Q}) + \left[ \frac{1}{2M} \nabla^2_{\mathbf{R}} - M \frac{q^2}{8} \mathbf{R}^2 \right] G'_{11}(\mathbf{R}, \mathbf{Q}) = \delta^{(2)}(\mathbf{R}), \quad (2.21)$$

which is readily recognizable as Green’s function equation for an isotropic two-dimensional harmonic oscillator (with the impulsive Dirac $\delta$-function driving term having its source point at the origin) in position–frequency representation. Its retarded solution in position–‘time’ ($\tau$) representation may be written as (Horing 1965; Horing & Liu 2009) ($\eta_+($) is the Heaviside unit step function)

$$G'_{11}(\mathbf{R}; \tau) = -\eta_+ (\tau) \frac{M \mathbf{Q}_c}{4\pi \sin(\mathbf{Q}_c \tau/2)} \exp \left\{ iM \mathbf{Q}_c [X^2 + Y^2] \right\} \frac{4 \tan(\mathbf{Q}_c \tau/2)}{4 \tan(\mathbf{Q}_c \tau/2)} \quad (2.22)$$
Consequently, in frequency ($\omega$) representation, we have (note that $\Omega$ is a convenient parameter here, not the actual frequency, $\omega$)

$$G'_{11}(\mathbf{R}; \Omega) = -iM\Omega c^4 \int_0^{\infty} \frac{e^{i\Omega \tau}}{\sin(\Omega c \tau/2)} \exp \left\{ \frac{iM\Omega c[X^2 + Y^2]}{4\tan(\Omega c \tau/2)} \right\},$$

(2.23)

with the identifications for $\nu = K$

$$\Omega = \omega + \frac{\gamma v}{\omega} eB = \omega - \frac{\gamma^2}{\omega} eB; \quad M = \frac{\omega}{2\gamma^2} \quad \text{and} \quad \Omega c = \frac{2\gamma^2}{\omega} eB.$$  

(2.24)

Expanding the $\tau$-integrand as a generator of Laguerre polynomials, $L_n$, we obtain

$$(Erdelyi \ et \ al. \ 1953b) \quad G'_{11}(\mathbf{R}; \nu) = \frac{eB}{2\pi} \omega \exp \left( -\frac{eB}{4} [X^2 + Y^2] \right) \sum_{n=0}^{\infty} \frac{L_n(eB/2[X^2 + Y^2])}{\omega^2 - 2n\gamma^2 eB}.$$  

(2.25)

Similar treatment for $G'_{22}(X, Y; \nu)_{K}$ yields

$$G'_{22}(\mathbf{R}; \nu)_{K} = G'_{11}(\mathbf{R}; \nu)_{K} = \frac{eB}{2\pi} \omega \exp \left( -\frac{eB}{4} [X^2 + Y^2] \right) \sum_{n=0}^{\infty} \frac{L_n(eB/2[X^2 + Y^2])}{\omega^2 - 2n\gamma^2 eB}.$$  

(2.26)

The energy spectrum of the infinite graphene sheet obtained from the frequency poles of equation (2.26) is given by

$$\omega' = \pm\sqrt{2n\gamma^2 eB},$$

(2.27)

as was found earlier by Ando (2005). Moreover, $G'_{21}$ and $G'_{12}$ are readily obtained from $G'_{11}$ and $G'_{22}$.

In the case $\nu = K'$, we have identifications in equation (2.21) as

$$\Omega = \omega + \frac{\gamma v}{\omega} eB = \omega - \frac{\gamma^2}{\omega} eB; \quad M = \frac{\omega}{2\gamma^2} \quad \text{and} \quad \Omega c = \frac{2\gamma^2}{\omega} eB,$$

(2.28)

and, proceeding as above, we obtain

$$G'_{11}(\mathbf{R}; \nu)_{K'} = G'_{22}(\mathbf{R}; \nu)_{K'} = \frac{eB}{2\pi} \omega \exp \left( -\frac{eB}{4} [X^2 + Y^2] \right) \sum_{n=0}^{\infty} \frac{L_n(eB/2[X^2 + Y^2])}{\omega^2 - 2(n + 1)\gamma^2 eB},$$

(2.29)

which has energy pole positions for the infinite graphene sheet at

$$\omega = \pm\sqrt{2(n + 1)\gamma^2 eB},$$

(2.30)

but the residues representing the relative strengths of the modes differ from those obtained above by a unit shift of the index of the $L_n(eB/2[X^2 + Y^2])$ amplitude.

Yet another interesting representation of the Landau-quantized graphene Green function can be derived by rewriting equation (2.21) in circular coordinates.
as (for either $K$ or $K'$)

$\left[ \frac{\partial^2}{\partial R^2} + \frac{1}{R} \frac{\partial}{\partial R} - \frac{\mathcal{M}^2 \Omega^2 R^2}{4} + 2\mathcal{M} \Omega \right] G'_{11}(R; \Omega) = \frac{\mathcal{M} \delta(R)}{R},$ \hspace{1cm} (2.31)

since there is no angular dependence. For $R > 0$, equation (2.31) has the form of the ‘Bessel wave equation’ (Moon & Spencer 1971)

$\left[ \frac{\partial^2}{\partial R^2} + \frac{1}{R} \frac{\partial}{\partial R} + \alpha^2 R^2 + q^2 - \frac{p^2}{R^2} \right] Z(R) = 0,$ \hspace{1cm} (2.32)

with $p = 0$, $\alpha^2 = -\mathcal{M}^2 \Omega^2 c^2/4$ and $q^2 = 2m\Omega$. The ‘Bessel wave function’ solutions (Moon & Spencer 1971) of equation (2.32) for the case at hand, $p = 0$, are denoted by $Z_1 = J_0(\alpha, q, R)$ having small $R$ behaviour as $Z_1 \approx 1 + 0(R^2)$; and the second solution is $Z_2 = Z_1 \ln(R) + 0(R^2)$ for small $R$. Thus, the solution of the homogeneous equation may be written as a linear combination of $Z_1$ and $Z_2$,

$G'_{11}(R; \Omega) = AZ_1 \left( \frac{i\mathcal{M} \Omega c}{2}, \sqrt{2\mathcal{M} \Omega}, R \right) + BZ_2 \left( \frac{i\mathcal{M} \Omega c}{2}, \sqrt{2\mathcal{M} \Omega}, R \right),$ \hspace{1cm} (2.33)

subject to the condition at small $R \to \varepsilon \to 0^+$ arising from the Dirac $\delta(R)$-function of equation (2.31),

$\frac{\partial}{\partial \varepsilon} G'_{11}(\varepsilon, \Omega) \approx \frac{\mathcal{M}}{2\pi \varepsilon} \text{ or } G'_{11}(\varepsilon, \omega) \approx \frac{\mathcal{M}}{2\pi} \ln(\varepsilon).$ \hspace{1cm} (2.34)

From this, it is clear that the coefficient $B$ in equation (2.33) must be $B = \mathcal{M}/2$. The coefficient $A$ must be chosen to prevent singular behaviour as $R \to \infty$. To examine the solutions further for large $R$, we note that the term $\Omega Z_1$ is negligible when compared with $(\mathcal{M} \Omega^2 R^2/8) G'_{11}$ in this limit, and equation (2.31) then becomes

$\left[ \frac{\partial^2}{\partial R^2} + \frac{1}{R} \frac{\partial}{\partial R} - \frac{\mathcal{M}^2 \Omega^2 R^2}{4} \right] G'_{11}(R, \Omega) = 0.$ \hspace{1cm} (2.35)

Carrying out an inverse Lommel transform (Erdelyi et al. 1953a) on equation (2.35), we obtain a modified Bessel equation of order 0, yielding the large-$R$ solution for $G'_{11}$ as

$G'_{11}(R, \Omega) \to \tilde{A}I_0 \left( \frac{\mathcal{M} \Omega c}{4} R^2 \right) + \tilde{B}K_0 \left( \frac{\mathcal{M} \Omega c}{4} R^2 \right).$ \hspace{1cm} (2.36)

Here, $I_0$ and $K_0$ are modified Bessel functions of the first and third kind, respectively, with the latter embodying a typical second solution log-singularity for finite $R$ but falling off for large $R$ as $K_0(z) \to \sqrt{\pi/2z} e^{-z}$, whereas the former solution of the first kind diverges as $I_0(z) \to \sqrt{\pi/2z} e^z$. On the basis of these considerations jointly with the log-requirement of equation (2.35), we conclude that

$G'_{11}(R; \Omega) = G'_{22}(R; \Omega) = \frac{\mathcal{M}}{2\pi} Z_2 \left( \frac{i\mathcal{M} \Omega c}{2}, \sqrt{2\mathcal{M} \Omega}, R \right),$ \hspace{1cm} (2.37)

with $Z_2$ as the second solution of the Bessel wave equation. ($G_{21}$ and $G'_{12}$ can be determined as indicated above.)
Graphene quantum dot Green’s function in a magnetic field

To represent the presence of a quantum dot on a planar graphene sheet, one may add a potential term of the form $U(r) = \alpha \delta^{(2)}(r)$ to the Hamiltonian above. This represents a quantum well in the potential profile at $r = 0$ (with $\alpha < 0$ being essentially the product of the well depth times its area), which can support just one sub-band state in the well in the absence of a magnetic field.

Green’s function $G'_{\text{dot}}(r_1, r_2; \omega)$ of the graphene sheet with its quantum well thus described can be determined analytically in terms of the infinite graphene sheet Green function $G'(r_1, r_2; \omega)$ as (Horing & Liu 2010) ($a$ is the dot radius and $G'_{\text{dot}}(r_1, r_2; \omega) \equiv G'(|r_1 - r_2| = a; \omega)$)

$$G'_{\text{dot}}(r_1, r_2; \omega) = G'(r_1, r_2; \omega) + \alpha G'(r_1, 0; \omega)[\hat{I} - \alpha G'(a; \omega)]^{-1} G'(0, r_2; \omega). \quad (2.38)$$

(A complete discussion of our derivation is available in Horing & Liu (2010).)

The energy spectrum is then given by the dispersion relation expressed in terms of the elements of the matrix Green function as

$$\Delta = [(1 - \alpha G'_{11}(a; \omega))(1 - \alpha G'_{22}(a; \omega)) - \alpha^2 G'_{12}(a; \omega)G'_{21}(a; \omega)] = 0. \quad (2.39)$$

It is readily seen from equation (2.39) that the magnetic field ‘splinters’ the single zero-field sub-band state into a proliferation of Landau-quantized levels, approximately given by

$$\omega_K = \frac{\alpha e B}{4\pi} e^{-eBa^2/4} L_n \left( \frac{eBa^2}{2} \right) \pm \frac{1}{2} \sqrt{\left( \frac{\alpha e B}{2\pi} \right)^2 e^{-eBa^2/2} \left( L_n \left( \frac{eBa^2}{2} \right) \right)^2 + 8n\gamma^2 eB} \quad (2.40)$$

and

$$\omega_{K'} = \frac{\alpha e B}{4\pi} e^{-eBa^2/4} L_n \left( \frac{eBa^2}{2} \right) \pm \frac{1}{2} \sqrt{\left( \frac{\alpha e B}{2\pi} \right)^2 e^{-eBa^2/2} \left( L_n \left( \frac{eBa^2}{2} \right) \right)^2 + 8(n + 1)\gamma^2 eB}. \quad (2.41)$$

The results of more accurate numerical calculations of the energy/frequency levels of a graphene quantum dot subject to Landau quantization for the $K$ and $K'$ nodes, based on equation (2.39), are shown as functions of the square root of the magnetic field in figures 1 and 2.

Another analysis of the energy spectrum of graphene quantum dots was carried out by Matulis & Peeters (2008), who found that Dirac fermions in a cylindrical quantum dot potential are not fully confined, but form quasi-bound states. Their line-broadening decreases with orbital momentum. It decreases dramatically for energies close to barrier height owing to total internal reflection of the electron wave at the dot edge.
Figure 1. Energy/frequency levels of a graphene quantum dot subject to Landau quantization for the $K$ node as a function of the square root of magnetic field. (Reprinted with permission from Horing & Liu (2010). Copyright © (2010), Institute of Physics). $U_0 = 200 \text{meV}; \ a = 10 \text{nm}; \ \gamma = 1.1 \times 10^6 \ \text{ms}^{-1}$.

Figure 2. Same as figure 1, for the $K'$ node (instead of the $K$ node). (Reprinted with permission from Horing & Liu (2010). Copyright © (2010), Institute of Physics). $U_0 = 200 \text{meV}; \ a = 10 \text{nm}; \ \gamma = 1.1 \times 10^6 \ \text{ms}^{-1}$.

3. Graphene dielectric function

For a translationally invariant graphene sheet, the equilibrium thermodynamic $2 \times 2$ matrix Green function may be written in terms of the spectral weight matrix (equation (2.12)) as

$$\vec{G}_0^{\lfloor \downarrow \rfloor}(\mathbf{p}, \omega) = i \left\{ \frac{f_0(\omega)}{-1 + f_0(\omega)} \right\} \vec{A}(\mathbf{p}, \omega),$$

(3.1)
where $f_0(\omega)$ is the Fermi–Dirac distribution function. (In the case of a uniform, constant magnetic field, this equation applies to $G'$ in place of $G$.) Within the framework of the random-phase approximation (RPA), the polarizability is given by

$$\alpha(p, \omega + i0^+) = -v_c(p) R(p, \omega),$$  \hspace{1cm} (3.2)

where the two-dimensional Coulomb potential is

$$v_c(p) = \frac{2\pi e^2}{p},$$  \hspace{1cm} (3.3)

and the RPA density perturbation response function, $R = \delta \rho / \delta V_{\text{eff}}$, is given by

$$R(p, \omega + i0^+) = \Im \left< -\Im^* \right>,$$  \hspace{1cm} (3.4)

$\Im^* = \int_0^\infty dt e^{-i(\omega - i0^+)t} \int \frac{d^2q}{(2\pi)^2} \text{Tr} \left[ \tilde{G}^<_q(t) \tilde{G}^>(q - p; t) \right]$ \hspace{1cm} (3.5)

and

$$\Im < = \int_{-\infty}^0 dt e^{-i(\omega + i0^+)t} \int \frac{d^2q}{(2\pi)^2} \text{Tr} \left[ \tilde{G}^>(\bar{q}; -t) \tilde{G}^<_q(q - p; t) \right].$$ \hspace{1cm} (3.6)

(Tr represents the trace over pseudo-spin.)

The explicit determination of $R(p, \omega + i0^+)$ has been carried out by several researchers (Shung 1986a, b; Ando 2006; Wünsch et al. 2006; Hwang & Das Sarma 2007) in the degenerate (zero-field) limit. We employ it in the notation of Wünsch et al. (2006), expressed in terms of the dimensionless quantities $x = p/p_F$, $n = \omega/E_F$ (not to be confused with $n \equiv s = \pm 1$ in §2) and $\tilde{R}(x, v) = R(p, \omega)/(E_F/v^2_F)$, where $E_F$ is the Fermi energy, $p_F$ is the Fermi wavenumber, $\gamma \equiv v_F$ is essentially the two-dimensional Fermi velocity (independent of density), $g = g_s g_v$ with $g_s = 2$ and $g_v = 2$ as the spin and valley degeneracies, respectively, and $\hbar \rightarrow 1$,

$$\tilde{R}(x, v) = \tilde{R}^{(0)}(x, v) + \tilde{R}^{(1)}(x, v),$$  \hspace{1cm} (3.7)

with

$$\tilde{R}^{(0)}(x, v) = -i\pi F(x, v)$$  \hspace{1cm} (3.8)

and

$$\tilde{R}^{(1)}(x, v) = -\frac{g}{2\pi} + F(x, v) \left\{ G\left(\frac{v + 2}{x}\right) - \theta\left(\frac{2 - v}{x} - 1\right) \left[ G\left(\frac{2 - v}{x}\right) - i\pi\right] - \theta\left(\frac{v - 2}{x} + 1\right) G\left(\frac{v - 2}{x}\right) \right\},$$  \hspace{1cm} (3.9)

where

$$F(x, v) = \frac{g}{16\pi} \frac{x^2}{\sqrt{v^2 - x^2}}$$  \hspace{1cm} (3.10)

and

$$G(z) = z\sqrt{z^2 - 1} - \ln(z + \sqrt{z^2 - 1}).$$  \hspace{1cm} (3.11)
The high-frequency local limit reduces to the familiar two-dimensional result \((v_F \equiv \gamma\) is the Fermi velocity\)

\[
R(0, \omega) = \sqrt{\frac{ng}{\pi}} \frac{v_F p^2}{2\hbar}\text{ or } \varepsilon(0, \omega) = 1 - v_c(p) R(0, \omega) = 1 - \frac{\omega_p^2}{\omega^2},
\]

(3.12)

where \(\omega_p \equiv \lambda \sqrt{p}\) with \(\lambda = (v_F \epsilon^2 \sqrt{n\pi g/\kappa \hbar})^{1/2}\), which is similar to the expression for the usual two-dimensional plasma with regard to the \(p^{1/2}\)-dependence, but differs with regard to \(n\)-density dependence for the case of graphene being proportional to \(n^{1/4}\).

Furthermore, the leading wavenumber correction to the graphene plasma frequency (\(p_{TF}\) is the Thomas–Fermi wavenumber),

\[
\omega = \omega_p \left(1 - \frac{p_{TF} p}{8 p_F^2}\right),
\]

(3.13)

reduces the plasma frequency (rather than increasing it as in a normal plasma).

In the zero frequency limit, the RPA static shielding dielectric function for graphene given above at zero temperature reduces to

\[
\varepsilon(p, \omega = 0) = 1 + \frac{p_{TF}}{p} \left\{ \begin{array}{ll}
1, & \text{if } p \leq 2p_F, \\
\frac{\pi p}{8p_F} - \frac{1}{2} \sqrt{1 - \left(\frac{2p_F}{p}\right)^2} - \frac{p}{4p_F} \sin^{-1} \left(\frac{2p_F}{p}\right), & \text{if } p > 2p_F,
\end{array} \right.
\]

(3.14)

where \((\kappa\) is the static background dielectric constant)

\[
p_{TF} = \frac{4e^2 p_F}{\hbar \kappa \gamma}
\]

(3.15)

is the two-dimensional Thomas–Fermi shielding wavevector for graphene. The associated shielded Coulombic impurity potential (in wavenumber representation)

\[
v_c(p, \omega = 0) = \frac{2\pi e^2}{p \varepsilon(p, \omega = 0)}
\]

(3.16)

has been employed in various transport calculations for graphene.

Stauber et al. (2009) have analysed the dynamic polarizability of graphene beyond the usual ‘Dirac cone’ low-energy description provided above, deriving an approximate analytical expression for it. Furthermore, inter-valley plasmons in graphene have been studied in the tight-binding approximation by Tudorovskiy & Mikhailov (2009), relating them to transitions between the two nearest Dirac cones. Moreover, Gangadharaiah et al. (2008) have found a novel plasmon mode in graphene based on ladder-type vertex corrections (beyond the RPA), and Liu & Willis (2010) have observed a strongly coupled plasmon–phonon mode in dispersion measurements in epitaxial graphene. In their analysis of double-layer graphene, Hwang & Das Sarma (2009) have found exotic plasmon modes. Finally, graphene plasmons having a linear dependence on wavenumber are discussed immediately below (Horing 2009).
4. Linear graphene plasmons

Plasmons in graphene and carbon nanotubes have been carefully examined experimentally (Stephan et al. 2002; Taverna et al. 2002, 2008; Eberlein et al. 2008; Kramberger et al. 2008; Trevisanutto et al. 2008), and the occurrence of a plasmon whose frequency is a linear function of $q$-wavenumber (in contrast to $\omega_p = \sqrt{\alpha q}$) has been attributed to local field effects (Kramberger et al. 2008). Considering other possible sources of linear plasmon dispersion, we found that such a plasmon may arise from the Coulombic interaction between the native graphene plasmon ($\omega \sim \sqrt{\alpha q}$) and the surface plasmon of a nearby thick substrate hosting a semi-infinite plasma.

The dynamic, non-local and spatially inhomogeneous screening function,

$$K(r_1, t_1; r_2, t_2) = \frac{\delta^{(3)}(r_1 - r_2)\delta(t_1 - t_2)}{d^{(3)}(r_1 - r_2)d(t_1 - t_2)},$$

provides the basic description of longitudinal dielectric response. Its frequency poles define the plasmon modes of the system, and the residues describe the relative excitation amplitudes (oscillator strengths) of these modes. Rewriting this equation in the form of an integral equation, we have

$$K(r_1, t_1; r_2, t_2) + \int d^{(3)}x\int d\tau \alpha_{\text{semi}}(r_1, t_1; x, \tau)K(x, \tau; r_2, t_2)$$

$$= \delta^{(3)}(r_1 - r_2)\delta(t_1 - t_2) - \int d^{(3)}x\int d\tau \alpha_{\text{2D}}(r_1, t_1; x, \tau)K(x, \tau; r_2, t_2),$$

in which we have considered $\alpha(r_1, t_1; r_2, t_2)$, the combined polarizability of the semi-infinite and two-dimensional graphene sheet constituents of the system, using an accurate and useful approximation (Horing et al. 2001) in writing the combined polarizability as the sum of the separate polarizabilities of (i) the semi-infinite plasma, $\alpha_{\text{semi}}(r_1, t_1; r_2, t_2)$, and (ii) the two-dimensional graphene plasma, $\alpha_{\text{2D}}(r_1, t_1; r_2, t_2)$. Equation (4.2) can also be rewritten in the useful form

$$K(r_1, t_1; r_2, t_2) = K_{\text{semi}}(r_1, t_1; r_2, t_2) - \int d^{(3)}x\int d\tau \int d^{(3)}x'\int d\tau' K_{\text{semi}}(r_1, t_1; x, \tau)$$

$$\times \alpha_{\text{2D}}(x, \tau; x', \tau')K(x', \tau'; r_2, t_2),$$

where $K_{\text{semi}}(r_1, t_1; r_2, t_2)$ is the corresponding screening function of the semi-infinite medium alone with no graphene sheet.

For a semi-infinite bulk plasma and a nearby parallel two-dimensional graphene sheet plasma, we Fourier transform in the surface plane of translational invariance.
(\vec{r}_1 - \vec{r}_2 \rightarrow \vec{q}, \text{ where } \vec{r} = \vec{r}, z) \text{ and time } (t_1 - t_2 \rightarrow \omega), \text{ obtaining in frequency representation (suppress } \vec{q}, \omega),

\begin{equation}
K(z_1, z_2) = K_{\text{semi}}(z_1, z_2) - \int dz_3 \int dz_4 K_{\text{semi}}(z_1, z_3) \alpha_{2\text{D}}(z_3, z_4) K(z_4, z_2). \quad (4.4)
\end{equation}

We have previously shown that the dynamic, non-local and spatially inhomogeneous screening function of the semi-infinite medium (occupying \(z = 0 \rightarrow \infty\)) is given by (Horing et al. 1985) \((\theta(z) = 1 \text{ for } z > 0; \ 0 \text{ for } z < 0; \ 1/2 \text{ for } z = 0)\)

\begin{equation}
K_{\text{semi}}(z_1, z_2) = \theta(-z_1) \left[ \delta(z_1 - z_2) - \frac{\varepsilon_\tilde{q}}{1 + \varepsilon_\tilde{q}} e^{i|\tilde{q}|z_1} \delta(z_2) + \frac{2\varepsilon_\tilde{q}}{1 + \varepsilon_\tilde{q}} K_0(z_2) e^{i|\tilde{q}|z_1} \theta(z_2) \right]
+ \theta(z_1) \left[ v_0(z_1) \left[ \frac{|\tilde{q}|\varepsilon_\tilde{q}}{1 + \varepsilon_\tilde{q}} \delta(z_2) - \frac{2|\tilde{q}|\varepsilon_\tilde{q}}{1 + \varepsilon_\tilde{q}} K_0(z_2) \theta(z_2) \right] \right]
+ \theta(z_1)[K_0(z_1 + z_2) + K_0(z_1 - z_2)] \theta(z_2), \quad (4.5)
\end{equation}

where \(\varepsilon_0(q_z, \tilde{q}; \omega)\) is the dynamic, non-local bulk dielectric function of the semi-infinite medium and

\begin{equation}
K_0(z_2) = \left( \frac{1}{\pi} \right) \int_0^\infty dq_z \cos(q_z z_2)[\varepsilon_0(q_z, \tilde{q}; \omega)]^{-1} \quad (4.6)
\end{equation}

and

\begin{equation}
v_0(z_2) = \frac{2}{\pi} \int_0^\infty dq_z \cos(q_z z_2)[(q_z^2 + |\tilde{q}|^2)\varepsilon_0(q_z, \tilde{q}; \omega)]^{-1}, \quad (4.7)
\end{equation}

with \(\varepsilon_\tilde{q}^{-1} = |\tilde{q}|v_0(0)\). We further define

\begin{equation}
J(z_0) = \int dz_3 K_{\text{semi}}(z_0, z_3)e^{-i|\tilde{q}|z_3}. \quad (4.8)
\end{equation}

For the thin two-dimensional sheet of graphene located at \(z_0\), the three-dimensional polarizability is described by (Horing et al. 1987)

\begin{equation}
\alpha_{2\text{D}}(z_1, z_2) = \delta(z_2 - z_0) e^{i|\tilde{q}|(z_1 - z_0)} \alpha_{2\text{D}}, \quad (4.9)
\end{equation}

with the last factor on the right, \(\alpha_{2\text{D}} = \alpha_{2\text{D}}(\tilde{q}, \omega)\), as the planar two-dimensional polarizability on the graphene sheet in two-dimensional wavevector–frequency representation. With this, we have solved the integral equation for the combined screening function of the two-component system exactly in closed form as

\begin{equation}
K(z_1, z_2) = K_{\text{semi}}(z_1, z_2) - \frac{\alpha_{2\text{D}} e^{i|\tilde{q}|z_0} J(z_1) K_{\text{semi}}(z_0, z_2)}{1 + \alpha_{2\text{D}} e^{i|\tilde{q}|z_0} J(z_0)}. \quad (4.10)
\end{equation}

Considering the local limit, we have \(\varepsilon_\tilde{q} = \varepsilon_0(\omega)\) for the semi-infinite medium,

\begin{equation}
K_0(z_2) = \frac{\delta(z_2)}{\varepsilon_0(\omega)} \quad (4.11)
\end{equation}

and

\begin{equation}
v_0(z_2) = \frac{e^{-i|\tilde{q}|z_2}}{(|\tilde{q}|\varepsilon_0(\omega))}. \quad (4.12)
\end{equation}
This leads to $K_{\text{semi}}(z_1, z_2)$ in the local limit as

$$K_{\text{semi}}(z_1, z_2) = \theta(-z_1) \left\{ \delta(z_1 - z_2) + \delta(z_2)e^{i\bar{q}|z_2|} \left( \frac{1 - \varepsilon_0(\omega)}{1 + \varepsilon_0(\omega)} \right) \right\} + \theta(z_1) \left\{ \frac{\delta(z_1 - z_2)}{\varepsilon_0(\omega)} + \delta(z_2)e^{-i\bar{q}|z_1|} \frac{1}{\varepsilon_0(\omega)} \left( \frac{\varepsilon_0(\omega) - 1}{\varepsilon_0(\omega) + 1} \right) \right\}. \quad (4.13)$$

The plasmon dispersion relation for the coupled system of the graphene sheet and the nearby semi-infinite plasma is given by the frequency poles of $K(z_1, z_2)$ above,

$$1 + \alpha_{2D}e^{i\bar{q}|z_0|} J(z_0) = 0. \quad (4.14)$$

Determining $J(z_0)$ in the local limit of $K_{\text{semi}}(z_0, z_3)$, we have

$$1 + \alpha_{2D} \left( 1 + e^{2i\bar{q}|z_0|} \left[ \frac{1 - \varepsilon_0}{1 + \varepsilon_0} \right] \right) = 0, \quad (4.15)$$

where $\varepsilon_0 = 1 - \omega_p^2/\omega^2$ for the local limit of the bulk dielectric function of the semi-infinite medium and $\alpha_{2D} = -\omega_{2D}^2/\omega^2$ for the graphene sheet. In this matter, we consider only intraband terms for doped graphene since we seek long wavelength modes $\omega \sim q$ at low wavenumbers, and interband contributions to the polarizability are negligible for such low frequency, low wavenumber terms with $\hbar\omega/E_F \ll 2$. With these remarks in view, we have

$$\omega^2 = \omega_{2D}^2 \left( 1 + e^{2i\bar{q}|z_0|} \frac{\omega_p^2}{2\omega^2 - \omega_{2D}^2} \right). \quad (4.16)$$

The two coupled plasmon frequencies given by the roots of equation (4.16) are ($\omega_s^2 = \omega_p^2/2$)

$$\omega_{\pm}^2 = \frac{1}{2}[\omega_s^2 + \omega_{2D}^2] \pm \frac{1}{2}\sqrt{[\omega_s^2 + \omega_{2D}^2]^2 - 4\omega_s^2\omega_{2D}^2[1 - e^{2i\bar{q}|z_0|}]}. \quad (4.17)$$

If $|\bar{q}|z_0 \rightarrow 0$ and also $\omega_{2D}^2 = \lambda^2|\bar{q}| \ll \omega_s^2$, the $\omega_+$-plasmon is approximately linear,

$$\omega_+ = \omega_s + \frac{\lambda^2|\bar{q}|}{2\omega_s}. \quad (4.18)$$

On the other hand, if $1 \gg |\bar{q}|z_0 \neq 0$ and $\omega_{2D} \ll \omega_s$, the mode $\omega_-$ is acoustic with

$$\omega_-^2 \approx 2\omega_{2D}^2|\bar{q}| |z_0| \sim |\bar{q}|^2. \quad (4.19)$$

Some aspects of these results have been discussed previously (Chaplik 1972; Lin et al. 1997; Ryzhii 2006, 2007), but they ignore the possibility of coupling the graphene plasmon to a surface plasmon by taking the thick substrate dielectric function to be a constant, independent of frequency, consequently omitting the $\pm \rightarrow +$ mode. Also, the results above provide the basis upon which non-locality of the thick substrate can be analysed in the coupled mode spectrum.
5. Energy-loss probes of graphene

(a) Power loss by a parallel-moving charged particle

In earlier work (Horing et al. 1987), we formulated the power loss by a charged probe particle moving in the \(x\)-direction with speed \(v\) at a distance \(H\) (not to be confused with the Hamiltonian) from a two-dimensional plasma sheet on the \(x-y\) plane at \(z=0\) as (\(Z\) is the charge number of the particle)

\[
\frac{dW}{dt} = - \frac{Z^2 e^2 v}{\kappa} \int \frac{d^2 p}{2\pi} e^{-2pH} \frac{p_x}{p} \text{Im} K^{2D}(p, -p \cdot v), \tag{5.1}
\]

where

\[
K^{2D}(p, \omega) = \left[\epsilon^{2D}(p, \omega)\right]^{-1} = \left[1 - \nu_c(p) R(p, \omega)\right]^{-1}. \tag{5.2}
\]

Expressed in terms of real and imaginary parts,

\[
\text{Im} K^{2D}(p, \omega) = - \frac{\alpha^{2D}(p, \omega)}{[\epsilon_1^{2D}(p, \omega)^2 + \alpha^{2D}_0(p, \omega)^2]}, \tag{5.3}
\]

and the ‘plasma-pole’ approximation describes the excitation of the plasmons by the work done by a high-velocity passing particle (\(\delta(x)\) is the Dirac delta function),

\[
\text{Im} K^{2D}(p, -p \cdot v) = \pi \delta \left(1 - \frac{\lambda^2 p}{\omega^2}\right) \text{sgn}(p_x). \tag{5.4}
\]

This yields the fast particle energy loss as

\[
\frac{dW}{dt} = \frac{Z^2 e^2}{2\kappa v} \frac{\partial}{\partial H} \left\{ \int_{(\lambda^2/\lambda^2)}^{\infty} dpe^{-2pH} \left[p_0 \left(p - \frac{\lambda^2}{\omega^2}\right)\right]^{-1/2} \right\}, \tag{5.5}
\]

which may be evaluated in terms of modified Bessel (Whittaker) functions, \(K_n(x)\), as

\[
\frac{dW}{dt} = - \frac{Z^2 e^2 \lambda^4}{2\kappa v^3} e^{-\left(\lambda^2 H/v^2\right)} \left[K_0 \left(\frac{\lambda^2 H}{v^2}\right) + K_1 \left(\frac{\lambda^2 H}{v^2}\right)\right]. \tag{5.6}
\]

For the case of a low-velocity particle, it is sufficient to calculate \(K^{2D}(p, -p \cdot v)\) to first order in \(v\), with the result

\[
\frac{dW}{dt} \approx - \frac{Z^2 e^2 v^2}{2\kappa} \int_0^{\infty} dpe^{-2pH} p^2 \frac{1}{[\epsilon^{2D}_1(p, 0)]^2} \frac{\partial \alpha^{2D}_0(p, \omega = 0)}{\partial \omega}. \tag{5.7}
\]

Written in terms of the stopping power \(S\) (energy loss per unit length of path traversed by the particle),

\[
S = \frac{1}{v} \frac{dW}{dt} = \frac{Z^2 \hbar v}{16gH^2 \pi F} \left[3 - 6\pi p_F H I_0(4p_F H) + (3 + 8p_F^2 H^2)\pi I_1(4p_F H)\right. \\
+ \left. 2\pi p_F H(3L_{-2}(4p_F H) - 4p_F H L_{-1}(4p_F H))\right], \tag{5.8}
\]

where \(I_n(x)\) is the modified Bessel function of the first kind (order \(n\)) and \(L_n(x)\) is the modified Struve function (order \(n\)).

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A complete discussion of the details of this work and improvement upon the plasma-pole approximation by considering $R(p, \omega)$ more accurately for both high- and low-incident particle velocities, using results discussed in §3, may be found in the paper by Horing & Fessatidis (2010a).

These results clearly indicate that the energy loss is dominated by plasmon excitations at large distances, whereas electron–hole excitations dominate at short distances.

(b) Energy loss by a perpendicular-moving charged particle

It is also of interest to discuss the energy loss of a charged probe particle moving perpendicular to the graphene sheet (Fessatidis et al. 2010) and through it with speed $v_z$. In this case, the work done by the passing particle is given by

$$W = \frac{4\pi}{\kappa} (Ze)^2 \int \frac{d^2\tilde{p}}{(2\pi)^2} \int_{-\infty}^{\infty} dp_z \frac{2p_z\tilde{p}}{2\pi (\tilde{p}^2 + p_z^2)^2} \text{Im} K^{2D}(\tilde{p}, \omega = p_z v_z).$$

(5.9)

In the high-velocity limit, the plasma-pole approximation yields

$$W = -\frac{4\pi}{\kappa} (Ze)^2 \int \frac{d^2\tilde{p}}{(2\pi)^2} \int_{0}^{\infty} dp_z \frac{p_z\tilde{p}}{2\pi (\tilde{p}^2 + p_z^2)^2} \frac{\omega_p}{v_z} \delta \left( p_z - \frac{\omega_p}{v_z} \right)$$

$$= -\frac{4\pi}{\kappa} \left( Ze \frac{\lambda}{v_z} \right)^2 \int_{0}^{\infty} \frac{d\tilde{p}}{2\pi (\tilde{p}^2 + (\tilde{p}\lambda/v_z)^2)^2},$$

(5.10)

and we employ an upper-limit cutoff, $p_c$, corresponding to the limitation of validity of the local plasma-pole approximation $p_c^{1/2} < \lambda/v_F$. The resulting total work is

$$W = \frac{2}{\kappa} \left( Ze \frac{\lambda}{v_z} \right)^2 \left( \frac{v_z^2}{v_z^2 + v_F^2} - \ln \left( 1 + \frac{v_z^2}{v_F^2} \right) \right).$$

(5.11)

On the other hand, for the case of low velocity, expansion of $\text{Im} K^{2D}$ to linear order in $v_z$ yields the result

$$|W| = \pi v_z \frac{D_0 p_F}{E_F} \left( \frac{Ze^2}{\kappa} \right)^2 \left[ c\pi - 4 - \frac{2(c^2 - 2)}{\sqrt{c^2 - 4}} \cos^{-1} \left( \frac{2}{c} \right) \right],$$

(5.12)

where we have defined

$$c = \frac{2\pi e^2 \sqrt{g_n g_e n/\pi}}{\kappa p_F^2} \quad \text{and} \quad D_0 = \frac{\kappa p_F c}{2\pi e^2}.$$  

(5.13)

Again, a complete discussion of the details of these calculations can be found in yet another paper by Fessatidis et al. (2010).

6. Graphene van der Waals interactions

The mutual polarization of non-overlapping neutral systems (such as an atom/molecule and a nearby surface) in a van der Waals (vdW) interaction also involves a graphene dielectric response in conjunction with its vdW attraction for a nearby atom/molecule. We have examined this vdW energy to second order in the Coulomb interaction between the graphene electrons and those of the
atom/molecule, with the result (Horing & Chen 2002; Horing 2004; Horing et al. in press) \((\epsilon_0 \equiv \kappa\) is the background dielectric constant here)

\[
E_{\text{vdW}}^{(2)} = \frac{4}{3\hbar \epsilon_0} \sum_n \int_0^\infty \frac{d u \omega_{n0} |D_{0n}|^2}{2\pi u^2 + \omega_{n0}^2} \int_0^\infty d p p^2 e^{-2p|Z|} \frac{\alpha^{2D}(p,iu)}{\epsilon_0 + \alpha^{2D}(p,iu)},
\]

where \(|Z|\) is the distance between the atom and the two-dimensional graphene sheet; \(\omega_{n0}\) is the energy difference of the unperturbed atomic electron levels, \(\omega_{n0} = E_n - E_{0n}^a\); \(D_{0n}\) is the matrix element of the atom’s dipole moment operator between atomic electron levels \(n, 0\); \(\alpha^{2D}(p, \omega)\) is the dynamic, non-local polarizability of the graphene sheet. The prime on \(\Sigma\) denotes omission of the \(n = 0\) term. Equation (6.1) is a useful point of departure to determine both local and non-local structure of the vdW interaction using \(\alpha^{2D}(p, \omega)\) of §3 for graphene. For the undoped case, \(\alpha^{2D}(p,iu)\) is given by

\[
\alpha^{2D}(p, iu) = - \left( \frac{g_s g_v \pi e^2}{8\epsilon_0 \hbar} \right) \frac{p}{\sqrt{u^2 + \gamma^2 p^2}}.
\]

It should be noted that an expansion of \(E_{\text{vdW}}\) in inverse powers of \(|Z|\) is not available since it would involve expanding the \(p\)-integral of equation (6.1) in powers of \(p/u\), which would cause divergence in the final \(u\)-integration. However, for atomic frequencies \((\omega_{n0})\), the polarizability is small, \(\alpha^{2D}(p, iu) \ll 1\), and we have the \(p\)-integral of equation (6.1) approximately as

\[
\int_0^\infty dp \ldots \approx - \left( \frac{g_s g_v \pi e^2}{8\epsilon_0 \hbar} \right) \int_0^\infty dp e^{-2p|Z|} \frac{p^3}{\sqrt{u^2 + \gamma^2 p^2}}.
\]

This integral can be evaluated using

\[
\int_0^\infty \frac{x e^{-\mu x}}{\sqrt{x^2 + \beta^2}} dx = \frac{\beta \pi}{2} [H_1(\beta \mu) - Y_1(\beta \mu)] - \beta,
\]

where \(H_1(x)\) is the Struve function and \(Y_1(x)\) is the Bessel function of the second kind, with the result (Horing et al. in press)

\[
\int_0^\infty dp \ldots \approx - \left( \frac{g_s g_v \pi e^2}{8\epsilon_0 \hbar} \right) \frac{u \pi}{8 \gamma^2} \frac{\partial^2}{\partial |Z|^2} \left[ H_1 \left( \frac{2|Z|}{\gamma} \right) u - Y_1 \left( \frac{2|Z|}{\gamma} u \right) \right].
\]

The vdW interaction of two graphene sheets (A and B; separation \(2z_0\)), sufficiently separated so that the interaction is solely Coulombic (and the sheets do not affect each other’s structure except for mutual carrier polarization owing to electrostatic interactions) is given by (Horing & Fessatidis 2010b)

\[
\frac{E_{\text{vdW}}}{\text{area}} = \frac{1}{\pi} \int_0^\infty \frac{d^2 \tilde{q}}{(2\pi)^2} \int d z_2 \int d z_3 K_A(z_2, z_3; \tilde{q}, iu) K_B(z_3, z_2; \tilde{q}, iu),
\]

where

\[
K_{A,B}(z_1, z_2; \tilde{q}, \omega) = -\delta(z_2 \pm z_0) e^{-|\tilde{q}| |z_1 \pm z_0|} \frac{\alpha^{2D}(q, iu)}{1 + \alpha^{2D}(q, iu)}
\]

(6.7)
Figure 3. Plot of plasmon and electron–hole contributions per unit area to $E_{\text{vdW}} \equiv E_{\text{int}}$ (in eV nm$^{-2}$) versus distance $z_0$ (in nm). The solid line represents the plasmon contribution and the dashed line represents the electron–hole estimate.

Figure 4. Ratio of plasmon contribution to $E_{\text{vdW}}$ relative to the electron–hole contribution as a function of $z_0$.

and $\alpha_{2D}(q, \omega)$ is the graphene single-sheet two-dimensional polarizability. In the plasma-pole approximation, this yields

$$\frac{E_{\text{vdW}}}{\text{area}} = \frac{(g_u g_v)^2 e^4}{4096 \kappa^2 \gamma \hbar |z_0|^3} \left[ \frac{\delta}{(\delta^2 - 1)} - \frac{1}{(\delta^2 - 1)^{3/2}} \ln \left( \frac{\delta + 1 + \sqrt{\delta^2 - 1}}{\delta + 1 - \sqrt{\delta^2 - 1}} \right) \right]$$

(6.8)

and $\delta = g_u g_v \pi e^2 / 8 \kappa \gamma \hbar = 1.432$. (The quantity in square brackets is approximately 0.528.) A comparative study of the vdW energy contributions owing to plasmons and electron–hole excitations is exhibited in figure 3 as a function of $z_0$, with the ratio shown in figure 4.

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7. Some other physical features of graphene

Of course, the dielectric response properties of graphene enter the determination of its electromagnetic normal modes. Mikhailov & Ziegler (2007) recently found a new transverse electric (TE) mode in graphene in the terahertz range,

\[ 1.667 < \frac{\hbar \omega}{E_F} < 2, \text{ or } 15 \text{ THz} \leq f \leq 18 \text{ THz}, \]  

and they also found a transverse magnetic (TM) plasmon–polariton mode described as

\[ \frac{\hbar \omega}{E_F} < 1.667. \]  

These authors have also examined the nonlinear electromagnetic response of graphene, including frequency multiplication and self-consistent field effects (Mikhailov & Ziegler 2008). Moreover, plasmonics in doped graphene have been examined and discussed by Jablan et al. (2009).

Needless to say, the plasmons of graphene play an important role in its correlation energy, and Das Sarma et al. (2007b) investigated the RPA-screened Coulombic self-energy, \( \Sigma_{\text{coul.}} \), of graphene \( 1 = \mathbf{r}_1, t_1, \text{ etc.} \),

\[ \Sigma_{\text{coul.}}(1, 2) \rightarrow -i V(1 - 2) G(1, 2), \]  

where the effective screened potential is given by

\[ V(1 - 2) = \int d^{(4)}K(2 - 3)v_c(1 - 3). \]  

Clearly, the plasma poles of the screening function, \( K \), make distinct contributions to the Coulombic self energy, \( \Sigma_{\text{coul.}} \). In this study, Das Sarma et al. (2007) found that intrinsic graphene is a marginal Fermi liquid, with the quasi-particle spectral weight vanishing near the Dirac point, but extrinsic graphene is a well-defined Fermi liquid owing to doping. Moreover, Tse & Das Sarma (2007) also examined the phonon-induced self energy, \( \Sigma_{\text{phonon}} \), of graphene,

\[ \Sigma_{\text{phonon}}(1, 2) \rightarrow -i V_{\text{eff}}(1, 2) G(1, 2), \]  

where

\[ V^{(1,2)}_{\text{eff}} = \Gamma_{\text{ep}}(\mathbf{x}_1) D_0(1, 2) \Gamma_{\text{ep}}(\mathbf{x}_2), \]  

with \( \Gamma_{\text{ep}} \) measuring electron–ion interaction strength, and \( D_0(1, 2) \) as the free phonon Green function. They found that the phonon-mediated carrier–carrier coupling of equation (7.6) gives rise to a large effect on graphene band-structure renormalization.

A particularly interesting aspect of graphene has been investigated by Isacsson (2008), who studied artificially corrugated graphene ribbons, showing that the ribbon curvature leads to an electronic superlattice with a period set by the corrugation wavelength. This facilitates the analysis of Dirac fermions in periodic potentials and opens yet another possible design configuration for an electronic

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device based on graphene. Yet another very interesting paper on graphene nanoribbons by Roslyak et al. (2010) addresses the relativistic phenomenon of Klein tunnelling, unimpeded in nanoribbons (Roslyak et al. 2010).

8. Graphene transport

(a) Background

The extraordinary nature of graphene’s very high mobility is matched by the extraordinary peculiarities of its theory. The measured conductivity rises almost linearly as a function of gate voltage away from its minimum (Novoselov et al. 2004, 2005; Gusynin & Sharapov 2005; Zhang et al. 2005). Remarkably, its minimum is finite at zero gate voltage, $V_g$, which is generally taken as a measure of carrier density; the non-zero minimum value of this ‘residual’ conductivity is approximately

$$\sigma_{\text{min}} \approx \frac{4e^2}{h}. \quad (8.1)$$

Moreover, graphene exhibits a quantum Hall effect at room temperature (Ludwig et al. 1994; Ziegler 1997; Gorbar et al. 2002; Gusynin & Sharapov 2005, 2006; Novoselov et al. 2007). There are other interesting effects of a magnetic field on conduction in graphene discussed in the literature (Goerbig 2010 and references therein), and ballistic transport in graphene nanoribbons in crossed magnetic and electric fields has recently been addressed by Roslyak et al. (2010).

There have been numerous attempts to form a theoretical explanation of $\sigma_{\text{min}} \neq 0$ at $V_g = 0$ using the Kubo formula and the Landauer formula, with differing results that include (Ziegler 1998; Gusynin & Sharapov 2006; Katsnelson 2006; Ostrovsky et al. 2006; Peres et al. 2006; Tworzydlo et al. 2006; Ziegler 2006; Cserti 2007; Falkovsky & Varlamov 2007; Ryu et al. 2007)

$$\sigma_{\text{min}} = \frac{e^2}{\pi h}; \quad \frac{8e^2}{\pi h}; \quad \frac{\pi e^2}{4h}. \quad (8.2)$$

The peculiarities of the theoretical analyses became obvious when Ziegler (2006) and Cserti (2007) demonstrated that, within the Kubo formalism, the magnitude of the residual conductivity is sensitive to the order in which the zero frequency (DC) and dissipationless limits are taken, yielding different results when the order of the limits is interchanged. Moreover, Adam & Das Sarma (2008) showed that the minimum residual conductivity can arise from a non-vanishing carrier density at zero gate voltage that is induced by impurity potentials: analysing random fluctuations of gate voltage, they provided a quantitative explanation of the experimentally observed residual conductivity. Furthermore, the mechanism of minimum conductivity has been discussed in terms of mesoscopically inhomogeneous graphene charge density (probably owing to fluctuations of charges trapped in the substrate, or on its surface), forming electron–hole puddles (Martin et al. 2007; Zhang et al. 2009), in combination with relativistic Klein tunnelling (Cheianov et al. 2007; Peres 2009). A recent review paper by Das Sarma et al. (2010) provides a well-documented review of the subject. In addition, other very recent reviews of theoretical approaches in graphene quantum transport are now available (Kailasvuori & Lüffe 2010;
Peres 2010). It should also be borne in mind that relativistic theory also provides for pair production that, in the case of massless graphene, supplies electron and hole charge carriers for conduction (Schwinger 1951; Schmidt et al. 1998; Lewkowicz & Rosenstein 2009).

We have developed a kinetic equation for graphene transport in the diffusive regime in which \( p_F \ell > 1 \) (\( \ell \) is the diffusion length), including the effect of interband polarization on conductivity (Liu et al. 2008). The current is expressed in terms of elements, \([\hat{\rho}]_{ij}\), of the distribution function, \(\hat{\rho}\), as (\(n\) is the normal vector to the graphene plane)

\[
J = g_\gamma e \sum_{p,s} \frac{1}{p} \left[ p(\hat{\rho}_1^{(s)})_{11}(p) - (\hat{\rho}_2^{(s)})_{22}(p) \right] + 2 sgn(s)[p \times n] \text{Im}[(\hat{\rho}_1^{(s)})_{12}(p)]
\]  
(8.3)
in the pseudo-helicity basis. Considering the impurity scattering mechanism (in pseudo-spin basis) owing to an isotropic potential, \(V(p-k)\), which scatters a carrier from state \(p\) to state \(k\), its counterpart in pseudo-helicity basis is given by

\[
\hat{T}_s(p,k) = [U_{s}^{(p)}]^+ V(|p-k|) U_{s}^{(k)},
\]  
(8.4)
where \(U_{s}^{(p)}\) is given by equation (2.3).

(b) DC conduction

The kinetic equation for the linear electric field part of the distribution function, \(\hat{\rho}_1^{(s)}(p)\), has the form (Liu et al. 2008)

\[
cE \cdot \nabla_p [\hat{\rho}_0^{(s)}]_{\mu\mu}(p) = -[\hat{I}_s^{(1)}]_{\mu\mu}
\]  
(8.5)
and \((\hat{\rho}_0^{(s)}(p)) = \text{diag}[n_F(\epsilon_1(p)), n_F(\epsilon_2(p))]\), where \(n_F^{(s)}\) is the unperturbed equilibrium Fermi distribution function

\[
2i\gamma p [\hat{\rho}_1^{(s)}]_{12}(p) = -[\hat{I}_s^{(1)}]_{12},
\]  
(8.6)
where \([\hat{I}_s^{(1)}]_{\mu\nu}\) are the linear field parts of the impurity scattering terms (which are presented in detail in Liu et al. (2008)). Defining

\[
v_{\mu}^{(s)}(p) = \nabla_p e_{\mu}^{(s)}(p) = \frac{(-1)^{\mu+1}\gamma p}{p},
\]  
(8.7)
the solution of the linear kinetic equation is given by

\[
[\hat{\rho}_1^{(s)}]_{\mu\mu}(p) = eE \cdot v_{\mu}^{(s)}(p) A_{\mu}^{(s)}(p),
\]  
(8.8)
for the diagonal elements of \(\hat{\rho}_1^{(s)}(p)\) to the first order in \(E\), while the off-diagonal elements take the linear form

\[
[\hat{\rho}_1^{(s)}]_{12}(p) = \frac{e\gamma}{p} [E \times p \cdot n] \Phi^{(s)}(p),
\]  
(8.9)
where the functions \( A_\mu^{(s)}(p) \) and \( \Phi^{(s)}(p) \) can be expressed in terms of microscopically calculated relaxation times as

\[
A_\mu^{(s)}(p) = -\tau_\mu^{(a)}(p) \frac{\partial [\hat{\rho}_0^{(s)}]_{\mu\mu}(p)}{\partial \varepsilon_\mu^{(s)}(p)} + \text{sgn}(s) \text{Im}[\Phi^{(s)}(p)],
\]

(8.10)

and

\[
\text{Re}[\Phi^{(s)}(p)] = -\frac{\text{sgn}(s)}{4\gamma^2 p^2} \sum_\mu \left\{ \gamma p \frac{\partial [\hat{\rho}_0^{(s)}]_{\mu\mu}(p)}{\partial \varepsilon_\mu^{(s)}(p)} \right\},
\]

(8.11)

with

\[
\text{Im}[\Phi^{(s)}(p)] = -\frac{\text{sgn}(s)}{16\gamma^3 p^3} \left[ \frac{1}{\tau_1^{(b)}(p)} + \frac{1}{\tau_2^{(b)}(p)} \right] \sum_\mu \left[ \gamma p \frac{\partial [\hat{\rho}_0^{(s)}]_{\mu\mu}(p)}{\partial \varepsilon_\mu^{(s)}(p)} \right].
\]

(8.12)

Finally, the microscopically determined conductivity is given by

\[
\sigma = -\frac{e^2}{2} \frac{\delta N}{\gamma^2} \sum_{p,\mu,s} \left\{ \left[ \tau_\mu^{(a)}(p) + \frac{1}{4\gamma^2 p^2 \tau_\mu^{(b)}(p)} \right] \frac{\partial [\hat{\rho}_0^{(s)}]_{\mu\mu}(p)}{\partial \varepsilon_\mu^{(s)}(p)} \right\},
\]

(8.13)

where the calculated relaxation times are given in terms of the impurity concentration \( N_i \) and the impurity scattering potential \( V \) as

\[
[\tau_\mu^{(a,b)}(p)]^{-1} = \pi N_i \sum_k |V(p - k)|^2 \delta[\varepsilon_\mu(p) - \varepsilon(k)] A^{(a,b)}(\phi_k),
\]

(8.14)

independent of node index \( s \), with \( A^{(a)}(\phi) = \sin^2 \phi \), \( A^{(b)}(\phi) = (1 - \cos \phi)^2 \) and

\[
[\tau_\mu^{(b)}(p)]^{-1} \equiv [\tau_1^{(b)}(p)]^{-1} + [\tau_2^{(b)}(p)]^{-1}.
\]

(8.15)

It should be noted that the conductivity involves not only a term proportional to \( (N_i)^{-1} \), but also a term linear in impurity density owing to \( [\hat{\rho}_1^{(s)}]_{12}(p) \), which describes interband coherence and correlation. At zero temperature, the diffusive conductivity is given by \( \sigma_F = \sqrt{4\pi N_i/e_0 g_0 \gamma} \), \( E_F = \gamma p_F \) and \( N_e \) is the carrier density

\[
\sigma|_{T=0} = \frac{e^2}{4\pi} \frac{\delta N}{\gamma^2} \gamma p_F \left[ \tau_1^{(a)}(p_F) + \frac{1}{4\gamma^2 p_F^2 \tau^{(b)}(p_F)} \right].
\]

(8.16)

Obviously, there is a minimum in the dependence of conductivity on the impurity density; correspondingly, there is also a conductivity minimum as a function of charge carrier density indicated here. This is of special physical interest as it arises from interband polarization associated with off-diagonal elements of the distribution function, i.e. electron–hole correlation. For a short-range (SR) scattering model, \( V(p - k) \approx \pi \gamma/(2p_F) \), the resulting conductivity is

\[
\sigma|_{T=0} = \frac{e^2}{\pi} \left[ \frac{16N_e}{\pi N_i} + \frac{3\pi N_i}{32N_e} \right].
\]

(8.17)

This yields a minimum conductivity at zero temperature given by

\[
\sigma|_{T=0} \geq \sigma_{\text{min}} = \frac{e^2 \sqrt{6}}{\pi} = \frac{2\sqrt{6}e^2}{\pi h} \approx \frac{4.9e^2}{h},
\]

(8.18)
and the critical-carrier density at which this minimum conductivity \( (\sigma|_{T=0} = \sigma_{\text{min}}) \) occurs is \( N_e \rightarrow N_e' = N_i \pi \sqrt{6}/32 \approx 0.24 N_i \). When \( N_e > N_e' \), the first term in \( \sigma|_{T=0} \) is dominant, giving rise to a linear dependence of conductivity on electron density.

The RPA-screened Coulombic impurity scattering model characterized by the two-dimensional scattering potential of equations (3.16) and (3.14) yields the zero temperature conductivity as

\[
\sigma_{|T=0}^{\text{RPA}} = \frac{e^2}{\pi} \left[ \frac{N_e}{N_i G(2r_s)} + \frac{N_i F(2r_s)}{4N_e} \right], 
\]

(8.19)

where \( r_s = e^2/(4\pi k \gamma) \) and \( G(x), F(x) \) are given by

\[
G(x) = \frac{x^2}{16} \int_0^{2\pi} \frac{d\theta}{\sin^2 \theta} \left[ \frac{\pi}{4} + 3x - \frac{3\pi}{2} x^2 + |x|(3x^2 - 2) \arccos \left( \frac{1}{x} \right) (x^2 - 1)^{-1/2}, \right.
\]

\[
\left. \quad \text{for } |x| > 1, \right. \\
\left. \frac{\pi}{4} + 3x - \frac{3\pi}{2} x^2 + x(3x^2 - 2) \text{Re} \left[ \arctanh \left( \frac{1}{\sqrt{1 - x^2}} \right) \right] (1 - x^2)^{-1/2}, \right.
\]

(8.20)

and

\[
F(x) = \frac{x^2}{8} \int_0^{2\pi} \frac{d\theta \left( (1 - \cos \theta)^2 \right)}{(\sin \theta/2 + x)^2} \left[ \frac{\pi}{2} - 4x + 3x^2 \pi - \frac{2x^3}{x^2 - 1} + x^3 |(8 - 6x^2) \arccos \left( \frac{1}{x} \right) (x^2 - 1)^{-3/2}, \right.
\]

\[
\left. \quad \text{for } |x| > 1, \right. \\
\left. \frac{\pi}{2} - 4x + 3x^2 \pi - \frac{2x^3}{x^2 - 1} - x^3 (8 - 6x^2) \right. \\
\left. \quad \times \text{Re} \left[ \arctanh \left( \frac{1}{\sqrt{1 - x^2}} \right) \right] (1 - x^2)^{-3/2}, \quad \text{for } 0 \leq x \leq 1. \right.
\]

(8.21)

For a typical graphene system on an SiO\(_2\) substrate with background dielectric constant \( \kappa \approx 2.45 \) and \( r_s = 0.813 \), the present linear diffusive-transport theory with RPA-screened impurity scattering leads to the minimum conductivity as

\[
\sigma_{|T=0,\text{min}}^{\text{RPA}} = \frac{4.42 e^2}{h}, 
\]

(8.22)

at the critical-carrier density value

\[
N_e^{\text{RPA}} \approx 0.11 N_i. 
\]

(8.23)
Figure 5. Dependencies on $r_s$ of the minimum conductivity (in units of $e^2/h$) and the critical-carrier density (relative to impurity concentration) for a RPA-screened Coulomb scattering potential. (Reprinted with permission from Liu et al. (2008). Copyright © (2008), American Institute of Physics). $\gamma = 1.1 \times 10^6 \text{ m s}^{-1}$.

Table 1. Critical electron densities and minimum conductivities for the short-range (SR) and RPA-screened Coulomb scattering potentials considered. (Reprinted with permission from Liu et al. (2008). Copyright © (2008), American Institute of Physics).

<table>
<thead>
<tr>
<th></th>
<th>$N_c/N_i$</th>
<th>$\sigma_{\text{min}}/(e^2/h)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SR</td>
<td>$\pi \sqrt{6}/32 \approx 0.24$</td>
<td>$2\sqrt{6} \approx 4.9$</td>
</tr>
<tr>
<td>RPA</td>
<td>$\sqrt{F(2r_s)G(2r_s)}/2$</td>
<td>$2[\sqrt{F(2r_s)/G(2r_s)}]$</td>
</tr>
</tbody>
</table>

We again find almost linear dependence of the conductivity on carrier density, in this case for $N_e > 0.11N_i$, above the critical density.

The minimum conductivity and critical density are presented as functions of $r_s$ for RPA screening in figure 5 (note: $N_i^\varepsilon \equiv N_c$). Furthermore, tables of $N_c/N_i$ and $\sigma_{\text{min}}/(e^2/h)$, exhibited as functions of $r_s$ analytically, are presented in table 1 for both RPA and SR models of impurity scatterer screening. These results are consistent with the experimental observations. However, this theory is limited to the diffusive regime and is not applicable in the limit of very low carrier density.

(c) Dynamic conductivity

For the case of an AC electric field, $\mathbf{E} = E_0 e^{-i\omega t}$, the linearized kinetic equation for $[\hat{\rho}_1^{(s)}]_{\mu\mu}$ in the diffusive regime may be written as (Liu et al. 2010)

$$i\omega [\hat{\rho}_1^{(s)}]_{\mu\mu}(\omega, \mathbf{p}) - eE_0 \cdot \nabla_p [\hat{\rho}_0^{(s)}]_{\mu\mu}(\mathbf{p}) = -[\hat{\tau}_1^{(1)}]_{\mu\mu},$$

(8.24)
and for $[\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p})$, we have
\[
\ii \omega [\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p}) + 2\ii \gamma \mathbf{p} [\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p}) = -[\hat{I}^{(s)}_{s}]_{12},
\]
(8.25)
with $[\hat{\rho}^{(s)}_{1}]_{\mu\nu}(\omega, \mathbf{p})$ and $[\hat{\rho}^{(s)}_{0}]_{\mu\nu}(\mathbf{p})$, respectively, as the elements of $\hat{\rho}^{(s)}_{1}(\omega, \mathbf{p})$ and $\hat{\rho}^{(s)}_{0}(\mathbf{p})$. The linear electric field part of the scattering term, $\hat{I}^{(s)}_{s}$, is composed of elements as follows: its diagonal elements, $[\hat{I}^{(s)}_{s}]_{\mu\mu}$, are given by
\[
[\hat{I}^{(s)}_{s}]_{\mu\mu} = \pi N_{i} \sum_{\mathbf{k}} |V(\mathbf{p} - \mathbf{k})|^{2} \delta[\epsilon^{(s)}_{\mu}(\mathbf{p}) - \epsilon^{(s)}_{\mu}(\mathbf{k})]
\]
\times \{[1 + \cos(\phi_{\mathbf{p}} - \phi_{\mathbf{k}})]\{[\hat{\rho}^{(s)}_{1}]_{\mu\mu}(\omega, \mathbf{p}) - [\hat{\rho}^{(s)}_{1}]_{\mu\mu}(\omega, \mathbf{k})] - (-1)^{\mu} \text{sgn}(s) \sin(\phi_{\mathbf{p}} - \phi_{\mathbf{k}}) \text{Im}[[\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p}) + [\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{k})]\},
\]
(8.26)
while the off-diagonal element, $[\hat{I}^{(s)}_{s}]_{12}$, takes the form
\[
[\hat{I}^{(s)}_{s}]_{12} = \frac{\pi N_{i}}{2} \sum_{\mathbf{k}, \mu} |V(\mathbf{p} - \mathbf{k})|^{2} \delta[\epsilon^{(s)}_{\mu}(\mathbf{p}) - \epsilon^{(s)}_{\mu}(\mathbf{k})]
\]
\times \{- \left[(-1)^{\mu+1} \text{sgn}(s) \sin(\phi_{\mathbf{p}} - \phi_{\mathbf{k}})\{[\hat{\rho}^{(s)}_{1}]_{\mu\mu}(\omega, \mathbf{p}) - [\hat{\rho}^{(s)}_{1}]_{\mu\mu}(\omega, \mathbf{k})]\}ight.
\times \{1 - \cos(\phi_{\mathbf{p}} - \phi_{\mathbf{k}})\} \{[\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p}) - [\hat{\rho}^{(s)}_{1}]_{21}(\omega, \mathbf{k})\}\}.
\]
(8.27)
Solution for the diagonal elements of $\hat{\rho}^{(s)}_{1}(\omega, \mathbf{p})$ can be written as
\[
[\hat{\rho}^{(s)}_{1}]_{\mu\mu}(\omega, \mathbf{p}) = e \mathbf{E}_{0} \cdot \mathbf{v}^{(s)}_{\mu}(\mathbf{p}) A^{(s)}_{\mu}(\omega, \mathbf{p}),
\]
(8.28)
while the off-diagonal element, $[\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p})$, is given by ($\mathbf{n}$ is the unit vector normal to the graphene sheet)
\[
[\hat{\rho}^{(s)}_{1}]_{12}(\omega, \mathbf{p}) = \frac{e \gamma}{p} [\mathbf{E}_{0} \times \mathbf{p} \cdot \mathbf{n}] \Phi^{(s)}(\omega, p),
\]
(8.29)
as above. However, the functions $A^{(s)}_{\mu}(\omega, p)$ and $\Phi^{(s)}(\omega, p)$ differ from their DC counterparts and are given in terms of the microscopically determined relaxation times $\tau^{(a,b)}_{\mu}(p)$ (given above) as
\[
\text{Re}[\Phi^{(s)}(\omega, p)] = 2\tau^{(b)}(p)(\omega + 2\gamma p) \text{Im}[\Phi^{(s)}(\omega, p)],
\]
(8.30)
\[
\text{Im}[\Phi^{(s)}(\omega, p)] = -\text{sgn}(s) \sum_{\mu} \left[ \frac{1}{2 \ii \omega \tau^{(a)}_{\mu}(p) - 1} \frac{i}{\ddot{\varepsilon}^{(s)}_{\mu}(\mathbf{p})} \right] \frac{1}{2 \tau^{(a)}_{\mu}(p)} + \sum_{\mu} \frac{1}{2 \tau^{(a)}_{\mu}(p)[i \omega \tau^{(a)}_{\mu}(p) - 1]} \right]^{-1}
\]
(8.31)
Figure 6. Density dependence of the real part of the dynamic conductivity for various frequencies of the AC field in the presence of SR scattering. (Reprinted with permission from Liu et al. (2010). Copyright © (2010), IEEE). $N_i = 1 \times 10^{16}$ m$^{-2}$; $T = 0$ K. Solid line, 10 THz; dotted line, 7 THz; dashed line, 5 THz; short dashed-dotted line, 3 THz; long dashed-dotted line, 1 THz.

In terms of these functions, the linear AC current of the diffusive regime is given by

$$J(\omega) = \frac{e^2}{2} g_s \gamma^2 E_0 \sum_{p,s} \frac{1}{i \omega \tau_{\mu}^{(a)}(p) - 1} \left\{ \tau_{\mu}^{(a)}(p) \frac{\partial \left[ \hat{\rho}_0^{(s)}(p) \right]}{\partial \delta_{\mu}^{(s)}(p)} + sgn(s) \text{Im} \left[ \Phi^{(s)}(\omega, p) \right] \right\}. \quad (8.32)$$

and

$$A_{\mu}^{(s)}(\omega, p) = -\frac{1}{i \omega \tau_{\mu}^{(a)}(p) - 1} \left\{ \tau_{\mu}^{(a)}(p) \frac{\partial \left[ \hat{\rho}_0^{(s)}(p) \right]}{\partial \delta_{\mu}^{(s)}(p)} + sgn(s) \text{Im} \left[ \Phi^{(s)}(\omega, p) \right] \right\}. \quad (8.33)$$

The conductivity calculated from this result takes account of electron–hole interband coherence, and exhibits a minimum as a function of electron density for both SR and long-range RPA-screened electron-impurity scatterings, provided that the frequency of the AC electric field is less than a critical value, $\omega_0$, in the terahertz regime. For SR scattering, $\omega_0 \approx 5$ THz, while for long-range RPA-screened scattering, $\omega_0 \approx 3$ THz. Again, the existence of such a minimum in the conductivity as a function of electron density is the result of interband coherence (Liu et al. 2010). However, for frequencies greater than the critical value, the dynamic conductivity decreases monotonically with decreasing electron density. These features are exhibited in figures 6 and 7.
Figure 7. Density dependence of the real part of the dynamic conductivity for various frequencies of the AC field in the presence of RPA-screened Coulomb scattering. (Reprinted with permission from Liu et al. (2010). Copyright © (2010), IEEE). $N_i = 1 \times 10^{16} \text{m}^{-2}$; $T = 0 \text{K}$. Solid line, 10 THz; dotted line, 7 THz; dashed line, 5 THz; short dashed-dotted line, 3 THz; long dashed-dotted line, 1 THz.

9. Summary

Graphene holds great promise to become the primary material of a new generation of electronics and sensors. Here, we have touched upon an eclectic selection of aspects of its theory, including its Green’s function with and without a magnetic field, as well as Green’s function for a graphene quantum dot and its Landau-quantized spectrum. Furthermore, its dynamic, non-local dielectric function has been discussed in the RPA, along with its application to plasma modes and some of their interactions. The latter includes discussion of the role of graphene plasmons in energy-loss probe spectroscopy and vdW interactions (as well as TE and TM electromagnetic modes): moreover, the role of plasmons (and phonons) in graphene self-energy is described. The important issue of charge transport in graphene has been addressed for both steady-state DC conduction and dynamic AC conductivity, for both SR and long-range RPA shielded impurity scattering.

Having a massless relativistic Dirac-like single-particle Hamiltonian and energy spectrum, graphene is also of great fundamental interest. The introduction of relativistic phenomenology such as Klein tunnelling and ‘zitterbewegung’
open the possibility of observing and measuring such relativistic effects under laboratory conditions that are actually non-relativistic. For example, the finite ‘residual’ conductivity of graphene may arise (in part) in connection with the relativistic phenomenon of pair production.

It is hardly necessary to point out that there is much, much more literature pertinent to graphene phenomenology that we have not discussed. Its meteoric rise in the world of science and technology has been documented by Geim & Novoselov (2007) and Barth & Marx (2008). Its extraordinary device-friendly potential, which we have briefly discussed above, is reviewed (along with its production and properties) by Soldano et al. (2010). Of particular importance, the current status of graphene transistors is discussed in detail by Lemme (2010). Finally, another very detailed review article on graphene theory is soon to be published by Abergel et al. (2010). The literature on graphene is vast.

This article barely scratches the surface of the huge flood of work on the subject, omitting many very interesting and important studies. However, this is not intended to be a comprehensive review, and we apologize to all the authors of such studies that are not cited here.

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