Electron–electron and electron–hole pairing in graphene structures

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The superconducting pairing of electrons in doped graphene owing to in-plane and out-of-plane phonons is considered. It is shown that the structure of the order parameter in the valley space substantially affects conditions of the pairing. Electron–hole pairing in a graphene bilayer in the strong coupling regime is also considered. Taking into account retardation of the screened Coulomb pairing potential shows a significant competition between the electron–hole direct attraction and their repulsion owing to virtual plasmons and single-particle excitations.

Keywords: graphene; pairing; massless fermions; superfluidity

1. Introduction

Electrons in graphene, a two-dimensional form of carbon, can be described by a two-dimensional Dirac-type equation for massless particles near the Fermi level (see Castro Neto et al. 2009 and references therein). Thereby, graphene offers a unique possibility to study effectively ultrarelativistic charged particles in condensed-matter phenomena (Katsnelson et al. 2006; Katsnelson & Novoselov 2007) and particularly in collective phenomena (Lozovik et al. 2008; Berman et al. 2008a, b). Absence of mass for electrons make it possible to achieve new regimes of quantum many-particle system behaviour in graphene. Therefore, it is interesting to search for various superconducting and superfluid phases in graphene and graphene-based structures, with their applications for dissipationless information transfer in nanoscale devices. In the present paper, we consider the Bardeen–Cooper–Schrieffer-like (BCS-like; Bardeen et al. 1957) phonon-mediated pairing of electrons in graphene, and the Coulomb pairing of electrons and holes in a graphene bilayer, taking into account the unusual electron dynamics.

Several possibilities for electron-pairing phenomena in graphene have been proposed. One possibility is the pairing of spontaneously created electrons in the conduction band and holes in the valence band, leading to the excitonic insulator state (Khveshchenko 2001). The results of numerical simulations in recent papers (e.g. Drut & Lähde 2008; Armour et al. 2009) show that graphene can turn into
an excitonic insulator state while being suspended in vacuum. Another possibility is electron–electron pairing in the graphene layer, mediated either by phonons, plasmons (Uchoa & Castro Neto 2007) or by Coulomb interaction, acting as attractive in certain channels (i.e. resonating valence bond mechanisms, proposed by Black-Schaffer & Doniach (2007) and Honerkamp (2008) or anisotropic electron scattering near the Van Hove singularity by González (2008)). The other two possible mechanisms of establishing a coherent state in graphene are proximity-induced superconductivity (Heersche et al. 2007; Beenakker 2008) and the pairing of spatially separated electrons and holes in the graphene bilayer (Lozovik & Sokolik 2008a; Min et al. 2008; Zhang & Joglekar 2008), analogous to electron–hole pairing in coupled quantum wells (Lozovik & Yudson 1975, 1976; Shevchenko 1994; Lozovik & Berman 1997; Lozovik & Poushnov 1997).

We consider electron–electron pairing owing to optical in-plane phonons, represented by two pairs of doubly degenerate modes (Piscanec et al. 2004; Basko & Aleiner 2008), and owing to out-of-plane (flexural) acoustical and optical modes; the out-of-plane modes interact with electrons quadratically (Mariani & von Oppen 2008; Khveshchenko 2009). We demonstrate that each phonon mode in graphene provides a contribution to effective electron–electron interaction, dependent on both its symmetry and the structure of the order parameter with respect to electron valleys. Estimates of the coupling constants show that out-of-plane phonons do not cause a pairing with any observable critical temperatures, however, the in-plane optical phonons can lead to the pairing in heavily doped graphene.

Electron–hole pairing in the graphene bilayer in the weak coupling regime is of BCS type, and affects only the conduction band of the electron-doped graphene layer and the valence band of the hole-doped layer (Lozovik & Sokolik 2008a). On increase of the coupling strength, the pairing becomes multi-band, involving also the valence band of the electron-doped layer and the conduction band of the hole-doped layer (Lozovik & Sokolik 2009, 2010a). Such an ‘ultrarelativistic’ regime of pairing occurs owing to absence of local pairs in graphene (Lozovik & Sokolik 2008b; Sabio et al. 2009)—in contrast to usual systems of attracting fermions, where crossover to a gas of local pairs at strong coupling occurs (Nozières & Schmitt-Rink 1985).

The estimates of a critical temperature in the graphene bilayer within the framework of a one-band BCS model, by taking into account static screening of electron–hole interaction, give unobservably small values (Kharitonov & Efetov 2008a, b). However, the estimates using unscreened interaction, or with a statically screened interaction, but within the multi-band model, provide much larger values of the critical temperature (Min et al. 2008; Zhang & Joglekar 2008; Lozovik & Sokolik 2009). In this paper, we consider the strong coupling regime within the framework of the multi-band model, taking into account a dynamical screening of the electron–hole interaction. The dynamical effects manifest themselves as virtual plasmons and single-particle excitations, the contribution to the interaction of which is repulsive and thus competes with the ‘direct’ Coulomb attraction.

The article is organized as follows. In §2, we derive and solve the gap equations for the phonon-mediated electron–electron pairing in graphene. In §3, we study electron–hole pairing in the graphene bilayer using Eliashberg-type equations; §4 is devoted to conclusions.
Pairing in graphene structures

2. Phonon-mediated electron–electron pairing in graphene

Electrons in graphene populate two interpenetrating triangular lattices $A$ and $B$, composing the bipartite graphene lattice, and two ‘valleys’ $K$ and $K' = -K$ in momentum space; therefore, it is convenient to describe electrons by the effective four-component wave function (Castro Neto et al. 2009). Analogous to Gusynin et al. (2007), we introduce the four-component electron destruction operator $\Psi_p = (a_{K+p}, b_{K+p}, b_{K'+p}, a_{K'+p})^T$, where the operators $a_p$ and $b_p$ correspond to sublattices $A$ and $B$, respectively. In the Heisenberg representation, $\Psi_p$ evolves according to the Dirac-type equation

$$p_\mu \gamma^\mu \Psi_p = 0, \quad \mu = 0, 1, 2. \quad (2.1)$$

The ‘covariant’ coordinates $p^0 = (i/v_F)(\partial/\partial t)$, $p^{1,2} = px, py$, $p_\mu = \{p^0, -p^1, -p^2\}$ are used, where $v_F \approx 10^6 \text{ m s}^{-1}$ is the Fermi velocity. The gamma matrices are in the Weyl representation

$$\gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma = \begin{pmatrix} 0 & -\sigma \\ \sigma & 0 \end{pmatrix} \quad \text{and} \quad \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. $$

The Hamiltonian of linear electron–phonon coupling can be written in the general form (see figure 1a)

$$H^{(\text{lin})}_{\text{el-ph}} = \frac{1}{\sqrt{S}} \sum_{pq\mu} g_{pq}^{(\mu)} \overline{\Psi}_{p+q} \Gamma_\mu \Psi_p \Phi_{q\mu}. \quad (2.2)$$

Here, $g_{pq}^{(\mu)}$ and $\Gamma_\mu$ are, respectively, the coupling amplitude and interaction vertex for the $\mu$th phonon mode, $\Phi_{q\mu} = c_{q\mu} + c_{q\mu}^+$, where $c_{q\mu}$ is the phonon destruction operator, $\overline{\Psi}_p = \Psi_p^+ \gamma^0$ is the Dirac-conjugated spinor and $S$ is the system area.

Figure 1. Diagrammatic representations of electron–phonon coupling Hamiltonians (2.2) and (2.4) for (a) linear and (b) quadratic couplings, respectively. The corresponding self-consistent gap equations (2.6) and (2.7) are shown in (c) and (d), respectively.
We take into account two pairs of degenerate in-plane optical phonon modes, most strongly coupled to graphene electrons (Piscanec et al. 2004; Basko & Aleiner 2008): $A_1$ and $B_1$ modes (we denote them by $\mu = 1, 2$) with the momentum $q = \pm K$ and energy $\omega_K \approx 0.170$ eV, and $E_{2x}$ and $E_{2y}$ modes ($\mu = 3, 4$) with $q = \Gamma$, $\omega_\Gamma \approx 0.196$ eV. The coupling constants (Piscanec et al. 2004) and interaction vertices (Basko & Aleiner 2008) for these modes are $g_{pq}^{(1,2)} \approx 1.34$ eV Å, $g_{pq}^{(3,4)} \approx 0.86$ eV Å, $\Gamma_1 = I$, $\Gamma_2 = i\gamma^5$, $\Gamma_3 = -\gamma^5\gamma^2$ and $\Gamma_4 = -\gamma^5\gamma^4$.

The Hamiltonian of quadratic interaction of graphene electrons with out-of-plane phonons is more complicated. The major part of the interaction, resulting from the deformation potential (Suzuura & Ando 2002; Mariani & von Oppen 2008) can be written in the form

$$H_{el-ph}^{(\text{quadr})} = \frac{1}{S} \sum_{pp'q\sigma\sigma'} \sum_{j=1}^{3} \left[ a_p^+ a_p + b_p^+ b_p e^{i(p-p')d_j} \right] \Phi_{q\sigma} \Phi_{q'\sigma'} \times \frac{\sqrt{3} g_1 \left[ e^{iqd_j} \varepsilon^B_{q\sigma} - \varepsilon^A_{q\sigma} \right] \left[ e^{i(q'-d_j)} \varepsilon^B_{q'\sigma'} - \varepsilon^A_{q'\sigma'} \right]}{4M \sqrt{\omega_{q\sigma} \omega_{q'\sigma'}}},$$

(2.3)

where $q' = p' - p - q$, $M$ is the carbon atom mass, $g_1 \approx 20–30$ eV and $d_j$ ($j = 1, 2, 3$) are the vectors connecting an atom from the A sublattice with its nearest neighbours. The summation over $p$, $p'$ and $q$ in equation (2.3) is performed over the first Brillouin zone of graphene; $\varepsilon^A_{q\sigma}$ and $\omega_{q\sigma}$ are polarizations and frequencies of acoustical ($\sigma = 1$) and optical ($\sigma = 2$) out-of-plane phonons branches.

Rewriting equation (2.3) in the four-component spinor notation requires splitting of the summation over electron momentums $p$ and $p'$ among the valleys $\pm K$. The result is (see figure 1b; see also Lozovik & Sokolik 2010b for details)

$$H_{el-ph}^{(\text{quadr})} = \frac{1}{S} \sum_{pp'q\sigma\sigma'} \sum_{Q=\Gamma,\pm K} \overline{\psi}_p V_{q\sigma\sigma'}^{(Q)} \psi_p \Phi_{q\sigma} \Phi_{Q+p'-p,\sigma'}$$

(2.4)

and

$$V_{q\sigma\sigma'}^{(Q)} = \frac{\sqrt{3} g_1}{8M \sqrt{\omega_{q\sigma} \omega_{q'\sigma'}}} \left[ \delta Q\Gamma \gamma^1\gamma^5 + \delta QK (1 + \gamma^5) + \delta Q_-\Gamma (1 - \gamma^5) \right] i\gamma^2 \times \sum_{j=1}^{3} \left[ \gamma^3 + \gamma^0 + (\gamma^3 - \gamma^0) e^{-iQd_j} \right] \left[ e^{iqd_j} \varepsilon^B_{q\sigma} - \varepsilon^A_{q\sigma} \right] \left[ e^{i(q'-d_j)} \varepsilon^B_{q'\sigma'} - \varepsilon^A_{q'\sigma'} \right],$$

where $q' = Q - q$.

Similar to Pisarski & Rischke (1999), we describe the pairing by the set of matrix Green functions in the Matsubara representation $G_{ij}(p, \tau) = -\langle T \psi_i^{(j)}(\tau) \overline{\psi}_p^{(j)}(0) \rangle$, where $\psi_p^{(1)} = \psi_p$, $\psi_p^{(2)} = \psi_C p \equiv C \overline{\psi}_{-p}^T$ is the charge-conjugated spinor and $C = i\gamma^2\gamma^0$ is the charge-conjugation matrix. The anomalous Green functions $G_{12}$ and $G_{21}$ are responsible for a Cooper pair.
condensate. The Gor’kov equations, describing the pairing in the mean-field approximation, are

\[ G_{ij}(p) = \delta_{ij} G_i^{(0)}(p) + G_i^{(0)}(p) \Delta_{i,3-i}(p) G_{3-i,j}(p), \quad (2.5) \]

where \( p = \{ p_0 = \pi T (2k + 1), p \} \), \( G_i^{(0)}(p) = [\gamma^0 (p_0 \pm \mu) - v_F \gamma^j p]^{-1} \) are the free-particle Green functions, following from equation (2.1), and \( \mu \) is the chemical potential in graphene.

The expressions for the anomalous self-energy \( \Delta_{21} \) (the other component \( \Delta_{12} = \gamma^0 \Delta_{21}^\dagger \gamma^0 \)) in equation (2.5) for the cases of linear (2.2) and quadratic (2.4) electron–phonon interaction Hamiltonians are, respectively (see figure 1c,d),

\[ \Delta_{21}(p) = -\frac{T}{S} \sum_{p', \mu} q_{\mu}^2 D_\mu (p - p') \bar{T}_\mu G_{21}(p') T_\mu \quad (2.6) \]

and

\[ \Delta_{21}(p) = \frac{2T^2}{S^2} \sum_{p', q} \sum_{Q, \sigma, \sigma'} D_\sigma (q) D_{\sigma'} (Q + p - p' - q) \bar{V}_{q, \sigma, \sigma'} (Q) G_{21}(p') V_{-Q, \sigma, \sigma'}. \quad (2.7) \]

Here, the charge-conjugated vertices \( \bar{T}_\mu = C^{-1} T_\mu C \) and \( \bar{V}_{q, \sigma, \sigma'} (Q) = C^{-1} V_{q, \sigma, \sigma'} (Q)^T C \) are introduced, and \( D_\mu (q) = 2\omega_{q\mu} / \left( q_0^2 - \omega_{q\mu}^2 \right) \) is the phonon Green function.

To solve the Gor’kov equations (2.5), we assume that the pairing is diagonal with respect to the conduction and valence bands, but suppose that the structure of the order parameter with respect to electron valleys is parameterized by arbitrary \( SU(2) \) matrix. The band-diagonal order parameter can be represented as a decomposition over projection operators \( P_{\pm}(\hat{p}) = (1 \pm \gamma^0 \gamma^\hat{p}) / 2 \) on conduction and valence bands, where \( \hat{p} = p / |p| \) (Pisarski & Rischke 1999). Further, rotation of the order parameter in the valley space can be performed by means of three generators \( T_1 = \gamma^5, T_2 = \gamma^3 \gamma^5 \) and \( T_3 = i\gamma^3 \), obeying the algebra of the Pauli matrices (Gusynin et al. 2007). Thus, the explicit form of \( \Delta_{21} \) is

\[ \Delta_{21}(p) = e^{i\pi T} [\Delta_+(p) P_+(\hat{p}) + \Delta_-(p) P_-(\hat{p})], \quad (2.8) \]

where \( \Delta_{\pm}(p) \) are the gaps in conduction and valence bands, and the three-dimensional vector \( \mathbf{v} \) defines the valley structure of the order parameter.

Substituting equation (2.8) in equations (2.6) and (2.7), we can derive the system of two coupled gap equations for \( \Delta_{\pm}(p) \) having the form

\[ \Delta_\alpha (p) = -\frac{T}{S} \sum_{p', \beta} \frac{\Delta_\beta (p')}{p_0^2 - E_\beta^2 (p')} A_{\alpha \beta} (p, p'; \mathbf{v}), \quad (2.9) \]

where \( E_\pm (p) = \sqrt{(v_F |p| \mp \mu)^2 + \Delta_\pm^2 (p)} \) are the energies of the Bogolyubov excitations in the conduction and valence bands. The effective intraband \((\alpha = \beta)\)
and interband \((\alpha = -\beta)\) interactions in the cases of linear and quadratic electron–phonon couplings are, respectively,
\[
A_{\alpha\beta}^{\mu}(p, p'; v) = \frac{1}{2} \sum_{\mu} g_{\mu}^2 D_{\mu}(p - p') \text{Sp}[\mathcal{P}_{\alpha}(\hat{p}) e^{-i\nu T \gamma^0_{\mu} \gamma^0} \mathcal{P}_{\beta}(\hat{p}') \gamma^0 D_{\mu}]
\]
(2.10) and
\[
A_{\alpha\beta}^{\mu}(p, p'; v) = -\frac{T}{S} \sum_{qQ} D_{\sigma}(q) D_{\sigma'}(q + p - p' - q)
\]
\[
\times \text{Sp}[\mathcal{P}_{\alpha}(\hat{p}) e^{-i\nu T \gamma^0_{q\sigma} \gamma^0} e^{i\nu T \mathcal{P}_{\beta}(\hat{p}') \gamma^0} V(-q)]
\] (2.11)

We can find analytical solutions of equations (2.9)–(2.11) in the regime of high doping of graphene, when \(\mu\) is greater than the characteristic phonon frequencies. Moreover, high doping facilitates the pairing owing to larger density of states at the Fermi level \(\mathcal{N} = \mu/2\pi v_F^2\). In this case, the pairing is effectively one band, and the Eliashberg equations at \(T = 0\), following from equation (2.9), can be derived by setting \(\Delta_+(p) = \Delta_0(\omega_0 - p_0)\), \(\Delta_- = 0\) (similar to Lozovik et al. 2010),
\[
1 = 2 \int_{0}^{\omega_0} \frac{d\omega}{\sqrt{\omega^2 - \Delta^2}} \int_{0}^{\infty} dv \frac{\alpha_{T}^2(v) F(v)}{\omega + v}.
\]
(2.12)

Here, \(\omega_0\) is a cutoff frequency of the order of phonon frequencies, and the Eliashberg functions \(\alpha_{T}^2(v) F(v)\) for in-plane and out-of-plane phonons, respectively, can be represented as
\[
\alpha_{T}^2(v) F(v) = \mathcal{N} g_{T}^2 \delta(v - \omega_T) R_{T}^{(1)}(v) + \mathcal{N} g_{K}^2 \delta(v - \omega_K) R_{K}^{(1)}(v)
\]
(2.13)
and
\[
\alpha_{T}^2(v) F(v) = Z_{T}(v) R_{T}^{(2)}(v) + Z_{K}(v) R_{K}^{(2)}(v).
\]
(2.14)

The partial Eliashberg functions of out-of-plane phonons can be calculated within the simple phonon model (see Lozovik & Sokolik 2010b) and reduced to dimensionless functions \(Z_{\mu}(v) = (81 \mathcal{N} g_{T}^2/2a^2 M^2 \omega_T^3) \tilde{Z}_{\mu}(x)\), where \(x = 6v/\omega_{T2}\), \(\omega_{T2} \approx 0.11\) eV. The functions \(\tilde{Z}_{\mu}(x)\) are shown in figure 2.

Equations (2.13)–(2.14) show that the Eliashberg functions consist of two parts, corresponding to phonon-mediated electron–electron interaction processes, leaving both electrons in their valleys (\(T\)-terms), and flipping both electrons into opposite valleys (\(K\)-terms). The factors \(R_{T,K}^{(1,2)}(v)\), dependent on the valley structure of the order parameter, determine the signs and amplitudes of these contributions,
\[
R_{T}^{(1)}(v) = -\cos^2 v + (1 - 2\hat{v}_T^2) \sin^2 v, \quad R_{T}^{(1)}(v) = -\cos^2 v + \hat{v}_T^2 \sin^2 v,
\]
\[
R_{T}^{(2)}(v) = 1 \quad \text{and} \quad R_{K}^{(2)}(v) = (-\hat{v}_T^2 + \hat{v}_T^2) \sin^2 v.
\]
(2.15)

All the factors in (2.15), except \(R_{T}^{(2)}\), can vary in the range from \(-1\) (the effective phonon-mediated repulsion) to \(+1\) (the effective attraction).
Figure 2. Partial dimensionless Eliashberg functions for out-of-plane phonons. Contributions of the two phonon processes, leaving the electron in its initial valley (Z_r, solid line), and flipping it into the opposite valley (Z_K, dotted line) are shown.

The system under pairing conditions should prefer the valley structure v of the order parameter, which provides the maximal gap and thus the maximal $\alpha_v^2(v)F(v)$. For in-plane phonons, the gap, found from equations (2.12)–(2.13), is $\Delta \sim \omega_{l,K} \exp[-1/\lambda]$, where the effective coupling constant $\lambda = 2\int_0^\infty (d\nu/\nu)\alpha^2_v(\nu)F(\nu)$ consists of the partial coupling constants $\lambda = \lambda_l R_l(v) + \lambda_K R_K(v)$, $\lambda_\mu = 2N g^{\mu}_\mu/\omega_\mu$. When $\lambda_K > 2\lambda_l$, the preferable pairing structure is $v = \{\pi/2, 0, 0\}$; in this case, $R_K = 1$ (scalar and pseudoscalar phonons give rise to effective electron–electron attraction) and $R_l = -1$ (pseudovector phonons cause repulsion). At $\lambda_K < 2\lambda_l$, we have $v = \{0, (\pi/2) \cos \phi, (\pi/2) \sin \phi\}$, and $R_l = 1$ (pseudovector phonons cause attraction), $R_K = 0$ (contributions from scalar and pseudoscalar modes cancel each other). Actually, at high values of dielectric permittivity of the surrounding medium, $\lambda_K < 2\lambda_l$; at lower permittivity, the Coulomb interaction renormalizes $\lambda_K$ towards higher values, so the relation $\lambda_K > 2\lambda_l$ can be satisfied (Basko & Aleiner 2008).

For out-of-plane phonons, the preferable valley structure of the order parameter is $v = \{0, 0, \pi/2\}$, when $R_l = R_K = 1$. Numerical estimates of the coupling constant for out-of-plane phonons show very small values ($10^{-3}$ by order of magnitude), thus out-of-plane phonons cannot provide any observable electron pairing in graphene. However, in-plane optical phonons can provide observable pairing at heavy doping of graphene.

3. Electron–hole pairing in the graphene bilayer

The pairing of spatially separated electrons and holes in the graphene bilayer occurs owing to Coulomb attraction. This longitudinally vectorial interaction is described by the vertex $\Gamma = \gamma^0$ within the framework of the matrix diagrammatic
technique employed in the previous section. Any interaction with such a vertex leads to an effective electron–electron interaction, independent of the valley structure of the order parameter. Under band-diagonal pairing, the system of self-consistent equations for the conduction- and valence-band gap functions \( \Delta_\pm(p) \) is similar to (2.9),

\[
\Delta_\alpha(p) = -\frac{T}{S} \sum_{\beta} \frac{1 + \alpha \delta \hat{p}'_\beta}{2} V(|p - p'|, p_0 - p'_0) F_\beta(p'),
\]

where \( F_\beta(p') = \Delta_\beta(p')/[p'_0 - E^2_\beta(p')] \) is the anomalous Green function and \( V(q, \omega) \) is the dynamically screened electron–electron interaction.

The system (3.1) can be solved in the spirit of BCS theory (Bardeen et al. 1957), i.e. in the static approximation, when one puts \( \omega = 0 \) in \( V(q, \omega) \) and assumes that \( \Delta_\pm(p, \omega) \) do not depend on \( \omega \) and are non-zero in some range of \( p \), corresponding to the neighbourhood of the Fermi surface. Such calculations (Lozovik & Sokolik 2009) showed that in the multi-band pairing regime, the gap depends exponentially on the energy width of the pairing region and thus can be very large. Here, we go beyond the static approximation and take into account the frequency dependence of the screened interaction.

The pairing interaction \( V(q, \omega) \) can be calculated in the random-phase approximation, well justified in the graphene bilayer owing to the large number of fermionic flavours, equal to eight (Kharitonov & Efetov 2008a, b; see also Apenko et al. 1982),

\[
V(q, \omega) = \frac{v_q e^{-qD}}{1 - 2v_q \Pi(q, \omega) + v_q^2 \Pi^2(q, \omega)(1 - e^{-2qD})},
\]

where \( v_q = 2\pi e^2/\varepsilon q \) is the bare Coulomb interaction, \( \varepsilon \) is a dielectric permittivity of the surrounding medium, \( \Pi(q, \omega) \) is a polarization operator of each graphene layer. Hereafter, we consider the case of a small interlayer distance \( D \), when \( p_F D \ll 1 \), \( p_F = \mu/v_F \) is the Fermi momentum. At \( \omega = 0 \), equation (3.2) reduces to the statically screened interaction, equal in dimensionless form to \( \mathcal{N} V(q, 0) = r_s/(q/p_F + 8r_s) \), where \( r_s = e^2/\varepsilon v_F \approx 2.19/\varepsilon \) determines the coupling strength.

There exist two plasmon branches in the system, corresponding to zeros of the denominator of equation (3.2): the lower branch with the dispersion \( \omega_-(q) \approx v_F q \) and the upper branch with the square-root dispersion \( \omega_+(q) \approx 2\mu \sqrt{r_s(q/p_F)} \) at small \( q \) and almost linear dispersion at large \( q \). When \( \omega_+(q) + v_F q > 2\mu \), the plasmons in graphene acquire a finite lifetime owing to interband transitions (Wunsch et al. 2006; Hwang & Das Sarma 2007). At \( \omega \to \infty \), the potential \( V(q, \omega) \) becomes unscreened: \( \mathcal{N} V(q, \infty) = r_s/(q/p_F) \).

Using the spectral representations of \( F_\beta(p') \) and \( V(q) \) in equation (3.1) and summing over \( p'_0 \) at \( T = 0 \), we get the Eliashberg-type equations

\[
\Delta_\alpha(p, \omega) = \sum_\beta \left[ \frac{d^{q'}}{(2\pi)^2} \frac{1 + \alpha \delta \hat{p}'_\beta}{2} \int_0^\infty \frac{d\omega'}{\pi} \text{Im} F_\beta(p', \omega') \right] \left\{ v_{p-p'} + \int_0^\infty \frac{d\nu'}{\pi} \right\}
\times \text{Im} V(p - p', \omega - \omega' + i\delta) \left( \frac{1}{\omega' + \nu + \omega + i\delta} - \frac{1}{\omega' + \nu - \omega - i\delta} \right),
\]

(3.3)
We assume that \( \Delta(p, \omega) \) is real (it is well justified near \( \omega = 0 \)); therefore, Im\( F_\beta(p') = -\pi\delta(\omega' - \beta(p')) \Delta_\beta(p')/2E_\beta(p') \). Then, we assume that the argument of the \( \delta \)-function in this expression vanishes at some unambiguous \( \omega' = \tilde{\omega}(p') \). This allows us to handle only ‘on-shell’ gap functions and Bogolyubov energies: \( \Delta_\alpha(|p|) \equiv \Delta_\alpha(p, \tilde{\omega}(p)) \) and \( E_\alpha(|p|) \equiv E_\alpha(p, \tilde{\omega}(p)) \). Rewriting equation (3.3) in terms of the on-shell quantities and assuming \( \alpha = +1 \), \( p = p_F \) on its left-hand side, we get

\[
\Delta_+(p_F) = \sum_\beta \int \frac{dp'}{(2\pi)^2} \frac{1 + \beta \hat{p'} \hat{p}}{2E_\beta(p')} \Delta_\beta(p') \\
\times \left\{ v_{p-p'} + \frac{2}{\pi} \int_0^\infty \frac{\mathrm{d}\nu}{E_\beta(p') + \nu} \right\}.
\]  
(3.4)

Here, we also neglected \( \omega = \Delta_+(p_F) \) in the second term in the braces.

To demonstrate the influence of dynamical screening of \( V(q, \omega) \) on the gap value, we will simplify equation (3.4) further. Firstly, we suppose that both on-shell gap functions \( \Delta_\beta(p) \) are equal to each other; this seems plausible at large \( r_s \), as discussed by Lozovik & Sokolik (2010a), and allows us to neglect the angular factor \( \hat{p'} \hat{p} \) in equation (3.4). Secondly, we assume \( \Delta_\pm(p) = \Delta f(p) \), where \( \Delta = \Delta_+(p_F) \) is the gap at the Fermi surface and \( f(p) \) is some trial function, equal to 1 at \( p = p_F \) and having the asymptotics \( f(p) \propto 1/p \) at \( p \to \infty \), caused by the leading contribution of the unscreened Coulomb interaction in equation (3.3). For computational purposes, it is also convenient to single out the contribution of undamped plasmons of the higher branch as Im\( V(q, \nu + i\delta) = \text{Im} V(q, \nu) - \pi\delta[\nu - \omega_+(q)]A(q) \). Here, the spectral weight of the higher branch plasmons is \( A(q) = -1/2[\partial \Pi(q, \omega)/\partial \omega]_{\omega=\omega_+(q)} \) when \( q + \omega_+(q) < 2\mu \) and zero otherwise. Thus, equation (3.4) for the gap reduces to

\[
1 = \frac{1}{2} \sum_\beta \int \frac{dp}{(2\pi)^2} \frac{\Delta_\beta(p)}{2E_\beta(p)} \left\{ v_{p-p_F} + \frac{2A(p-p_F)}{E_\beta(p) + \omega_+(p-p_F)} \right\} \\
+ \frac{2}{\pi} \int_0^\infty \frac{\mathrm{d}\nu}{E_\beta(p) + \nu}.
\]  
(3.5)

The expression in braces in equation (3.5) is the effective on-shell interaction, which incorporates the effects of dynamical screening of the pairing interaction. It differs from the statically screened interaction \( V(q, \omega) \), employed by Lozovik & Sokolik (2009, 2010a) and is naturally divided into three contributions (see figure 3): (i) an attractive unscreened Coulomb interaction, (ii) a repulsive contribution owing to virtual undamped higher-branch plasmons, and (iii) a repulsive contribution owing to virtual damped higher-branch plasmons and single-particle intra- and interband excitation continuums at \( \omega < v_Fq \) and \( \omega + v_Fq > 2\mu \), respectively, (Wunsch et al. 2006; Hwang & Das Sarma 2007). However, strictly on the Fermi surface (at \( \beta = +1 \), \( p = p_F \)) the effective on-shell interaction coincides with the statically screened one.

Assuming that the characteristic momentum, at which the on-shell gap \( \Delta_\pm(p) \) decays, is of the order of the Fermi momentum and employing \( f(p) = p_F/(|p-p_F| + p_F) \) as a trial function, we can study the influence of dynamical screening of the pairing interaction on the gap value \( \Delta \). Figure 4 shows the
Figure 3. On-shell interaction, represented by the expression in the braces of equation (3.5), in the intraband channel \((\beta = +1)\) at \(r_s = 2\). Solid line, full on-shell interaction; dashed-dotted line, unscreened Coulomb interaction only; dotted line, unscreened Coulomb interaction with the contribution of undamped plasmons; dashed line, statically screened interaction.

Results of the numerical solution of equation (3.5) by taking into account various contributions to the effective on-shell interaction. Taking into account only the unscreened Coulomb attraction results in huge gap values, reported previously by Phil. Trans. R. Soc. A (2010).
Min et al. (2008) and Zhang & Joglekar (2008). The addition of the undamped plasmons repulsive contribution eliminates the logarithmic singularity of the effective interaction on the Fermi momentum (figure 3), but does not change the gap values essentially at large $r_s$. Finally, the contribution of the damped plasmons and single-particle excitations lowers the gap down to the values of the order of 0.01$\mu$ at maximum (several Kelvins at $\mu \sim 0.1$ eV).

When the on-shell interaction is replaced by the statically screened one $V(q,0)$, the gap is unobservably small, if we use the trial function $f(p)$, spread over the momentums of the order of $p_F$; this is in agreement with the BCS-type estimates by Kharitonov & Efetov (2008a,b). However, as shown by Lozovik & Sokolik (2009), the pairings tend to occupy much larger regions of the momentums of the order of $8r_sp_F$ and result in large gap values, if we use the statically screened potential as the pairing potential. In our case, when we take into account the dynamical effects and naturally assume that the on-shell gaps $\Delta_\pm(p)$ decay at $p \sim p_F$, the gap turns out to take the values several orders of magnitude smaller than these with unscreened Coulomb interactions, but, at the same time, several orders of magnitude larger than the BCS-type estimates.

4. Conclusions

We have considered electron–electron pairing in graphene, mediated by in-plane and out-of-plane phonons, and electron–hole pairing in the graphene bilayer, mediated by the screened Coulomb interaction. In both cases, we consider the generally multi-band pairing with the $s$-wave order parameter, diagonal with respect to valence and conduction bands of paired particles. Moreover, we take into account the frequency dependence of the pairing interaction in both cases, deriving and solving two-band Eliashberg-type equations.

The consideration of phonon-mediated pairing is performed by resolution of the electron–phonon interaction with respect to sublattice and valley degrees of freedom of electrons in graphene and taking into account a possibility of different structures of the order parameter in valley space. We demonstrate that contributions of different phonon modes in graphene to effective electron–electron interactions, entering the Eliashberg-type equations, depend both on symmetries of these modes and on the structure of the order parameter in valley space.

The coupling of graphene electrons with out-of-plane (flexural) phonon modes is quadratic and leads to unusual forms of effective electron–electron phonon-mediated interactions, which include integration on frequency and integration on momentum over the whole Brillouin zone within the phonon loop. The estimates of effective coupling constants show that the pairing owing to in-plane phonon modes can occur at high doping of graphene, while the pairing owing to out-of-plane phonons does not occur at observable temperatures.

Eliashberg-type equations for electron–hole pairing in the graphene bilayer, written in the present paper in terms of the ‘on-shell’ gap functions, allow us to estimate the role of dynamical effects. The effective on-shell dynamically screened interaction, entering the gap equations, can be represented as a sum of attractive unscreened Coulomb interactions, repulsive contributions owing to undamped virtual plasmons and combined repulsive contributions of the damped plasmons and of the continuum of single-particle excitations.
The unscreened Coulomb interaction on its own provides large values of the gap, which are only slightly reduced by taking into account the undamped plasmons. Inclusion of the damped plasmons and single-particle excitations lower the gap by several orders of magnitude. This result demonstrates the significant competition between the bare Coulomb attraction and virtual excitations in the system, responsible for its dynamical screening. However, the estimates of the gap, calculated by taking into account the full on-shell potential, are by several orders of magnitude larger than the BCS-type estimates and can reach several Kelvins at strong coupling.

References


