Multicomponent electron-hole superfluidity and the BCS-BEC crossover in double bilayer graphene

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Superfluidity in coupled electron-hole sheets of bilayer graphene is predicted here to be multi-component because of the conduction and valence bands. We investigate the superfluid crossover properties as functions of the tunable carrier densities and the tunable energy band gap \( E_g \). For small band gaps there is a significant boost in the two superfluid gaps, but the interaction driven excitations from the valence to the conduction band can weaken the superfluidity, even blocking the system from entering the BEC regime at low densities. At a given larger density, a band gap \( E_g \approx 40-60 \text{ meV} \) can carry the system into the strong-pairing multiband BCS-BEC crossover regime, the optimal range for realization of high-\( T_c \) superfluidity.

The recent fabrication of two very close, but electrically isolated, conducting bilayer graphene sheets, one containing electrons and the other holes [1][3], raises exciting possibilities of observing high-temperature superconductivity [4], since the electrons form pairs with the holes through very strong Coulomb attraction [5][6].

In bilayer graphene, the Fermi energy can be tuned continuously relative to the average strength of the Coulomb interactions between carriers [7]. Metal gates can be used to change the carrier densities [8] so as to tune each sheet from the high-density regime of weak interactions, to the low-density regime where the average Coulomb interactions between carriers are much larger than their kinetic energies. However, the touching of the conduction and valence bands at the semi-metallic point means that at low densities, carriers from the two bands can strongly affect each other, and this weakens the superfluid pairing. A tunable energy band gap inserted between the conduction and valence bands by application of electric fields perpendicular to the sheets [9], can be used to decouple the conduction and valence bands at the semi-metallic point. We find that the crossover properties depend sensitively on both the carrier densities and the band gap.

Our effective Hamiltonian is,

\[
H = \sum_{\mathbf{k},\gamma} \left\{ \varepsilon^{(e)}_{\mathbf{k}\gamma} c^{\dagger}_{\mathbf{k}\gamma} c_{\mathbf{k}\gamma} + \varepsilon^{(h)}_{\mathbf{k}\gamma} d^{\dagger}_{\mathbf{k}\gamma} d_{\mathbf{k}\gamma} \right\} \\
+ \sum_{\mathbf{k},\mathbf{k}',\gamma,\gamma'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}+\gamma/2} d^{\dagger}_{\mathbf{k}'-\gamma/2} d_{\mathbf{k}'+\gamma/2} c_{\mathbf{k}'+\gamma/2}. 
\]  

\[
\Delta_{\gamma} = -\sum_{\mathbf{k}',\gamma'} F_{\gamma\gamma'}^{\gamma} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\gamma'}}{2E_{\gamma'}}. 
\]  

\[
E_{\mathbf{k}}^{\gamma} = \sqrt{(\varepsilon_{\mathbf{k}}^{(e)} + \Delta_{\gamma})^2 + (\xi_{\mathbf{k}}^{(h)} + \varepsilon_{\mathbf{k}}^{(h)})^2}, \\
\xi_{\mathbf{k}}^{(h)} = \frac{1}{2} \left( \varepsilon_{\mathbf{k}}^{(e)} + \varepsilon_{\mathbf{k}}^{(h)} \right). 
\]  

The band index \( \gamma = \pm \) labels the conduction and valence bands of each bilayer sheet. \( c_{\mathbf{k}\gamma}^{\ast} \) and \( d_{\mathbf{k}\gamma}^{\ast} \) are the creation operators in band \( \gamma \) for the electrons and holes in their respective bilayer sheets, and \( e_{\mathbf{k}}^{\gamma} \) and \( d_{\mathbf{k}}^{\gamma} \) the corresponding destruction operators. Spin indices are implicit. We make the standard transformation so the bands of the p-doped bilayer are filled with positively charged holes up to the Fermi level located in the conduction band. \( V_{\mathbf{k},\mathbf{k}'} \) is the electron-hole interaction. \( \xi_{\mathbf{k}'}^{(h)} = \varepsilon_{\mathbf{k}'}^{(h)} - \mu \), where \( \mu \) takes the single-particle energy dispersions of the conduction and valence bands for each bilayer graphene sheet \( \varepsilon_{\mathbf{k}}^{\gamma} \) to be identical and parabolic: \( \varepsilon_{\mathbf{k}}^{(e)} = \hbar^2 k^2/2m^* \) and \( \varepsilon_{\mathbf{k}}^{(h)} = -\hbar^2 k^2/2m^* - E_g \). We take the effective mass for electrons and holes equal, \( m^* = m^*_e = m^*_h = 0.04m_e \) [12]. We set the chemical potential \( \mu \) equal in the two bilayer sheets, considering only equal electron and hole densities.

We consider intraband pairing and Josephson-like pair transfer between the conduction and valence bands. The neglect of crosspairing will be justified later in the paper. The coupled zero temperature gap equations are [13],

\[
F_{\gamma\gamma'} = 2\left[ 1 + \gamma \gamma' (\cos \alpha_k \cos \alpha_{k'} + \sin \alpha_k \sin \alpha_{k'} \cos 2\phi) \right] \]  

is the form factor for the overlap of the single-particle state \( |k\rangle \) in band \( \gamma \) with \( |k'\rangle \) in band \( \gamma' \), \( \phi = \cos^{-1}(\mathbf{k}\cdot\mathbf{k'}) \), and \( \alpha_k = \tan^{-1} \left( \hbar^2 k^2/(m^* E_g) \right) \) [14]. We note the dependence of \( F_{\gamma\gamma'} \) on \( E_g \). To determine the chemical potential \( \mu \), we take for the density control parameter for each bilayer sheet [15][16],

\[
n_{0\gamma}^\pm = g_x g_v \sum_k \left[ (v_k^\gamma)^2 - (u_k^\gamma)^2 \right]. 
\]
$g_s = g_v = 2$ are the spin and valley degeneracy for bilayer graphene. $\mu$ is then obtained by solving Eqs. 2 to 4, $n_0^+$ is defined as the number of carriers in the conduction band, $n^+ = g_s g_v \sum_k (u_k^+)^2$, less the number of carriers in the conduction band that have been excited from the valence band. The number of such excited carriers in the conduction band equals the number of unoccupied states left behind in the valence band, $g_s g_v \sum_k (u_k)^2$.

The reason for this choice of control parameter (Eq. 5) is due to the influence of the valence band on the conduction band. The presence of the valence band means that the overall number of carriers in the conduction band, $n^+$, is no longer controlled purely by doping or using the metal gates, as is the case for the single band system, since now there are additional carriers in the conduction band excited from the valence band due to interactions. This increase in the number of carriers in the conduction band will push up the Fermi energy. We use $n^+$ to define an effective Fermi momentum $k_F^* = \sqrt{4 \pi n^+ / g_s g_v}$, and effective Fermi energy in the conduction band $E_F^* = (h k_F^*)^2 / 2 m^*$.

For large $n_0^+$, the average kinetic energy of the carriers in the conduction band $\langle K \rangle$ is large relative to the average strength of the Coulomb interactions $\langle V \rangle$, and, since $\sum_k (u_k^+)^2 \gg \sum_k (u_k)^2$, there are only a negligible number of carriers excited out of the valence band. However, small $n_0^+$ does not necessarily imply that $\langle K \rangle \ll \langle V \rangle$, since for sufficiently small $E_g$, both $\sum_k (u_k^+)^2$ and $\sum_k (u_k)^2$ can be large but nearly equal. We will see that both $n_0^+$ and $E_g$ play important roles in determining the relative strength of the Coulomb interactions.

We take the interaction term in Eq. 2 as unscreened,

$$V_{kk'} = \frac{-2 \pi e^2}{\epsilon |k - k'|},$$

(6)

where $d$ is the thickness of the insulating barrier separating the two bilayer sheets. A hexagonal Boron Nitride insulating barrier with dielectric constant $\epsilon = 3$ and thickness $d \geq 1$ nm can electrically isolate the two bilayer sheets [17][18]. We set $d = 1$ nm.

Neglecting screening is an excellent approximation in the BEC regime where the strong interactions tightly bind the pairs, making them compact on the scale of the average inter-carrier separations $r_0$ [19]. For example, at a carrier density of $1 \times 10^{11}$ cm$^{-2}$, $r_0 = 18$ nm which is much larger than our $d$. In this case, the superfluid gap in the excitation spectrum is large on the scale of $E_F^*$, and this suppresses the low energy excitations responsible for screening [20]. The unscreened approximation continues to be remarkably good even in the BCS-BEC crossover regime at intermediate densities [3], predicting superfluid gaps correctly to within $\sim 20\%$ [19]. However, at larger densities, $n_0^+ \geq 5 \times 10^{11}$ cm$^{-2}$, the unscreened approximation is known to completely break down, since at such densities, onset of very strong screening completely suppresses superfluidity in what would otherwise have been the BCS regime [20]. For this reason we will restrict our results to densities $n_0^+ \leq 5 \times 10^{11}$ cm$^{-2}$.

We omit intralayer electron-electron and hole-hole interactions. This approximation can be justified by comparing the gaps calculated including correlations between like-species [21], with the gaps calculated neglecting these correlations [22]. The intralayer correlations have at most a 10-20\% effect on the superfluid gap.

In general, the regimes of the crossover phenomena in a one-band system are conveniently characterized by the superfluid condensate fraction $c$ [23]. $c$ is defined as the fraction of carriers bound in pairs relative to the total number of carriers. The usual classification is: for $c > 0.8$ the condensate is in the BEC regime, for $c < 0.2$ in the BCS regime, and otherwise in the crossover regime.

However, we have here two partial condensate fractions, $c^+$, for the conduction and valence bands. For the conduction band, the usual one-band expression is readily generalized to the number of pairs divided by the total number of carriers in the conduction band,

$$c^+ = \frac{\sum_k (u_k^+)^2}{\sum_k (u_k)^2},$$

(7)

but for the valence band the corresponding definition of $c^-$ is the ratio of the number of pairs in the valence band to the number of anti-particles in the valence band,

$$c^- = \frac{\sum_k (u_k)^2}{\sum_k (u_k)^2}.$$

(8)

(We use the term anti-particle to refer to an empty single-particle state in the valence band, since we reserve the term hole to refer to the hole-doped bilayer sheet.) At zero temperature, the valence band anti-particles are generated exclusively as a result of the effect of interactions that excite carriers out of the valence band up into the conduction band. The pairs in the valence band are formed from pairing of anti-particles of the two sheets.

![Figure 1. Relative number of condensate pairs in conduction band (solid lines) and valence band (dashed lines) as functions of $n_0^+$ for different values of the energy band gap $E_g$.](image-url)
Figure 2. The condensate fraction and the chemical potential as functions of $n_0^+$ for different values of $E_g$, as labeled. In the upper panels, the solid and dashed lines indicate the condensate fraction in the conduction and valence band, respectively. In the lower panels, the solid lines show the chemical potential $\mu$ and the dashed lines the effective Fermi energy $E_F^*$. The light shaded area represents the energy band gap. Screening $E$ is because there are very few anti-particles in the valence band condensate. For $E_g = 0$ and small $n_0^+$, the peaks in $\Delta_k^\pm$ is very broad, characteristics of the BEC regime.

Figure 3. The superfluid gap energy $\Delta_k^\pm$ in the conduction and valence bands, for different values of energy band gap $E_g$. The results are for low density $n_0^+ = 0.5 \times 10^{11}$ cm$^{-2}$ (dotted lines), intermediate density $n_0^+ = 1.5 \times 10^{11}$ cm$^{-2}$ (dotted lines), and high density $n_0^+ = 5 \times 10^{11}$ cm$^{-2}$ (solid lines).

Excitations from the valence band now significantly increase the total population of carriers in the conduction band. The chemical potential $\mu$ therefore goes negative only at very low $n_0^+$. It is interesting that in the zero $n_0^+$ limit, $\mu$ now approaches the mid-point of the energy band gap, $\mu \approx -E_g/2$ instead of $-\epsilon_B/2$, behavior analogous to the low density limit in a conventional semiconductor.
Figure 4. The maximum superfluid gap energy $\Delta^\pm$ in the conduction and valence bands as functions of the energy band gap $E_g$. Dotted lines: $n_0^+ = 0.5 \times 10^{11} \text{ cm}^{-2}$; dashed lines: $n_0^+ = 1.5 \times 10^{11} \text{ cm}^{-2}$; solid lines: $n_0^+ = 5 \times 10^{11} \text{ cm}^{-2}$.

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