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The Kohn–Luttinger superconductivity in idealized doped graphene

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ABSTRACT

Idealized graphene monolayer is considered neglecting the van der Waals potential of the substrate and the role of the nonmagnetic impurities. The effect of the long-range Coulomb repulsion in an ensemble of Dirac fermions on the formation of the superconducting pairing in a monolayer is studied in the framework of the Kohn–Luttinger mechanism. The electronic structure of graphene is described in the strong coupling Wannier representation on the hexagonal lattice. We use the Shubin–Vonsowsky model which takes into account the intra- and intersite Coulomb repulsions of electrons. The Cooper instability is established by solving the Bethe–Salpeter integral equation, in which the role of the effective interaction is played by the renormalized scattering amplitude. The renormalized amplitude contains the Kohn–Luttinger polarization contributions up to and including the second-order terms in the Coulomb repulsion. We construct the superconductive phase diagram for the idealized graphene monolayer and show that the Kohn–Luttinger renormalizations and the intersite Coulomb repulsion significantly affect the interplay between the superconducting phases with f-, $d+id$-, and $p+ip$-wave symmetries of the order parameter.

1. Introduction

One of the most interesting properties of graphene is controllability of the position of its chemical potential by an applied electric field, which allows the change of the carrier type (electrons or holes) [1,2]. It was experimentally demonstrated that short graphene samples placed between superconducting contacts could be used for constructing Josephson junctions [3]. This indicates that Cooper pairs can coherently propagate in graphene. The question now arises of whether graphene can be structurally or chemically modified to become a magnet [4] or even a true superconductor.

Theoretically, a model with the conical dispersion requires the minimum intensity of the pairing interaction to develop the Cooper instability [5]. In view of this fact, a number of attempts were made to theoretically analyze possible implementation of the superconducting state in doped graphene. In paper [6], the role of topological effects in implementation of the Cooper pairing in this material was investigated. In paper [7], using the mean field approximation, the plasmon type of superconductivity in graphene was investigated, which leads to the low critical temperatures in the s-wave channel for realistic electron densities. The possibility of inducing superconductivity in graphene by electron correlations was studied in [8,9]. In paper [10], the interplay of the superconducting phase with the $d+id$-wave symmetry of the order parameter and the spin density wave phase depending on the position of the chemical potential with respect to van Hove singularity in the electron density of states of graphene was investigated using the functional renormalization group. Near the van Hove singularity, the superconducting phases with $d+id$- and f-wave symmetries of the order parameter were found.

In paper [11], the situation was considered when the Fermi level is located near one of the van Hove singularities in the density of states of graphene. It is known that these singularities can enhance the magnetic and superconducting fluctuations [12]. According to the scenario described in [11], the Cooper instability occurs due to the strong anisotropy of the Fermi contour at van Hove filling n_{vH}, which, as a matter of fact, originates from the Kohn–Luttinger mechanism [13] proposed in 1965 suggesting the appearance of the superconducting pairing in systems with the purely repulsive interaction. According to the estimation made in [11], the Cooper instability of this type in idealized graphene can increase the critical temperatures of the superconducting transition up to 10 K, depending on whether the chemical potential level is close to the van Hove singularity. It should be noted that in the calculation only the Coulomb repulsion of electrons on one site was taken into account. In paper [14], the possible interplay and coexistence of the Pomeranchuk instability and the

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Kohn–Luttinger superconducting pairing in graphene were discussed. The authors of [15] demonstrated using a renormalization group approach within the Kohn–Luttinger mechanism that in a monolayer of the doped graphene the superconducting $d+id$-pairing can be implemented.

In this paper, an idealized monolayer of graphene is considered neglecting the van der Waals potential of the substrate and the role of the nonmagnetic impurities. The Cooper instability in a monolayer is investigated in the weak coupling limit of the Born approximation by implementing the Kohn–Luttinger mechanism with respect to the Coulomb repulsion of electrons localized not only on one, but also on the nearest-neighbor carbon atoms. In the evaluation of the effective interaction in the Cooper channel, we take into account the polarization contributions caused by the Coulomb repulsion between electrons belonging to both one and different branches of the graphene energy spectrum.

The necessity to account for the long-range Coulomb repulsion in the calculation of the physical characteristics of graphene was dictated by the results of paper [16], where in the ab initio calculation of the effective many-body model of graphene and graphite the values of the partially screened frequency-dependent Coulomb repulsion were determined. It was demonstrated that the value of the onsite repulsion in graphene is $U=9.3$ eV and the Coulomb repulsion of electrons localized on the neighboring sites is $V=5.5$ eV, which indicates the principle importance to take into account the nonlocal Coulomb interaction. Note that other researchers consider the values of U and V to be much smaller.

2. Theoretical model

Since there are two carbon atoms per each unit cell of the graphene lattice, the latter can be divided in two sublattices A and B. In the Wannier representation, the Hamiltonian of the Shubin–Vonsowsky model (the extended Hubbard model) [17] for graphene with respect to electron hoppings between the nearest-neighbor and next-to-nearest-neighbor atoms and the Coulomb repulsion of electrons located at one and at neighboring sites has the form

$$\hat{H}=\hat{H}_0+\hat{H}_{int}, \tag{1}$$

$$\hat{H}_0=-\mu\sum_f(\hat{n}_f^A+\hat{n}_f^B)-t_1\sum_{\langle fm\rangle\sigma}(a_{f\sigma}^\dagger b_{m\sigma}+\text{h.c.}) -t_2\sum_{\langle\langle fm\rangle\rangle\sigma}(a_{f\sigma}^\dagger a_{m\sigma}+b_{f,\sigma}^\dagger b_{m,\sigma}+\text{h.c.}), \tag{2}$$

$$\hat{H}_{int}=U\sum_f(\hat{n}_{f\uparrow}^A\hat{n}_{f\downarrow}^A+\hat{n}_{f\uparrow}^B\hat{n}_{f\downarrow}^B)+V\sum_{\langle fm\rangle}\hat{n}_f^A\hat{n}_m^B. \tag{3}$$

Here $a_{f\sigma}^\dagger(a_{f\sigma})$ are the operators that create (annihilate) an electron with the spin projection $\sigma=\pm1/2$ at site f of the sublattice A, $\hat{n}_f^A=\sum_\sigma\hat{n}_{f\sigma}^A=\sum_\sigma a_{f\sigma}^\dagger a_{f\sigma}$ are the operators of the numbers of fermions at site f of the sublattice A (the analogous notations are used for the sublattice B), μ is the chemical potential of the system, t_1 is the hopping integral between neighboring atoms (hoppings between different sublattices), t_2 is the hopping integral between the next-to-nearest-neighbor atoms (within one sublattice), U is the parameter of the Coulomb repulsion of electrons located at one site and having the opposite spin projections (Hubbard repulsion), and V is the Coulomb repulsion of electrons located at neighboring atoms. In the Hamiltonian, $\langle\rangle$ denotes the summation over the nearest neighbors only, $\langle\langle\rangle\rangle$ denotes the summation over the next to nearest neighbors.

After the transition to the momentum state and the Bogoliubov transformation

$$\alpha_{i,k,\sigma}=w_{i1}(k)a_{k,\sigma}+w_{i2}(k)b_{k,\sigma},\quad i=1,2, \tag{4}$$

the Hamiltonian $\hat{H}_0$ is diagonalized and acquires the form

$$\hat{H}_0=\sum_{i=1}^{2}\sum_{k\sigma}E_{i,k}\alpha_{i,k,\sigma}^\dagger\alpha_{i,k,\sigma}. \tag{5}$$

The two-band energy spectrum of graphene is described by the expressions [18]

$$E_{1,k}=t_1|u_k|-t_2f_k,\quad E_{2,k}=-t_1|u_k|-t_2f_k, \tag{6}$$

where the notations

$$f_k=2\cos(\sqrt{3}k_y)+4\cos\left(\frac{\sqrt{3}}{2}k_y\right)\cos\left(\frac{3}{2}k_x\right),$$
$$u_k=\sum_\delta e^{ik\delta}=e^{-ik_x}+2e^{(i/2)k_x}\cos\left(\frac{\sqrt{3}}{2}k_y\right),\ \left|u_k\right|=\sqrt{3+f_k} \tag{7}$$

were used. The Bogoliubov transformation parameters have the form:

$$w_{1,1}(k)=w_{22}^*(k)=\frac{1}{\sqrt{2}}r_k^*,\quad r_k=\frac{u_k}{|u_k|},$$
$$w_{12}(k)=-w_{21}(k)=-\frac{1}{\sqrt{2}}. \tag{8}$$

In the Bogoliubov representation of quasiparticles, the interaction operator (3) is determined by the expression containing $\alpha_{1,k,\sigma}$ and $\alpha_{2,k,\sigma}$ as

$$\hat{H}_{int}=\frac{1}{N}\sum_{\substack{i,j,l,m\\k,p,q,s,\sigma}}\Gamma_{ij;lm}^{\parallel}(kp|qs)\alpha_{ik\sigma}^\dagger\alpha_{jp\sigma}^\dagger\alpha_{lq\sigma}\alpha_{ms\sigma}\Delta(k+p-q-s) +\frac{1}{N}\sum_{\substack{i,j,l,m\\k,p,q,s}}\Gamma_{ij;lm}^{\perp}(kp|qs)\alpha_{ik\uparrow}^\dagger\alpha_{jp\downarrow}^\dagger\alpha_{lq\downarrow}\alpha_{ms\uparrow}\Delta(k+p-q-s), \tag{9}$$

where the initial amplitudes

$$\Gamma_{ij;lm}^{\parallel}(kp|qs)=V_{ij;lm}(kp|qs)=Vu_{q-p}w_{i1}(k)w_{j2}(p)w_{l2}^*(q)w_{m1}^*(s), \tag{10}$$

describe the intensity of the interaction of Fermi quasiparticles with the parallel spins and the initial amplitudes

$$\Gamma_{ij;lm}^{\perp}(kp|qs)=V_{ij;lm}(kp|qs)+V_{ji;ml}(pk|sq)+U_{ij;lm}(kp|qs);$$
$$U_{ij;lm}(kp|qs)=U(w_{i1}(k)w_{j1}(p)w_{l1}^*(q)w_{m1}^*(s) +w_{i2}(k)w_{j2}(p)w_{l2}^*(q)w_{m2}^*(s)), \tag{11}$$

describe the interaction of Fermi quasiparticles with antiparallel spins. Indices i,j,l,m can take the values of 1 or 2. Note that as far as the terms $\alpha_{ik\sigma}^\dagger\alpha_{jp\sigma}^\dagger\alpha_{lq\sigma}\alpha_{ms\sigma}$ and $\alpha_{jp\sigma}^\dagger\alpha_{ik\sigma}^\dagger\alpha_{ms\sigma}\alpha_{lq\sigma}$ correspond to the same process, the effective interaction $\Gamma^{\parallel}$ should be written as

$$\Gamma_{ij;lm}^{\parallel}(kp|qs)=V_{ij;lm}(kp|qs)+(1-\delta_{ij}\delta_{lm})V_{ji;ml}(pk|sq). \tag{12}$$

3. Effective interaction in the Cooper channel and the equation for the order parameter

The utilization of the weak coupling Born approximation in the evaluation of the scattering amplitude in the Cooper channel allows us to limit the consideration up to the second order diagrams in the effective interaction for two electrons with the opposite values of the momentum and spin and use the quantity $\tilde{\Gamma}(p,k)$. This quantity is graphically determined as a sum of the diagrams shown in Fig. 1. Solid lines with the light (dark) arrows correspond to Green's function of the electrons with spin projections equal to $+\frac{1}{2}(-\frac{1}{2})$. It is well-known that the possibility of the Cooper pairing is determined by the characteristics of the energy spectrum close to the Fermi level and the effective interaction of