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Particle–hole pair states of layered materials

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HIGHLIGHTS

- The excitonic states and their wave functions in gapped graphene and in MoS_2 are presented.
- The Schrodinger equation in gapped graphene, in a single-layer MoS_2 and in bilayer graphene was solved.
- In the graphene in the MoS_2 the electron–hole pairing leads to the exciton insulator states.

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ABSTRACT

In the paper a theoretical study of both the quantized energies of excitonic states and their wave functions in gapped graphene and in monolayer of MoS_2 is presented. An integral two-dimensional Schrödinger equation of the electron–hole pairing for particles with electron–hole symmetry of reflection is analytically solved. The solutions of Schrödinger equation in momentum space in gapped graphene and in the direct band monolayer of MoS_2 by projection the two-dimensional space of momentum on the three-dimensional sphere are found. We analytically solve an integral two-dimensional Schrödinger equation of the electron–hole pairing for particles with electron–hole symmetry of reflection and with strong spin–orbit coupling. In monolayer of MoS_2 as well as in single-layer graphene (SLG) the electron–hole pairing leads to the exciton insulator states. Calculating an integral two-dimensional Schrödinger equation of the electron–hole pairing for bilayer graphene, exciton insulator states with a gap 3 meV are predicted. The particle–hole symmetry of Dirac equation of layered materials allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the valence band and conduction band and hence driving the Cooper instability.

1. Introduction

The graphene and graphene-like systems as well as the MX_2 (M=Mo, W, X=S, Se) [1–9] present a new state of matter of layered materials. The energy bands for graphite were found using "tight-binding" approximation by Wallace [10]. In the low-energy limit the single-particle spectrum is a Dirac cone similar to the light cone in relativistic mechanics, where the light speed is replaced by the Fermi velocity v_F.

In the paper we present a theoretical investigation of excitonic states as well as their wave functions in gapped graphene and in a direct band MoS_2. An integral form of the two-dimensional Schrödinger equation of Kepler problem in momentum space is solved exactly by the projection of the two-dimensional space of momentum on the three-dimensional sphere in the paper [12].

The integral Schrödinger equation was analytically solved by the projection of the three-dimensional momentum space onto the surface of a four-dimensional unit sphere by Fock in 1935 [11].

We consider the pairing between oppositely charged particles with complex dispersion. The Coulomb interaction leads to the electron–hole bound states scrutiny study of which acquire significant attention in the explanations of superconductivity.

If the exciton binding energy is greater than the flat band gap in narrow-gap semiconductor or semimetal then at sufficiently low temperature the insulator ground state is instable with respect to the exciton formation [13,14]. And excitons may be spontaneously created. A system undergoes a phase transition into a exciton insulator phase similar to Bardeen–Cooper–Schrieffer (BCS) superconductor. In a single-layer graphene (SLG) and in a single-layer MoS_2 the electron–hole pairing leads to the exciton insulator states [15].

In the paper an integral two-dimensional Schrödinger equation of the electron–hole pairing for particles with complex dispersion is analytically solved. Complex dispersions lead to fundamental difference in exciton insulator states and their wave functions.

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A crossing direct-gap like dispersion of single layer of graphene and single layer of MoS_2 does not lead to the fundamental differences in the many-particle effects in comparison with würtzite semiconductors [16,17].

We analytically solve an integral two-dimensional Schrödinger equation of the electron–hole pairing for particles with electron–hole symmetry of reflection.

For graphene in vacuum the effective fine structure parameter $\alpha_G = e^2/v_F\hbar\epsilon\sqrt{\pi} = 1.23$. For graphene in substrate $\alpha_G = 0.77$, the permittivity of graphene in substrate is estimated to be $\varepsilon = 1.6$ [18], which means the prominent Coulomb effects [19].

It is known that the Coulomb interaction leads to the semimetal-exciton insulator transition, where gap is opened by electron–electron exchange interaction [14,20–22]. The perfect host combines a small gap and a large exciton binding energy [13,14].

In graphene as well as in MoS_2 the existing of bound pair states is still subject matter of researches [23–27].

It is known [28] in the weak-coupling limit [29], exciton condensation is a consequence of the Cooper instability of materials with electron–hole symmetry of reflection inside identical Fermi surface. The identical Fermi surfaces are a consequence of the particle–hole symmetry of the Dirac equation. The room temperature superfluidity is shown to be calculated for bilayer graphene [13,28].

The particle–hole symmetry of the Dirac equation allows perfect pairing between electron Fermi sphere and hole Fermi sphere in the opposite layer and hence driving the Cooper instability. In the weak-coupling limit in graphene with the occupied conduction-band states and empty valence-band states inside identical Fermi surfaces in band structure, the exciton condensation is a consequence of the Cooper instability.

2. Theoretical study

2.1. Graphene

In the honeycomb lattice of graphene with two carbon atoms per unit cell the space group is D_{3h}^1 [30]:

D_{3h}^1	$\{E\|0\}$	$\{C_3^{(+,-)}\|0\}$	$\{C_2'^{(A,B,C)}\|0\}$	$\{\sigma_h\|\tau\}$	$\{S_3^{(-,+)}\|\tau\}$	$\{\sigma_v^{(A,B,C)}\|\tau\}$	
K_3^+	2	−1	0	2	−1	0	
g^2	$\{E\|0\}$	$\{C_3^{(+,-)}\|0\}$	$\{E\|0\}$	$\{E\|0\}$	$\{S_3^{(-,+)}\|\tau\}$	$\{E\|0\}$	
$\chi^2(g)$	4	1	0	4	1	0	$K_1^+ + K_2^+ + K_3^+$
$\chi(g^2)$	2	−1	2	2	−1	2	
$\frac{1}{2}[\chi^2(g) + \chi(g^2)]$	3	0	1	3	0	1	$K_1^+ + K_3^+$
$\frac{1}{2}\{\chi^2(g) - \chi(g^2)\}$	1	1	−1	1	1	−1	K_2^+

The direct production of two irreducible presentations of wave function and wave vector of difference $\kappa - K$ or $\kappa - K'$ expansion is $K_3^+ \times K_3^{+\star}$ and can be expanded on

$$p^\alpha: \tau_\psi \times \tau_k = (K_1^+ + K_2^+ + K_3^+) \times K_3^+ = K_3^+ \times K_3^+. \tag{1}$$

In the low-energy limit the single-particle spectrum is Dirac cone. The Hamiltonian of graphene [10]

$$\hat{H} = \frac{\Delta}{2}\hat{\sigma}_z + v_F(\tau\, q_x\hat{\sigma}_x + q_y\hat{\sigma}_y), \tag{2}$$

where Δ is the band gap of graphene, q_x and q_y are Cartesian components of a wave vector, $\tau = \pm 1$ is the valley index, $v_F = 1 \times 10^6$ m/s is the graphene Fermi velocity, $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are Pauli matrices (here we assume that $\hbar = 1$).

The dispersion of energy bands may be found in the following form [10]:

$$\epsilon_\pm = \pm\frac{\Delta}{2}\sqrt{1 + \frac{4v_F^2q^2}{\Delta^2}}, \tag{3}$$

where $q = \sqrt{q_x^2 + q_y^2}$.

The Schrödinger equation for calculating of exciton states can be written in the following general form:

$$(\epsilon(\mathbf{q}^2) + q_0^2)\Phi(\mathbf{q}) = \frac{1}{\pi}\int\frac{\Phi(\mathbf{q}')}{|\mathbf{q} - \mathbf{q}'|}d\mathbf{q}', \tag{4}$$

where $q_0^2 = -\epsilon$, ϵ is a quantized energy. We look for the bound states and hence the energy will be negative (Figs. 1–8).

An integral form of the two-dimensional Schrödinger equation in momentum space for the gapped graphene is solved exactly by the projection of the two-dimensional space of momentum on the three-dimensional sphere (Tables 1–5).

For the gapped single layer graphene

$$\frac{\epsilon(q^2) + q_0^2}{q^2 + q_0^2} = \pm\frac{\Delta}{4q_0^2}\sqrt{(1 - \cos\theta)^2 + \frac{4v_F^2}{\Delta^2}q_0^2(\sin\theta)^2} + \frac{1 - \cos\theta}{2}, \tag{5}$$

where an each point on sphere is defined of two spherical angles θ and ϕ, which are knitted with a momentum $\mathbf{q}$ [11,12]. A space angle Ω may be found as a surface element on sphere $d\Omega = \sin(\theta)d\theta\, d\phi = (2q_0/(q^2 + q_0^2))^2 d\mathbf{q}$ [11,12]. A spherical angle θ and a momentum $\mathbf{q}$ are shown [11,12] to be knitted as

$$\cos\theta = \frac{q^2 - q_0^2}{q^2 + q_0^2}, \quad \sin\theta = \frac{2qq_0}{q^2 + q_0^2}, \quad q^2 = q_0^2\left(\frac{1 + \cos\theta}{1 - \cos\theta}\right). \tag{6}$$

Using spherical symmetry the solution of integral Schrödinger equation can look for in the following form:

$$\Phi(\mathbf{q}) = \sqrt{q_0}\left(\frac{2q_0}{q^2 + q_0^2}\right)^{3/2}\sum_{l=0}^{\infty}A_lY_l^0(\theta, \phi), \tag{7}$$

where

$$Y_l^0(\theta, \phi) = \sqrt{\frac{2l + 1}{4\pi}}P_l^0(\cos\theta). \tag{8}$$

Since [12]

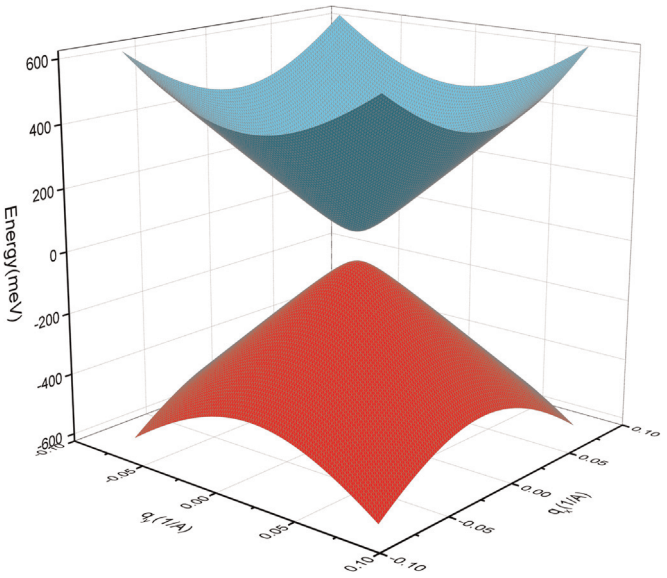

Fig. 1. Single-particle spectrum of gapped graphene.