Particle-hole pair states of layered materials.

Lyubov E. Lokot

Institute of Semiconductor Physics, NAS of Ukraine, 41, Nauky Ave., Kyiv 03028, Ukraine

In the paper a theoretical study the 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 a particles with electron-hole symmetry of reflection is analytically solved. The solutions of Schrödinger equation in momentum space is solved exactly 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, an 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.

PACS number(s): 81.05.ue, 81.05.U-, 71.30.+h, 71.10.-w.

I. INTRODUCTION

The graphene and graphene-like systems as well as the MX$_2$ (M=Mo, W, X=S, Se) [1] present a new state of matter of layered materials. The energy bands for graphite was found using "tight-binding" approximation by P.R. Wallace [10]. In the low-energy limit the single-particle spectrum is Dirac cone similarly 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 projection 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 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 stable with respect to the exciton formation [13,14]. And excitons may be spontaneously created. In a system undergo a phase transition into a exciton insulator phase similarly 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 [13].

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

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 wurtzite 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 $\alpha_G = \frac{2}{v_F \hbar^2 \sqrt{\pi}} = 1.23$. For graphene in substrate $\alpha_G = 0.77$, when the permittivity of graphene in substrate is estimated to be $\varepsilon = 1.6$ [18]. It 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 are 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 is a consequence of the particle-hole symmetry of Dirac equation. The room temperature superfluidity are shown to be calculated for bilayer graphene [13, 28].

The particle-hole symmetry of 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 the Cooper instability.
II. THEORETICAL STUDY

A. Graphene

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

| $D_{3h}^1$ | $\{E|0\}$ | $\{C^1_{3}^{+,-}\}|0\}$ | $\{C^1_{2}^{A,B,C}\}|0\}$ | $\{\sigma_h|\tau\}$ | $\{S^1_{3}^{(-,+)}|\tau\}$ | $\{\sigma^1_{l}|A,B,C\}|\tau\}$ |
|---|---|---|---|---|---|---|
| $K^+_3$ | 2 | -1 | 0 | 2 | -1 | 0 |
| $\Delta^2$ | $\{E|0\}$ | $\{C^1_{3}^{+,-}\}|0\}$ | $\{E|0\}$ | $\{S^1_{3}^{(-,+)}|\tau\}$ | $\{E|0\}$ |
| $\chi^2(g)$ | 4 | 1 | 0 | 4 | 1 | 0 |
| $\chi(g^2)$ | 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 $K^+_2$

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

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

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

where $q_0^2 = -\epsilon$, $\epsilon$ is a quantized energy. We look for the bound states and hence the energy will be negative.

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

For the gapped single layer graphene

$$ \epsilon(q^2) + q_0^2 + \frac{3\hbar^2}{4m^*} q_0^4 (\sin \theta)^2 + \frac{3\hbar^2}{4m^*} q_0^4 \cos^3 \theta, $$

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

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

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

$$ \Phi(q) = \sqrt{q_0^2(\frac{2q}{q^2 + q_0^2})^{3/2}} \sum_{l=0}^{\infty} A_l Y_l^0(\theta, \phi), $$

where

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

Since [12]
\[
\frac{(q^2 + q_0^2)^{1/2} (q^2 + q_0^2)^{1/2}}{2q_0} = \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \frac{4\pi}{2\lambda+1} Y_{\lambda}^{\mu}(\theta, \phi) Y_{\lambda}^{\mu, *}(\theta', \phi'),
\]
then substituting (7), (9) in (4), can find equation
\[
\varepsilon(q^2 + q_0^2) \sum_{l=0}^{\infty} a_l Y_l^0(\theta, \phi) = \frac{2}{q_0} \sum_{l=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \int \frac{1}{2\lambda+1} Y_{\lambda}^{\mu}(\theta, \phi) Y_{\lambda}^{\mu, *}(\theta', \phi') Y_l^0(\theta', \phi') A_l \left( \frac{2q_0}{q^2 + q_0^2} \right)^2 dq'.
\]

The integral equations for gapped SLG based on Eq. (5) may be found in the form
\[
\int (1 - \cos \theta)^2 + \frac{4q^2}{q_0^2} \sum_{l=0}^{\infty} a_l Y_l^0(\theta, \phi) Y_l^{\mu, *}(\theta, \phi) d\Omega = \frac{2}{q_0} \sum_{l=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \int \frac{1}{2\lambda+1} Y_{\lambda}^{\mu}(\theta, \phi) Y_{\lambda}^{\mu, *}(\theta', \phi') Y_l^0(\theta', \phi') Y_l^0(\theta', \phi') A_l \left( \frac{2q_0}{q^2 + q_0^2} \right)^2 dq'.
\]
Since \[\text{[31]}\]

\[
\cos \theta P_l^m(\cos \theta) = \frac{\sqrt{l + l + \mu}}{\sqrt{4l - 1}} P_{l+1}^m(\cos \theta) + \frac{\sqrt{l + 1 - \mu}}{\sqrt{4l - 1}} P_{l-1}^m(\cos \theta),
\]

\[
\sin \theta P_l^m(\cos \theta) = \frac{\sqrt{l - l - 1}}{\sqrt{4l - 1}} P_{l+1}^m(\cos \theta) + \frac{\sqrt{l + 1 - m}}{\sqrt{4l - 1}} P_{l-1}^m(\cos \theta),
\]

then solutions of the integral equation (10) for the energies and wave functions correspondingly can be found analytically with taken into account the normalization condition \(\frac{1}{2\pi} \int q_0^2 |\Phi(q)|^2 dq = 1\).

From equation (11) one can obtain the eigenvalue and eigenfunction problem and using a condition \(\frac{4q^2}{q_0^2} q_0^2 >> 1\) one can find recurrence relation
\[
\frac{1}{2} (l + \frac{1}{2}) A_l + \frac{1}{2} A_{l-1} (l + \frac{1}{2}) a_l + \frac{1}{2} A_{l+1} (l + \frac{1}{2}) b_l = 0.
\]

The solutions of the quantized series in excitonic Rydberges where \(\text{Ry} = m_e e^2 / (\epsilon^2 \hbar^2) = 34.72 \text{ meV}\), \(m_e\) is the reduced mass of an electron-hole pair, and wave functions of the integral equation (11) one can find in the form
\[
\epsilon_0 = -\frac{1}{(\frac{1}{2} + \frac{1}{2} a_1)^2},
\]
\[
\epsilon_1 = -\frac{1}{(\frac{1}{2} (1 + \frac{1}{2}) + \frac{1}{2} b_0 + \frac{1}{2} (2 + \frac{1}{2} a_2)^2)},
\]
\[
\epsilon_2 = -\frac{1}{(\frac{1}{2} (2 + \frac{1}{2}) + \frac{1}{2} (1 + \frac{1}{2}) b_1 + \frac{1}{2} (3 + \frac{1}{2} a_3)^2)},
\]
\[
\epsilon_3 = -\frac{1}{(\frac{1}{2} (3 + \frac{1}{2}) + \frac{1}{2} (2 + \frac{1}{2}) b_2 + \frac{1}{2} (4 + \frac{1}{2} a_4)^2)},
\]
\[
\Phi_l(\cos \theta) = \sqrt{\frac{2\pi}{(2q_0)^3}} \sum_{n=0}^{\infty} (1 - \cos \theta)^{3/2} P_n^0(\cos \theta),
\]

FIG. 2: Single-particle spectrum of the two-degenerated conduction band and spin-orbit splitting upper valence band of MoS_2

Table 1. Quantized spectral series of the excitonic states in meV, band gap of graphene in meV, effective reduced mass of electron-hole pair, the effective fine structure parameter, excitonic Rydberg in meV.

\[
a_l = \frac{1}{2\pi} \sqrt{\frac{2(l - 1) + 1}{2}} \sqrt{\frac{2}{2l + 1}} \frac{l}{\sqrt{4l^2 + 1}},
\]
\[
b_l = \frac{1}{4\pi} \sqrt{2(l + 1) + 1} \sqrt{2l + 1} \frac{l + 1}{\sqrt{4(l + 1)^2 - 1}}.
\]
κ can be expanded on κ of wave function and wave vector of difference

For the two-degenerated conduction band and spin-orbit splitting lower valence band one can find

For the two-degenerated conduction band and spin-orbit splitting upper valence band one can find

The Hamiltonian of MoS₂ [32]:

The dispersion of bands may be found in the form:

The direct production of two irreducible presentations of wave function and wave vector of difference κ − K or κ − K’ expansion with taken into account time inversion can be expanded on

The space group is

2 1

B. MoS₂

In the honeycomb lattice of MoS₂ the space group is

C₃h [32]:

FIG. 3: Single-particle spectrum of the two-degenerated conduction band and spin-orbit splitting lower valence band of MoS₂

FIG. 3: Single-particle spectrum of the two-degenerated conduction band and spin-orbit splitting lower valence band of MoS₂

\[ p^\alpha : \tau_v \times \tau_\psi = (B_1^+ + B_2^+) \times (A^+ + B_1^+ + B_2^+) = B_1^+ \times B_1^+ + B_2^+ \times B_2^+. \]

\[ \{ p^\alpha p^\beta \} : (A^+) \times (A^+ + B_1^+ + B_2^+) = A^+ \times A^+. \]
The integral equation for the two-degenerated conduction band and spin-orbit splitting upper valence band may be found correspondingly in the form substituting (27) in (10)

\[
\int \left( \frac{\Delta}{4q_0^2} \sqrt{(1 - \cos \theta)^2 + \frac{4a^2q_0^2}{\Delta}(\sin \theta)^2 + \frac{1 - \cos \theta}{2}} \right) \sum_{l=0}^{\infty} A_l Y_0^l(\theta, \phi) Y_{n^*}^{\mu^*}(\theta, \phi) d\Omega = \\
\frac{2}{q_0} \int \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \sum_{n'=0}^{\infty} Y_\lambda^\mu(\theta, \phi) Y_{n'}^{\mu^*}(\theta', \phi') Y_0^{n^*}(\theta, \phi) Y_k^{\mu^*}(\theta, \phi) d\Omega d\Omega'.
\]

(29)

From equation (29) one can obtain the eigenvalue and eigenfunction problem and using a condition \( \frac{a^2q_0^2}{\Delta} \gg 1 \) one can find

\[
\frac{1}{2} (l + \frac{1}{2}) A_l + \frac{1}{q_0} A_l + \frac{1}{2} A_{l-1} (l + \frac{1}{2}) a_l + \frac{1}{2} A_{l+1} (l + \frac{1}{2}) b_l = 0.
\]

(30)

The solutions of the quantized spectral series in excitonic Rydbergs where \( R_y = m_r e^4/(\epsilon^2\hbar^2) = 342.16 \text{ meV} \), \( m_r \) is the reduced mass of an electron-hole pair, and wave functions of the integral equation (29) one can find in the form

\[
\epsilon_0 = -\frac{1}{(\frac{1}{4} + \frac{1}{2}(1 + \frac{1}{2})a_1)^2},
\]

(31)

\[
\epsilon_1 = -\frac{1}{(\frac{1}{2}(1 + \frac{1}{2}) + \frac{1}{2}b_0 + \frac{1}{2}(2 + \frac{1}{2})a_2)^2},
\]

(32)

\[
\epsilon_2 = -\frac{1}{(\frac{1}{2}(2 + \frac{1}{2}) + \frac{1}{2}(1 + \frac{1}{2})b_1 + \frac{1}{2}(3 + \frac{1}{2})a_3)^2},
\]

(33)

\[
\Phi_l(\cos \theta) = \sqrt{\frac{2\pi}{(q_0)^2}} \sum_{n=0}^{\infty} (1 - \cos \theta)^{1/2} P_n^0(\cos \theta).
\]

(35)

FIG. 4: Wave function for graphene and single-particle spectrum of the two-degenerated conduction band and spin-orbit splitting upper valence band of MoS\(_2\) for quantum number \( l = 0 \)

FIG. 5: Wave function for single-particle spectrum of the two-degenerated conduction band and spin-orbit splitting lower valence band of MoS\(_2\) for quantum number \( l = 0 \)

Table 2. Quantized spectral series of the excitonic states in meV for the two-degenerated conduction band and spin-orbit splitting upper valence band, effective reduced mass of electron-hole pair, excitonic Rydberg in meV.

| \( \epsilon_0 \) | \( \epsilon_1 \) | \( \epsilon_2 \) | \( \epsilon_3 \) | \( m_r \) | \( R_y \) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 4338.78 | 479.60 | 155.06 | 70.37 | 0.146 | 342.16 |
The integral equation for the two-degenerated conduction band and spin-orbit splitting lower valence band may be found correspondingly in the form substituting (28) in (10)

\[
\int \left( \pm \frac{\nu}{g_0} \sqrt{\left(1 - \cos \theta \right)^2 + \frac{\omega^2}{\omega_0^2 + \Delta^2}} q_0^2 \sin \theta \right) + \frac{1 - \cos \theta}{\omega_0^2} \sum_{n=0}^{\infty} A_l Y_l^0(\theta, \phi) Y_k^{n,\ast}(\theta, \phi) d\Omega = 0.
\]

From equation (36) one can obtain the eigenvalue and eigenfunction problem and using a condition \(\frac{4a^2}{\Delta} q_0^2 >> 1\) one can find

\[
\frac{1}{2} \left( l + 1 \right) A_l + \frac{1}{2} A_{l-1} \left( l + \frac{1}{2} \right) a_l \left( 1 - \frac{\nu}{4q_0^2} \right) + \frac{1}{2} A_{l+1} \left( l + \frac{1}{2} \right) b_l \left( 1 - \frac{\nu}{4q_0^2} \right) = 0.
\]

The solutions of the quantized energies and wave functions of the integral equation one can find in the form

\[
\epsilon_{0\pm} = -\frac{9a^2 \nu^2}{64 \left( -1 \pm \sqrt{1 + \frac{3}{16} a_1 \nu (3a_1 + 1)} \right)^2}, \quad \Phi_l (\cos \theta) = \sqrt{\frac{2\pi}{(q_0 n)}} \sum_{n=0}^{\infty} (1 - \cos \theta)^{3/2} P_n^0 (\cos \theta).
\]

Table 3. Quantized spectral series of the excitonic states in meV for the two-degenerated conduction band and spin-orbit splitting lower valence band.

| | \(\epsilon_0\) | \(\epsilon_1\) | \(\epsilon_2\) | \(\epsilon_3\) |
|---|---|---|---|---|
| | 4305.39 | 446.29 | 123.45 | 41.32 |

C. Bilayer graphene

In the bilayer graphene the space group is \(D_{\text{h}}^3\), the point group of \(K\) point is \(D_3\) [94]:

| | \(D_3\) | \(E\{0\}\) | \(C_3^{(+,-)}\{0\}\) | \(C_2^{(A,B,C)}\{0\}\) |
|---|---|---|---|---|
| \(\tau_y\) | 2 | 1 | 0 | \(\Gamma_3\) |
| \(g^2\) | \{E\{0\}\} | \{C_3^{(+,-)}\{0\}\} | \{E\{0\}\} |
| \(\chi^2(g)\) | 4 | 1 | 0 |
| \(\chi(g^2)\) | 2 | -1 | 2 |
| \(\chi \left( \chi^2(g) + \chi(g^2) \right)\) | 3 | 0 | 1 | \(\Gamma_1 + \Gamma_3\) |
| \(\frac{1}{2} \left( \chi^2(g) - \chi(g^2) \right)\) | 1 | 1 | -1 | \(\Gamma_2\) |

| | \(D_4\) | \(E\{0\}\) | \(C_3^{(+,-)}\{0\}\) | \(C_2^{(A,B,C)}\{0\}\) | \(Q\{E\{0\}\}\) | \(Q\{C_3^{(+,-)}\{0\}\}\) | \(Q\{C_2^{(A,B,C)}\{0\}\}\) |
|---|---|---|---|---|---|---|---|
| \(\tau_y\) | 2 | 1 | 0 | -2 | -1 | 0 | \(\Gamma_4\) |
| \(g^2\) | \{E\{0\}\} | \{C_3^{(+,-)}\{0\}\} | \{E\{0\}\} | \{E\{0\}\} | \{C_3^{(+,-)}\{0\}\} | \{E\{0\}\} |
| \(\chi^2(g)\) | 4 | 1 | 0 | 4 | 1 | 0 |
| \(\chi(g^2)\) | 2 | -1 | -2 | 2 | -1 | -2 |
| \(\chi \left( \chi^2(g) + \chi(g^2) \right)\) | 3 | 0 | -1 | 3 | 0 | -1 | \(\Gamma_2 + \Gamma_3\) |
| \(\frac{1}{2} \left( \chi^2(g) - \chi(g^2) \right)\) | 1 | 1 | 1 | 1 | 1 | 1 | \(\Gamma_1\) |
The direct production of two irreducible presentations of wave function and wave vector of difference \( \kappa - K \) or \( \kappa - K' \) expansion for the wave vector including time inversion can be expanded on

\[
p^\alpha \tau \times \tau_q = (\Gamma_1 + \Gamma_3) \times (\Gamma_2 + \Gamma_3) = \Gamma_3 \times \Gamma_3, \quad (43)
\]

for the square of wave vector

\[
p^\beta \tau \times \tau_{q^2} = (\Gamma_1 + \Gamma_3) \times (\Gamma_1) = \Gamma_1 \times \Gamma_1. \quad (44)
\]

The Hamiltonian of bilayer graphene

\[
\hat{H} = \frac{\Delta}{2} \sigma_z + \zeta A q^2 \hat{I} + v_F (\tau q_x \sigma_x + q_y \sigma_y), \quad (45)
\]

where \( \Delta \) is band gap of graphene, \( \zeta = \pm \) is the particle index, \( m = 1/A \) is effective mass, \( \hat{I} \) is unit matrix, \( q_x, q_y \) are Cartesian components of a wave vector, \( \tau = \pm 1 \) is the valley index, \( v_F = 1 \times 10^6 \text{ m/s} \) is the graphene Fermi velocity, \( \sigma_x, \sigma_y, \sigma_z \) are Pauli matrices (here we assume that \( \hbar = 1 \)).

The dispersion of energy bands may be found in the form

\[
\epsilon_\pm = \pm (Aq^2 \pm \frac{\Delta}{2} \sqrt{1 + \frac{4\zeta^2 q^2}{\Delta^2}}),
\]

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

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

\[
(\epsilon(q^2) + q^2_0)\Phi(q) = \frac{1}{i} \int \frac{\Phi(q')}{|q - q'|} dq',
\]

(47)

then substituting (50), (52) in (47), can find equation

\[
\epsilon(q^2) + q^2_0 \sum_{l=0}^{\infty} A_l Y_l^0(\theta, \phi) = \frac{2}{q_0} \sum_{l=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \int \frac{1}{2\lambda+1} Y_\lambda^\mu(\theta, \phi) Y_\lambda^{\mu*}(\theta', \phi') Y_l^0(\theta', \phi') A_l (\frac{2q_0}{q^2 + q_0^2})^2 dq'.
\]

(53)
The integral equations for bilayer graphene based on Eq. (49) may be found in the form

$$\int (\pm \frac{e}{Aq_0^2} \sqrt{(1 - \cos \theta)^2 + \frac{4e^2}{\Delta^2}} q_0^2 (\sin \theta)^2 \pm A + (1 \mp A)(\frac{1 - \cos(\theta)}{2})) \sum_{l=0}^{\infty} A_l Y_l^m(\theta, \phi) Y_n^{*m}(\theta, \phi) d\Omega =$$

$$= \frac{2}{Aq_0^2} \int \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \sum_{l'=0}^{\infty} \frac{1}{\Delta^{1/2}} Y_{\lambda}^m(\theta, \phi) Y_{l'}^{*m}(\theta', \phi') Y_{n}^{*m}(\theta, \phi) d\Omega d\Omega' A_{l'}.$$  (54)

Since [31]

$$\cos \theta P_l^m(\cos \theta) = \sqrt{(l^2 - m^2) / 4l^2 - 1} P_{l-1}^m(\cos \theta) + \sqrt{(l^2 + m^2) / 4l^2 - 1} P_{l+1}^m(\cos \theta),$$

$$\sin \theta P_l^m(\cos \theta) = \sqrt{(l^2 - m^2) / 4l^2 - 1} P_{l-1}^{m+1}(\cos \theta) + \sqrt{(l^2 + m^2) / 4l^2 - 1} P_{l+1}^{m+1}(\cos \theta).$$  (55, 56)

Then solutions of the integral equation (54) for the energies and wave functions correspondingly can be found analytically with taken into account the normalization condition \( \int \frac{q_0^2}{2\lambda^2} |\Phi(q)|^2 dq = 1. \)

From equation (54) one can obtain the eigenvalue and eigenfunction problem and using a condition \( \frac{4e^2}{\Delta^2} q_0^2 \gg 1 \) one can find recurrence relation

$$\frac{1}{2} A_l + \frac{1}{2} A_{l+1} + A_{l-1} \left( \frac{1}{2} A_l + \frac{1}{2} A_{l+1} \right) (l + \frac{1}{2}) b_l = 0.$$  (57)

The solutions of the quantized series in excitonic Rydbergs and wave functions of the integral equation (54) one can find in the form

$$\epsilon_{0 \pm} = -\frac{1}{\left( \frac{1}{4} + \frac{1}{2} A_l + \frac{1}{4} A_{l+1} \right) \cdot (1 + \frac{1}{2}) a_l^2}.$$  (58)

$$\epsilon_{1 \pm} = -\frac{1}{\left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) \cdot \left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) b_0 + \frac{1}{2} A_l \cdot \frac{1}{2} A_{l+1} \cdot (2 + \frac{1}{2}) a_l^2}.$$  (59)

From equation (54) one can obtain the eigenvalue and eigenfunction problem and using a condition \( \frac{4e^2}{\Delta^2} q_0^2 \gg 1 \) one can find recurrence relation

$$\frac{1}{2} A_l + \frac{1}{2} A_{l+1} + A_{l-1} \left( \frac{1}{2} A_l + \frac{1}{2} A_{l+1} \right) (l + \frac{1}{2}) b_l = 0.$$  (57)

The solutions of the quantized series in excitonic Rydbergs and wave functions of the integral equation (54) one can find in the form

$$\epsilon_{2 \pm} = \frac{1}{\left( \frac{1}{4} + \frac{1}{2} A_l + \frac{1}{4} A_{l+1} \right) \cdot \left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) a_l^2 \cdot \left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) b_0 + \frac{1}{2} A_l \cdot \frac{1}{2} A_{l+1} \cdot (2 + \frac{1}{2}) a_l^2}.$$  (60)

$$\epsilon_{3 \pm} = \frac{1}{\left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) \cdot \left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) \cdot \left( \frac{1}{4} A_l + \frac{1}{2} A_{l+1} \right) \cdot \left( 3 + \frac{1}{2} \right) a_l^2 \cdot \left( 3 + \frac{1}{2} \right) b_0 + \frac{1}{2} A_l \cdot \frac{1}{2} A_{l+1} \cdot \left( 3 + \frac{1}{2} \right) a_l^2}.$$  (61)

$$\Phi_l(\cos \theta) = \sqrt{\frac{2\pi}{|q_0|^2}} \sum_{n=0}^{\infty} (1 - \cos \theta) \chi_l(\cos \theta),$$  (62)

where \( q_0^2 = -\epsilon_l, \quad l = 0, 1, 2, 3, 4, \ldots, \) excitonic Rydberg \( \text{Ry} = m_e e^4 / (\epsilon_l^2 \hbar^2) = 346.61 \text{ meV}, \) \( m_e \) is the reduced mass of an electron-hole pair, \( m = \frac{2m_e}{\omega^2} \) is the electron (hole) mass.

Table 4. Quantized spectral series of the excitonic states in meV, band gap of graphene in meV, effective reduced mass of electron-hole pair, excitonic Rydberg in meV.
In a SLG as well as in a single-layer MoS$\text{\textsubscript{2}}$ exciton insulator phase similarly to BCS superconductor.

Of excitons. In a system undergo a phase transition into a exciton formation with follow up spontaneous production the insulator ground state is instable concerning to the conductor or semimetal then at sufficiently low temperature greater than the flat band gap in narrow-gap semiconductivity.

Which acquire significant attention in the explanations of leads to the electron-hole bound states scrutiny study of particles in gapped graphene. The Coulomb interaction large exciton binding energy [13, 14].

20–22. The perfect host combines a small gap and a opened by electron-electron exchange interaction [14, 20–22]. The perfect host combines a small gap and a large exciton binding energy [13, 14].

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

It is known [13, 14] 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 concerning to the exciton formation with follow up spontaneous production of excitons. In a system undergo a phase transition into a exciton insulator phase similarly to BCS superconductor.

In a SLG as well as in a single-layer MoS$\text{\textsubscript{2}}$ and in bilayer graphene the electron-hole pairing leads to the exciton insulator states.

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. 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 the Cooper instability.

### III. RESULTS AND DISCUSSIONS

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

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

A crossing direct-gap like dispersion of single layer of graphene as well as in single layer of MoS$\text{\textsubscript{2}}$ does not lead to the fundamental differences in the many-particle effects in comparison with wurtzite 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.

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].

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

It is known [13, 14] 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 concerning to the exciton formation with follow up spontaneous production of excitons. In a system undergo a phase transition into a exciton insulator phase similarly to BCS superconductor.

In a SLG as well as in a single-layer MoS$\text{\textsubscript{2}}$ and in bilayer graphene the electron-hole pairing leads to the exciton insulator states.

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. 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 the Cooper instability.

### IV. CONCLUSIONS

In this paper we found the solution the integral Schrödinger equation in a momentum space of two interacting via a Coulomb potential Dirac particles that form the exciton in gapped graphene, in a single-layer MoS$\text{\textsubscript{2}}$ and in bilayer graphene.

In low-energy limit this problem is solved analytically. We obtained the energy dispersion and wave function of the exciton in gapped graphene, in monolayer MoS$\text{\textsubscript{2}}$ and in bilayer graphene. The excitons were considered as a system of two oppositely charge Dirac particles interacting via a Coulomb potential.

We solve this problem in a momentum space because on the whole the center-of-mass and the relative motion of the two Dirac particles can not be separated.

We analytically solve an integral two-dimensional Schrödinger equation of the electron-hole pairing for particles with electron-hole symmetry of reflection. An integral form of the two-dimensional Schrödinger equation in momentum space for gapped graphene, for monolayer MoS$\text{\textsubscript{2}}$ and in bilayer graphene is solved exactly by projection the two-dimensional space of momentum on the three-dimensional sphere.

In the SLG as well as in the monolayer MoS$\text{\textsubscript{2}}$ the electron-hole pairing leads to the exciton insulator states. The exciton insulator states with a gap 3 meV are shown to be found calculating an integral two-dimensional Schrödinger equation of the electron-hole pairing for bilayer graphene.

### V. APPENDIX

Table 6. The irreducible representational of $D_{3h}^1$ [33].

| $D_{3h}^1$ | $E|0\rangle$ | $C^+_2|+\rangle|0\rangle$ | $C^\alpha|A,B,C\rangle|0\rangle$ | $\sigma_0|\tau\rangle$ | $S_3^+|+\rangle|\tau\rangle$ | $\sigma_\alpha^\alpha(A,B,C)|\tau\rangle$ |
|----------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| $K_1^+$  | 1               | 1              | 1               | 1              | 1              | 1              |
| $K_2^+$  | 1               | 1              | -1              | 1              | 1              | -1             |
| $K_3^+$  | 2               | -1             | 0               | 2              | -1             | 0              |
| $K_4^+$  | 1               | 1              | 1               | -1             | -1             | 1              |
| $K_5^+$  | 1               | 1              | -1              | -1             | 1              | z              |
| $K_6^+$  | 2               | -1             | 0               | -2             | 1              | 0              |
| $J_x$    |                  |                | $x^2 + y^2$, $z^2$ |                |                |                |
| $J_y$    |                  |                |                  |                |                | $(x, y)$       |
| $J_z$    |                  |                |                  |                |                | $(x^2 - y^2, xy, (J_x, J_y))$ |
Table 7. The irreducible representational of \( C_{3h} \) [33].

\[
\begin{array}{cccccc}
\{E|0\} & \{C_3|0\} & \{C_2^x|0\} & \{\sigma_h|\tau\} & \{S_3|\tau\} & \{S_3^z|\tau\} \\
A^+ & 1 & 1 & 1 & 1 & 1 & J_z, x^2 + y^2, z^2 \\
A^- & 1 & \varepsilon & \varepsilon^2 & -1 & -1 & \varepsilon \\
B^+_1 & 1 & \varepsilon & \varepsilon^2 & 1 & \varepsilon & x + iy \\
B^-_1 & 1 & \varepsilon & \varepsilon^2 & -1 & -\varepsilon & J_x + iJ_y \\
B^+_2 & 1 & \varepsilon^2 & \varepsilon & 1 & \varepsilon^2 & \varepsilon & x - iy \\
B^-_2 & 1 & \varepsilon^2 & \varepsilon & -1 & -\varepsilon & J_x - iJ_y \\
\end{array}
\]

\( \varepsilon = \exp(2\pi i/3) \)

Table 8. The irreducible representational of \( D_3 \) [33].

\[
\begin{array}{cccccc}
\Gamma_1 & 1 & 1 & x^2 + y^2, z^2 \\
\Gamma_2 & 1 & 1 & J_z, z \\
\Gamma_3 & 2 & -1 & 0 & (xz, yz) (x^2 - y^2, xy), (x, y), (J_x, J_y) \\
\end{array}
\]

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, Science 306, 666, (2004).
[2] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, A. A. Firsov, Nature 438, 197, (2005).
[3] F.T. Vasko, V.V. Mitin, V. Ryzhii, T. Otsuji, Phys. Rev. B 86, 235424, (2012).
[4] T. Cheiwchanchamnangij, W.R.L. Lambrecht, Y. Song, H. Dery, arXiv:1308.2733v1 [cond-mat.mtrl-sci] (2013).
[5] Hannu-Pekka Komsa, Arkady V. Krasheninnikov, Phys. Rev. B 84, 241201(R), (2012).
[6] Z.Y. Zhu, Y.C. Cheng, U. Schwingenschl"ogl, Phys. Rev. B 84, 153402, (2011).
[7] H. Pellaers, C.G. Van de Walle, Phys. Rev. B 86, 241401(R), (2012).
[8] T. Cheiwchanchamnangij, W.R.L. Lambrecht, Phys. Rev. B 85, 205302, (2012).
[9] A. Ramanabramamian, Phys. Rev. B 86, 115409, (2012).
[10] P.R. Wallace, Phys. Rev. 71, 622, (1947).
[11] V.A. Fock, Z. Phys. 98, 145 (1935).
[12] D.G.W. Parfitt, M.E. Portnoi, J. Math. Phys. 43, 4681 (2002). arXiv:math-ph/0205031v1 (2002).
[13] T. Stroucken, J.H. Grönlund, S.W. Koch, Phys. Rev. B 87, 245428, (2013). arXiv:1305.1780v1 [cond-mat.mes-hall] (2013).
[14] D. Jerome, T.M. Rice, W. Kohn, Phys. Rev. 158, 462, (1967).
[15] Lyubov E. Lokot, arXiv:1409.0303v1 [cond-mat.mes-hall] (2014).
[16] L.E. Lokot, arXiv:1402.5794v2 [cond-mat.mes-hall] (2014).
[17] L.E. Lokot, Ukr. J. Phys. 58, 56, (2013). arXiv:1302.2783v1 [cond-mat.mes-hall] (2013).
[18] J. Alicea, M.P.A. Fisher, Phys. Rev. B 74, 075422, (2006).
[19] V.P. Gusynin, S.G. Sharapov, J.P. Carbotte, Inter. J. Mod. Phys. 21, 4611, (2007).
[20] T. Stroucken, J.H. Grönlund, S.W. Koch, Phys. Rev. B 84, 205445, (2011).
[21] Faris Kadi, Ermin Malic, Phys. Rev. B 89, 045419, (2014).
[22] Ermin Malic, Torben Winzer, Evgeny Bobkin, Andreas Knorr, Phys. Rev. B 84, 205406, (2011).
[23] O.V. Gamayun, E.V. Gorbar, V.P. Gusynin, Phys. Rev. B 80, 165429, (2009).
[24] O.V. Gamayun, E.V. Gorbar, V.P. Gusynin, Ukr. J. Phys. 56, 688, (2011).
[25] O.L. Berman, R.Ya. Kezerashvili, K. Ziegler, Phys. Rev. A 87, 042513, (2013). arXiv:1302.4505v1 [cond-mat.mes-hall] (2013).
[26] O.L. Berman, R.Ya. Kezerashvili, K. Ziegler, arXiv:1110.0744v2 [cond-mat.mes-hall] (2011).
[27] R.R. Hartmann, I.A. Shelykh, M.E. Portnoi, Phys. Rev. B 84, 035437, (2011). arXiv:1012.5517v2 [cond-mat.mes-hall] (2011).
[28] Hongki Min, Rafi Bistritzer, Jung-Jung Su, A.H. MacDonald, Phys. Rev. B 84, 205445, (2011).
[29] Josep Sak, Phys. Rev. B 5, 3081, (1972).
[30] L.M. Malard, D.L. Mafra, M.H.D. Guimaraes, M.S.C. Mazzoni, A. Jorio, arXiv:0812.1293v1 [cond-mat.mes-hall] (2008).
[31] V.A. Fock, Fundamentals of Quantum Mechanics (Mir, Publishers, Moscow, 1976).
[32] D. Xiao, G.B. Liu, W. Feng, X. Xu, W. Yao, Physical Review Letters 108, 196802, (2012).
[33] A.J. Mildred, S. Dresselhaus, Gene Dresselhaus Group theory: application to the physics of condensed matter (Springer, 2008).