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Research Article

Weakly Bound States of Elementary Excitations in Graphene Superlattice in Quantizing Magnetic Field

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The spectrum of allowed energy of electron in graphene superlattice in the quantizing magnetic field is investigated. Such spectrum consists of number of so-called magnetic minibands. The width of these minibands depends on the superlattice barriers power and on the magnetic field intensity. The explicit form of electron spectrum is derived in the case of weak magnetic field. The possibility of electron-electron and electron-phonon bound states is shown. The binding energies of these states are calculated. The binding energy is shown to be the function of magnetic field intensity.

1. Introduction

The interactions of electrons with elementary excitations in crystal lattice have fundamental implications on properties of materials and lead to such many-body phenomena as superconductivity and charge-density waves. Such interactions take an unusual form in graphene [1–3] which can be described by the Dirac-like form of the effective Hamiltonian. A new area for investigations of chiral massless fermions is induced by discovery of this 2D material. So, interactions of Dirac electrons with elementary excitations which lead to the emergence of the bound states (BS) are under the intensive theoretical [4–7] and experimental study [8–10] last time.

Renormalization of Dirac spectrum due to interactions of electrons with lattice vibrations was obtained in [11–15]. Formations of polarons, plasmon-phonon complexes, and electron-hole pares are investigated in [4, 16–20], where BSs were shown to appear if energy of quasiparticles interaction exceeds a threshold value. In [19], the modification of Dirac spectrum near the threshold of optical phonon emission was studied. The spectrum characteristics of the electron-phonon quasiparticles (in particular, the electron-phonon binding energy versus the coupling parameter $g_{\text{el-ph}}$) were found in [19] within the theory, taking into account the singular vertex corrections beyond perturbation theory. Such corrections lead to the spectrum that remains below the optical phonon energy and corresponds to the electron-phonon BS in comparison with that obtained within the Wigner-Brillouin perturbation theory [11–13].

Influence of various factors (geometry parameters, spin-orbit interaction, charge impurities, etc.) on BS properties in graphene-based structures was studied in [4, 5, 21–27]. From an application technological point of view, the tunability of graphene electronic and optical properties by external fields is of particular importance [21, 28–32]. So, the effect of electric and magnetic fields on the properties of the BSs in graphene structures is of high interest among the researchers now [20, 21, 33–35]. The influence of Landau level mixing on the energy of magnetoexcitons and magnetoplasmons in graphene was studied in [36], where dispersions of the excitations were shown to be changed by virtual transitions between Landau levels, caused by Coulomb interaction (electron-hole channel). In [20], the effect of the magnetic field on the electron-phonon BSs was studied. The electron-phonon binding energy was shown to diverge at the resonant values of the magnetic field intensity. Such divergences corresponded to the electron-phonon hybrid states formed in the spectrum between the graphene Landau levels. These resonance states were obtained within the perturbation theory from the poles of the two-particle Green function and determine the structure of the magnetophonon resonance [37–39].

Presently, among the different graphene structures, the special attention is paid to graphene superlattices (GSLs) [40–44]. Intensive investigations of electric and optical properties of GSL are explained by their different possible experimental and technological applications [31, 45–49]. Below we obtain the binding energies of electron-electron and electron-phonon coupling in GSL in the quantizing magnetic field and determine the binding energy dependence on the magnetic field intensity and on the coupling parameters $g_{\text{el-el}}$ and $g_{\text{el-ph}}$.

2. Electron Spectrum of GSL in Quantizing Magnetic Field

In this section, we obtain the effective electron spectrum of GSL in quantizing magnetic field. We consider a GSL which is in the plane xy (Figure 1). Near the Dirac point, the electron spectrum of GSL has the explicit form [40]:

$$\varepsilon_{\text{GSL}}(\mathbf{p}) = \sqrt{u_F^2 p_x^2 + \Delta^2 \sin^2 \frac{p_y d}{2\hbar}}, \tag{1}$$

where Oy is the GSL axis (Figure 1), $u_F = v_F \sin\eta/\eta$ is the Fermi velocity along the axis Ox, $\eta = V_0 d/4\hbar v_F$ is the dimensionless power of SL barriers [40], V_0 is the barrier height, $d = 2 \cdot 10^{-6}$ cm is the GSL period, $\Delta = 2\hbar v_F/d$, and $v_F = 10^8$ cm/s is the Fermi velocity in graphene. Linearized equation (equation analogous to the Dirac equation), which describes the motion of an electron in the GSL, takes the form [50, 51]:

$$\left(u_F \sigma_x \hat{\pi}_x + \Delta \sigma_y \sin \frac{\hat{\pi}_y d}{2\hbar}\right)\psi = \varepsilon\psi. \tag{2}$$

Here, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrixes, ψ is spinor function describing the electron states in GSL, $\hat{\boldsymbol{\pi}} = \hat{\mathbf{p}} + e\mathbf{A}/c$, $\hat{\mathbf{p}} = -i\hbar(\partial_x, \partial_y)$, $\mathbf{A} = (0, Hx)$ is the vector potential, and $\mathbf{H}$ is the intensity of magnetic field which is supposed to be perpendicular to the GSL plane. Indeed, in the absence of magnetic field, the substitution of spinor for free charge carrier [52] into (2) gives the dispersion law (1).

In nonzero quantizing magnetic field ($\hbar v_F/\lambda_H \gg T$, $\lambda_H = \sqrt{c\hbar/eH}$ is the Larmor radius, and T is the temperature) we represent $\psi = e^{iky}\chi$, where χ is spinor which is equal to

$$\chi = \begin{pmatrix} \chi_1(x) \\ \chi_2(x) \end{pmatrix}. \tag{3}$$

χ_1 and χ_2 describe electron states in the first and second graphene sublattice correspondingly. After acting on the spinor ψ twice with the operator

$$\hat{H}_{\text{GSL}} = u_F \sigma_x \hat{\pi}_x + \Delta \sigma_y \sin \frac{\hat{\pi}_y d}{2\hbar}, \tag{4}$$

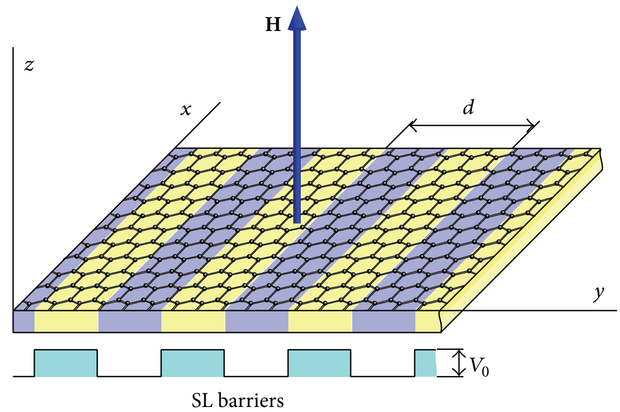

Figure 1: Schematic of the studied system.

using the next correlations $\hat{H}_{\text{GSL}}^2 \psi = \varepsilon^2\psi$, $\sigma_x\sigma_y = -\sigma_y\sigma_x = i\sigma_z$, and making a shift of the argument $k\lambda_H^2 + x \to x$, we derive the following:

$$-\hbar^2 u_F^2 \partial_x^2 \chi + \Delta U(x)\chi = \left(\varepsilon^2 - \Delta\Delta_H \sigma_z\right)\chi. \tag{5}$$

Here, we define $\Delta_H = 2\pi\hbar u_F/\Lambda_H$, $\Lambda_H = 4\pi\lambda_H^2/d$, and

$$U(x) = \Delta \sin^2\left(\frac{2\pi x}{\Lambda_H}\right) - 2\Delta_H \sin^2\left(\frac{\pi x}{\Lambda_H}\right)\sigma_z. \tag{6}$$

To find the eigen values of ε in (5) for the considered direction of vector $\mathbf{H}$ with respect to GSL axis, we use the method developed in [53]. It is easy to see from (6) that $U(x + \Lambda_H) = U(x)$ and therefore $\chi(x)$ satisfies the Bloch theorem. Thus, we can write

$$\chi(x) = \sum_n e^{inq\Lambda_H} \chi_0(x - n\Lambda_H), \tag{7}$$

where χ_0 is the eigenspinor of the next operator $\hat{H}_0^2 = -\hbar^2 u_F^2 \partial_x^2 + \Delta U(x)$ and corresponds to the electron state near the nth minimum of the function $U(x)$ [53]. Generally, the spectrum of allowed energy ε consists of a number of minibands (magnetic minibands [53]). Having made some transformations, we derive

$$\begin{aligned} &\varepsilon^2 - \left\langle \chi_0 \left| \hat{H}_0^2 \right| \chi_0 \right\rangle \\ &\quad = 4\hbar^2 u_F^2 \chi_0^+ \left(\frac{\Lambda_H}{2}\right) \partial_x \chi_0 \left(\frac{\Lambda_H}{2}\right) \cos q\Lambda_H. \end{aligned} \tag{8}$$

For the weak magnetic fields ($\Delta_H \ll \Delta$), the minima of $U(x)$ are separated by the wide barriers. In this case, the components of eigenspinor χ_0 for the operator $\hat{H}_0^2$ are close to the functions of the harmonic oscillator localized near the nth minimum of the function $U(x)$. Further, we consider that electron is in the lowest Landau level. Thus, we obtain instead (8)

$$\varepsilon(q) = \sqrt{\Delta\Delta_H} - D_H \cos q\Lambda_H, \tag{9}$$

where

$$D_H = 8\sqrt{\pi}\Delta \exp\left(-\frac{2\pi^2\Delta}{\Delta_H}\right). \qquad (10)$$

The width of allowed miniband is seen from (10) to depend on the GSL barriers power and on the magnetic field intensity.

3. Emergence of the BS of Two Electrons in GSL

Here, we show that in GSL with electron spectrum (9) in the presence of quantizing magnetic field the appearance of BS of two electrons is possible at arbitrarily weak repulsion between them. Equation that defines the dispersion law of the BS can be obtained by determining the poles of the two-particle Green function [54]:

$$\frac{g_{\text{el-el}}}{2\pi}\int_{-\pi/\Lambda_H}^{+\pi/\Lambda_H}\frac{dq}{E-\varepsilon_1(q-p/2)-\varepsilon_2(q+p/2)+i0} = 1, \qquad (11)$$

where $g_{\text{el-el}}$ is the effective coupling parameter of quasiparticles with dispersion lows $\varepsilon_1(q)$ and $\varepsilon_2(q)$ and p is the momentum of BS. We use (11) in the case of electron-electron interaction in GSL in the presence of quantizing magnetic field. Equation (11) has undamped solutions if $g_{\text{el-el}} > 0$ (repulsion) and $E > 2\sqrt{\Delta\Delta_H} + 2D_H$. After integration in (11), we obtain the dispersion law of BS:

$$E(p) = 2\sqrt{\Delta\Delta_H} + \sqrt{\frac{g_{\text{el-el}}^2}{\Lambda_H^2} + 4D_H^2\cos^2\frac{p\Lambda_H}{2}}. \qquad (12)$$

It is seen from (12) that electrons can bind if energy E is close to the top of conduction band where effective masses are negative. This fact explains the possibility of electrons binding while $g_{\text{el-el}} > 0$. Binding energy is

$$E_0 = \sqrt{\frac{g_{\text{el-el}}^2}{\Lambda_H^2} + 4D_H^2} - 2D_H. \qquad (13)$$

For weak repulsion between electrons ($g_{\text{el-el}} \ll D_H\Lambda_H$), the binding energy is proportional to square of $g_{\text{el-el}}$: $E_0 = g_{\text{el-el}}^2/4D_H\Lambda_H^2$. For intensive repulsion between electrons ($g_{\text{el-el}} \gg D_H\Lambda_H$), we have $E_0 = -2D_H + g_{\text{el-el}}/\Lambda_H$. The binding energy dependence on the magnetic field intensity is shown in Figure 2 for different values of coupling parameter.

4. Emergence of the Electron-Phonon BS in GSL

Now, we obtain the possibility of electron-optical phonon BS in GSL in the quantizing magnetic field. The equation that determines the dispersion law of such BS is [54]

$$\frac{g_{\text{el-ph}}}{2\pi}\int_{-\pi/\Lambda_H}^{+\pi/\Lambda_H}\frac{dq}{E-\hbar\omega_0-\varepsilon(q)+i0} = 1. \qquad (14)$$

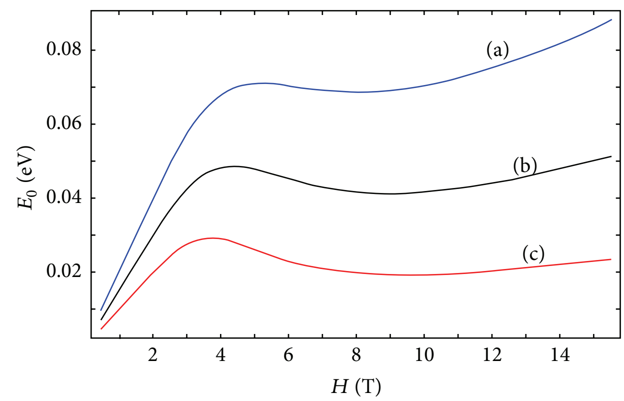

Figure 2: Binding energy E_0 versus the magnetic field intensity H. (a) $g_{\text{el-el}} = 2\hbar u_F$, (b) $g_{\text{el-el}} = 1.5\hbar u_F$, and (c) $g_{\text{el-el}} = \hbar u_F$.

Here, the coupling parameter $g_{\text{el-ph}} < 0$ and corresponds to the attraction between electron and phonon and ω_0 is the frequency of optical phonon which is assumed to be dispersionless. The undamped solution of (14) is possible if $E < \hbar\omega_0 + \sqrt{\Delta\Delta_H} - D_H$. Dispersionless of optical phonon leads to the fact that electron-phonon BS appears at all values of quasiparticle momentum. In this case, the binding energy is

$$E_0 = \sqrt{\frac{g_{\text{el-ph}}^2}{\Lambda_H^2} + D_H^2} - D_H. \qquad (15)$$

In comparison with that obtained for electron-phonon coupling in graphene in the absence of magnetic field [19], the binding energy (15) does not exhibit exponential dependence on the coupling constant $g_{\text{el-ph}}$.

5. Conclusion

Above we have investigated the spectrum of allowed energy of electron in GSL in the presence of quantizing magnetic field ($\hbar v_F/\lambda_H \gg T$). Generally, such spectrum consists of number of so-called magnetic minibands. The width of these minibands depends on the GSL barriers power and on the magnetic field intensity. For our calculations, we assume that electron is in the magnetic miniband which corresponds to the lowest harmonic oscillator state. The explicit form of electron spectrum in this case is (9). The formula (9) is adequate if magnetic field satisfies the next condition: $\Delta_H \ll \Delta$, which is true up to $H = 15$ T (the power of GSL barriers is of $\eta \sim 3.136$ [40]). For such magnetic fields, temperature should not exceed 100 K. Nitrogen boiling point is suitable to this end. Moreover, the upper limit of magnetic field can be increased by changing the power of GSL barriers η.

Thus, experimental measurements could confirm the suggested theory if one uses the GSL with the period $d = 2 \cdot 10^{-6}$ cm (typical value for superlattices [41, 45]) and with the height of barrier $V_0 \sim 0.392$ eV (in this case, $\eta \sim 3.136$). To this end, the GSL obtained by a sheet of graphene deposited on a banded substrate formed by periodically alternating layers of SiC and hexagonal BN is suitable one [41]. Another suitable structure could be obtained by periodical insertion of hydrogenated graphene (graphane [55]) between gapless graphene strips. For such material barrier height consists of $V_0 \sim 2.7$ eV [41, 55]. If $V_0 \sim 2.7$ eV, then $\eta \sim 22$ and the condition $\Delta_H \ll \Delta$ will be also performed up to $H = 15$ T.

Using (9), we have shown the possibility of electron-electron and electron-phonon BSs and have calculated the binding energy of these states, which is the function of magnetic field (Figure 2). In the case of electron-optical phonon coupling, the binding energy does not exhibit exponential dependence on the coupling constant $g_{\text{el-ph}}$ in comparison with that obtained for graphene in the absence of magnetic field [19]. Electron-phonon BS appears at all values of quasiparticle momentum. This feature is explained by the dispersionless of optical phonon.

In [20], the electron-phonon binding energy was shown to diverge in graphene at the resonant values of the magnetic field intensity. Such divergences correspond to the electron-phonon hybrid states formed in the spectrum between the graphene Landau levels. As it is shown above in GSL electron-phonon binding energy (15) has the finite maximum as well as electron-electron binding energy (Figure 2). It is obtained instead of divergence of the binding energy as it was for the case of single-layer graphene [20]. Finite maximum of the electron-electron and electron-phonon binding energy in GSL in quantizing magnetic field is due to the broadening of energy levels (Landau levels). Such broadening takes place if quantizing magnetic field is applied perpendicularly to the superlattice axis [53].

In the case of electron-electron coupling, BSs correspond to the Bose-Einstein statistics. At low temperatures (under the critical temperature), such electron system can form a superfluid gas [56]. The presence of additional potential in graphene in this case is essential for the following reason. Electrons can bind if energy E is close to the top of conduction band of GSL where effective masses are negative (12). This fact explains the possibility of electrons binding while $g_{\text{el-el}} > 0$. In the absence of additional potential (at the linear dispersion limit), there are no regions with negative effective masses. So, "repulsive" electron-electron interaction cannot form bound states in such limit.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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