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Impurity States in Gated Graphene Bilayer in a Magnetic Field

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Abstract. We develop a variational approach in momentum space for an impurity electron in bilayer graphene with an energy gap opened by perpendicular electric field. The binding energy of an impurity electron in gapped bilayer graphene is studied by this method and it is shown that the energy is monotonically increasing with the increase of the gap value. The dependence of the binding energy on the interlayer hopping parameter is also investigated. The method is extended for the investigation of impurity ground state energy in an external magnetic field.

Keywords: bilayer graphene, impurity states, binding energy, variational approach, magnetic field

1. Introduction

Graphene monolayer is a gapless semimetal where the electrons are massless Dirac fermions and exbibits a linear dispersion near the Dirac point [1]. The graphene bilayer, which is constructed of two stacked graphene planes, demonstrates more intriguing properties: the charge carriers here are chiral quasiparticles with nonzero effective mass and dominantly parabolic dispersion [2]. Theoretical and experimental investigations have shown that the electric field modifies band structure of the system near the K point, and may open an energy gap in the electronic spectrum from zero to midinfrared energies [3]. So, differently from monolayer and unbiased bilayer graphene, which are zero-gap semiconductors, a biased graphene bilayer is a semiconductor with energy gap between valence and conduction bands tunable by a perpendicular electric field. The gap may be opened also by chemical doping, that creates a potential difference between layers.

More reach physics is expected for graphene multilayers [4], where the magnitude of gap strongly depends on the number of graphene layers and its stacking order [5]. In [5, 6] we studied theoretically electric field induced band gap dependence in graphene multilayers on different ways of stacking between consecutive graphene planes. Coulomb problem in gapped graphene systems was considered in [7, 8]. In [9], using tight-binding approach with second quantized Hamiltonian, we investigated the binding energy of excitons created by an electromagnetic field in bilayer graphene with opened energy gap.

It is interesting to investigate the impurity states in bilayer graphene, where the binding energy of impurity and its localization lengths can be controlled by external electric and magnetic fields.

For fundamental physics as well as for different applications it is interesting to develop transparent analytical methods for a better understanding the physics of a single impurity in graphene systems and the influence of band structure parameters on the impurity electron binding energy, oscillator strengths etc.

In this paper we develop a clear variational approach in momentum space for calculation of the ground state energy of an impurity electron in bilayer graphene with opened energy gap.

The plan of the paper is as follow. Section 2 presents our variational method for an impurity electron in gapped graphene bilayer. In Section 3 we obtain the form of Hamiltonian in external magnetic field in coordinate as well as in momentum space. Section 4 presents main results and discussions. Our conclusions are presented in Section 5.

2. Variational approach in momentum space

The Hamiltonian for bilayer graphene in the vicinity of *K* point in the case of two band model has the following form:

$$H_0 = \begin{pmatrix} -U/2 & v_3(p_x + ip_y) - (1/2m)(p_x - ip_y)^2 \\ v_3(p_x - ip_y) - (1/2m)(p_x + ip_y)^2 & U/2 \end{pmatrix}, \tag{1}$$

where U is the gap induced by a static perpendicular electrical field, $v_3 = \sqrt{3}\gamma_3 a/2\hbar \approx 0.1 \mathrm{v_F}$ is the effective velocity, and $\mathrm{v_F}$ is the Fermi velocity in monolayer graphene (here we omit the real spin and valley quantum numbers), and a is the lattice constant. Tight-binding parameter γ_3 describes the interaction between different *B* atoms in neighboring layers ($\gamma_3 \approx 0.31eV$).

The equation for determination of hydrogen-like impurity energy spectrum in gapped graphene bilayer can be presented in the form

$$H_0 \begin{pmatrix} \phi \\ \chi \end{pmatrix} = \left(E + \frac{Ze^2}{r} \right) \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \tag{2}$$

with H_0 given by Eq. (1). From the system of two equations (Eq. (2)) we obtain one equation for the spinor component ϕ:

$$\left[\frac{U^2}{4} + (v_3 \hat{p})^2 - \frac{v_3 \hat{p}^3}{m} \cos 3\theta + \left(\frac{\hat{p}^2}{2m} \right)^2 \right] \phi = \left(E + \frac{Ze^2}{r} \right)^2 \phi, \tag{3}$$

where $\theta(p) = \arctan(p_y / p_x)$. In this work we do not take into account the azimuthal asymmetry of the bands, so, in Eq. (3) we ignore the term $(-v_3 \hat{p}^3 \cos 3\theta / m)$ that is responsible for the trigonal warping of the bands [5, 6]. We omit also the term $Z^2 e^4 / r^2$ in Eq. (3), which becomes crucial for small values of the energy gap, when impurity level is not shallow.

In momentum representation, the operators $\hat{\mathbf{p}}^2$ and $\hat{\mathbf{p}}^4$ have the form p^2 and p^4 correspondingly. The potential energy $V(r) = -Ze^2/\chi r$ (χ is the dielectric constant) that is the operator of multiplication in the coordinate space, becomes in the momentum space the integral operator with the kernel $V(\mathbf{p},\mathbf{p}') = V(\mathbf{p}-\mathbf{p}') = V(\mathbf{q})$ defined as [10]:

$$V(\mathbf{q}) = \frac{1}{(2\pi\hbar)^2}\int V(\mathbf{r})\exp(-i\mathbf{qr}/\hbar)dV\ .$$

In the momentum space, taking into account the above-mentioned approximations, the equation (3) for determination of impurity electron energy in bilayer graphene become

$$(v_3{}^2 p^2 + p^4/4m^2)\phi(p) - (E^2 - U^2/4)\phi(p) + 2E\iint V(\mathbf{p}-\mathbf{p}')\phi(p')p'dp'd\vartheta = 0, \qquad (4)$$

where $V(|\mathbf{p}-\mathbf{p}'|) = -4\pi a_B R^*/\sqrt{p^2 + p'^2 - 2pp'\cos\vartheta}$ is Fourier transform of two-dimensional Coulomb interaction with $R^* = \mu e^4/2\chi^2\hbar^2$ being effective Rydberg energy, and $a_B = \hbar^2\chi/\mu e^2$ is effective Bohr radius,

Using dimensionless units of $\tilde{E} = E/R^*$, $\tilde{U} = U/R^*$ the equation for energy of an impurity electron can be presented in the form

$$\left((\tilde{E}^2 - \frac{\tilde{U}^2}{2})\phi + \frac{2\tilde{E}}{\pi}\int\int \frac{k'dk'\phi(k')d\varphi}{\sqrt{k^2 + k'^2 - 2kk'\cos\vartheta}}\right)\phi(k) = k^2\left(\frac{4}{\alpha^2} + \left(\frac{\mu}{m}\right)^2 k^2\right)\phi(k), \qquad (6)$$

$\alpha = e^2\chi^2/\hbar^2 v_3^2$ is effective fine structure constant that corresponds to the velocity v_3; the mass m is defined by the expression $m = \gamma_1/2v_F^2$ [2, 3] and in the expression for effective Rydberg we use $\mu = 0.02m_0$ with m_0 is free electron mass.

Since there is no analytical solution for Coulomb problem in bilayer graphene with opened energy gap (Eq.3), here we develop a variational approach in momentum space. For ground state energy of an impurity electron we choose variational function in the form

$$\phi(k) = N/(k^2 + \lambda^2)^2\ , \qquad (7)$$

where λ is variational parameter and N is the normalization constant. Using this trial function, the energy of an impurity electron can be obtained from the equation:

$$\tilde{E}^2 - \tilde{U}^2 + \frac{2\tilde{E}}{\pi}\int\phi\, kdk\int\int \frac{k'dk'\phi(k')d\varphi}{\sqrt{k^2 + k'^2 - 2kk'\cos\vartheta}} - \frac{4}{\alpha^2}\int k^3\phi^2(k)dk - \left(\frac{\mu}{m}\right)^2\int k^5\phi^2(k)dk = 0. \qquad (8)$$

3. Impurity states in a magnetic field

In external magnetic field the energy states can be obtained from Eq. (3) where instead of $\hat{\mathbf{p}}^2$ and $\hat{\mathbf{p}}^4$ one should take $(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^2$ and $(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^2(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^2$ correspondingly. In cylindrical coordinates we choose vector-potential $\mathbf{A}$ in the form $A_\varphi = B\rho/2,\ A_\rho = A_z = 0$. In the case, when we are interested to calculate the ground state energy of an impurity electron we find

$$(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^2\psi(\rho) = (\hat{\mathbf{p}}^2+\kappa\rho^2)\psi(\rho),$$

$$(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^4\psi(\rho) = (\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^2(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A})^2\psi(\rho) = (\hat{\mathbf{p}}^4+2\kappa\rho^2\hat{\mathbf{p}}^2+4\kappa+\kappa^2\rho^4)\psi(\rho), \quad (9)$$

where $\kappa = m^2\omega^2/4,\ \omega = eB/mc$. Taking into account expression (9), the equation for impurity states in a magnetic field in bilayer graphene (in the absence of the trigonal warping effect) in coordinate space becomes

$$\left[\frac{U^2}{4}+v_3{}^2(\hat{\mathbf{p}}^2+\kappa\rho^2)+\frac{\hat{\mathbf{p}}^4+2\kappa\rho^2\hat{\mathbf{p}}^2+4\kappa+\kappa^2\rho^4}{(2m)^2}\right]\phi = \left(E+\frac{Ze^2}{r}\right)^2\phi \quad (10)$$

In momentum space $(\hat{\mathbf{p}})^2$ and $(\hat{\mathbf{p}})^4$ have the form p^2 and p^4 while ρ^2, ρ^4 and $\frac{Ze^2}{r}$ one should change to integral operators [10]. The variational function can be chosen here in the form $\psi = N\exp(-\lambda p^2)$.

4. Results and Discussions

In our previous work [11] we investigated the binding energy of an impurity electron in gapped bilayer graphene using variational approach in coordinate space. The difficulty of such method is connected with the presence of the term, proportional to $\hat{\mathbf{p}}^4$ (see Eq.(3)) that was considered in [11] as a double action of the operator $\hat{\mathbf{p}}^2$ in the consecutive order. Note that this approach leads to enough complicated calculations.

The variational method developed in ***p***-space gives better results than [11] and is more convenient for systems with complicated dispersion of charge carriers law, *e.g.* for graphene systems. After minimization of the energy, obtained as the solution of Eq (8) on the parameter λ, we obtain the dependence of total energy (counted out from the middle of the gap in effective Rydberg R^*) on the gap value and for different values of tight-binding parameter γ_1.

The binding energy is defined as $E_B = U/2 - E$. As is shown in Fig.1, the binding energy monotonically increases with the increase of the gap value, and in the case of fixed gap, to larger values of the interlayer hopping parameter γ_1 correspond larger values of E_B.

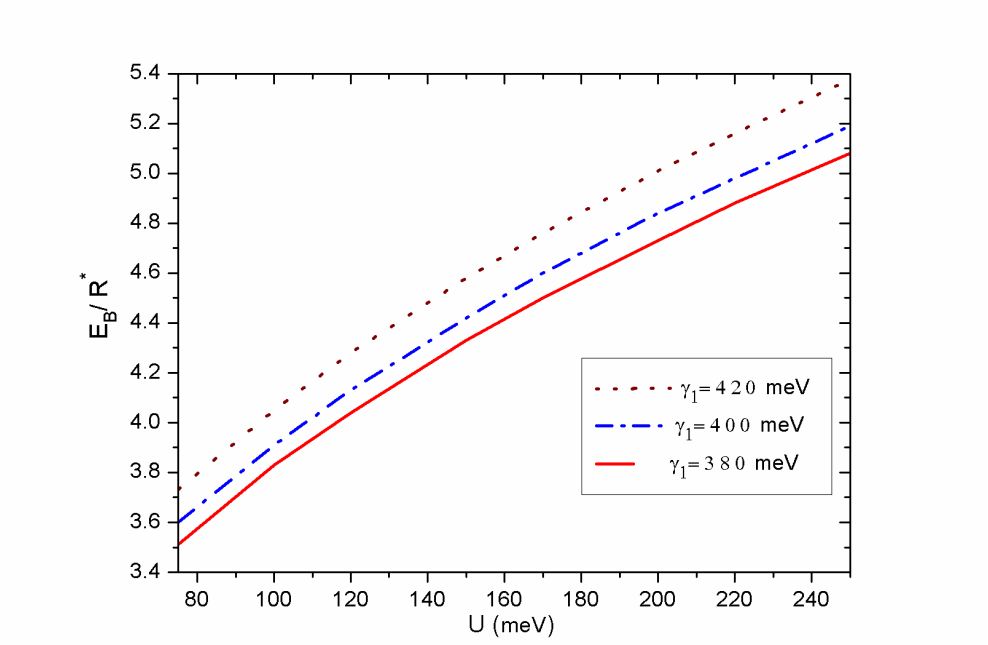

Figure 1. Dependence of the binding energy of an impurity electron in effective Rydberg ($R^* = 2\ meV$) on the gap value U for different values of the parameter γ_1: solid line corresponds to the value of $\gamma_1 = 380\,mev$, dot-dashed line is for $\gamma_1 = 400\,mev$, and dotted line is for $\gamma_1 = 420\,mev$

The variational method in momentum space gives better results for an impurity electron binding energy in comparison with results obtained in coordinate space: for the gap value $U = 150 mev$ and $\gamma_1 = 380\,mev$ the binding energy obtained by the first method is larger by 3%.

5. Conclusion

In this paper we develop a variational method for calculation of an impurity electron binding energy in momentum space in bilayer graphene. This approach is generalized for the investigation of binding energy of an impurity in a magnetic field. The suggested method is more appropriate for systems with complicated dispersion law of charge carriers, e.g. for a graphene bilayer. The possibility of impurity energy tuning by external fields and by changing band structure parameters can be promising for applications in nano- and optoelectronics for construction of new devices.

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