Magnetoexciton dispersion in graphene bilayers embedded in a dielectric

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A study of the magnetoexciton binding energy in graphene bilayers embedded in a dielectric is presented. The calculations are based on the relativistic Bethe-Salpeter equation assuming a strong magnetic field regime where the lowest Landau-level approximation takes place. It is shown that in graphene bilayer structures the magnetoexciton mass (binding energy) is four times lower (higher) than the corresponding magnetoexciton mass (binding energy) in coupled quantum wells with parabolic dispersion.

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I. INTRODUCTION

A lot of experimental and theoretical studies in recent years are focusing on the unusual relativistically kinematic properties of the electronic states in graphene predicted theoretically decades ago.[1,2] A major breakthrough was done in 2004 when Novoselov and co-workers[3,4] tested and confirmed that the graphitic monolayer has anomalous relativistic properties. Because electrons and holes in a graphene behave like massless Dirac particles, there are a number of unusual properties, such as high charge-carrier mobility,[4] the graphene's conductivity never falls below a minimum value,[5,6] and the presence of an anomalous quantum Hall effect.[7]

Bilayer graphene systems, where carriers in one layer are electrons and carriers in the other are holes, have been considered as ideal candidates for observing superfluid properties at room temperature.[8–10] It is expected that the excitons will behave as neutral bosons at low densities, and therefore, they can undergo Bose-Einstein condensation (BEC) when the interlayer distance is comparable to the distance between the particles within each layer. However, when we separate electrons and holes by introducing a dielectric between them, we reduce the exciton binding energy and so the critical temperature for condensation decreases. A possible way to increase the binding energy is to apply a magnetic field perpendicular to the layers. In parabolic band semiconductors the binding energy varies as the square root of the strength of the magnetic field, and therefore, it is reasonable to expect that the critical temperature in the presence of a magnetic field should increase.

Turning our attention to magnetoexciton dispersion in nonrelativistic systems, such as coupled quantum wells (CQWs) with parabolic dispersions ($E_{c,v}=\hbar^2k^2/2m_{c,v}$), we find that the following Hamiltonian,[11]

$$\hat{H}=-\frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2+\frac{\imath e\gamma\hbar}{2\mu c}(\mathbf{B}\times\mathbf{r})\cdot\nabla_{\mathbf{r}}+\frac{e^2B^2}{8\mu c^2}\mathbf{r}^2-V(\mathbf{r}+\mathbf{R}_0),$$

is used to obtain the magnetoexciton dispersion. Here μ is the exciton-reduced mass, $\gamma=(m_v-m_c)/(m_c+m_v)$, and $\mathbf{R}_0=R^2\mathbf{Q}_0$, [where $\mathbf{Q}_0=(-Q_y,Q_x,0)$], and $R=(\hbar c/eB)^{1/2}$ is the magnetic length. $V(\mathbf{r})=e^2/(\varepsilon_0\sqrt{|\mathbf{r}|^2+d^2})$ represents the electron-hole Coulomb attraction screened by the dielectric constant ϵ_0. Since the Coulomb term in the Hamiltonian is the only term which depends on the exciton momentum $\mathbf{Q}=(Q_x,Q_y,0)$, the magnetoexciton dispersion does not depend on the electron and hole masses and the magnetoexciton mass is determined only by Coulomb interaction. In strong magnetic fields one can apply the lowest Landau-level (LLL) approximation. In the LLL approximation the binding energy E_{CQW} and the magnetoexciton mass M_{CQW} are as follows:

$$\frac{M_{\mathrm{CQW}}}{M_{\mathrm{2D}}}=\left[\left(1+\frac{d^2}{R^2}\right)e^{(d^2/2R^2)}\mathrm{erfc}\left(\frac{d}{\sqrt{2}R}\right)-\sqrt{\frac{2}{\pi}}\frac{d}{R}\right]^{-1},$$

$$E_{\mathrm{CQW}}=E_b\exp\left(\frac{d^2}{2R^2}\right)\mathrm{erfc}\left(\frac{d}{\sqrt{2}R}\right).$$

Here $\mathrm{erfc}(x)$ is the complementary error function, and $E_b=\sqrt{\pi}e^2/(\sqrt{2}\varepsilon_0R)$ and $M_{\mathrm{2D}}=2^{3/2}\varepsilon_0\hbar^2/(\sqrt{\pi}e^2R)$ are the two-dimensional ($d=0$) magnetoexciton binding energy and magnetoexciton mass, respectively.[12]

In what follows we examine how both the magnetoexciton binding energy and magnetoexciton mass in graphene bilayer systems vary with the magnetic field and the separation d between the layers in the LLL approximation. It is worth mentioning that the calculations done by treating the Coulomb interaction as a perturbation[13] provide in the LLL approximation a number of extra terms which do not exist in the case of CQWs. From a general point of view, we have to expect that the binding energy is *exactly* four times higher than E_{CQW}, while the magnetoexciton mass is *exactly* four times lower than M_{CQW}. The physical reason for the above statement lies in the fact that in the LLL approximation we have a dimensional reduction in the dynamics of the electron-hole pairing from two space variables plus a time variable to zero space variable and a time variable. Because of this $2+1\rightarrow0+1$ reduction the results should be insensitive to the type of the band dispersion. The factor 4 is due to the four-component-spinor description used in the relativistic case.

The plan of this Brief Report is as follows. In Sec. II, we present a formalism based on the Bethe-Salpeter (BS) equation for describing the bound states between two relativistic particles. In Sec. III, we discuss our results.

II. BETHE-SALPETER EQUATION

The system under consideration is made from two graphene sheets embedded in a dielectric and separated by

distance d. Each of the two graphene layers has two Dirac-type linear dispersion $\hbar v_F k$ bands centered at two inequivalent points $\mathbf{K}$ and $\mathbf{K}'$, where v_F is the Fermi velocity of electrons in graphene. Since the layers are embedded in a dielectric, there is no hopping of π electrons between the layers. There is a potential difference $\pm V_g/2$ (gate voltage) applied to each of the two layers which allows us to adjust the charge density in the layers. We assume that the potential difference is chosen in such a manner that the electrons are in the top layer (pseudospin index $\tau=1$) and the same number of holes in the bottom layer ($\tau=2$).

The unit cell of graphene has two atoms, A and B, each belonging to a different sublattice. The operator $\psi^{(\tau)\dagger}_{\sigma,A,\alpha}(\mathbf{r})$ [$\psi^{(\tau)\dagger}_{\sigma,B,\alpha}(\mathbf{r})$] creates an electron of spin $\sigma=\uparrow,\downarrow$ on the atom A (atom B) of the unit cell in layer τ defined by the position vector $\mathbf{r}$. We present four-component spinors

$$\Psi^{(\tau)}_{\sigma}(\mathbf{r})=\begin{pmatrix}\psi^{(\tau)}_{\sigma,A,\mathbf{K}}(\mathbf{r})\\ \psi^{(\tau)}_{\sigma,B,\mathbf{K}}(\mathbf{r})\\ \psi^{(\tau)}_{\sigma,B,\mathbf{K}'}(\mathbf{r})\\ \psi^{(\tau)}_{\sigma,A,\mathbf{K}'}(\mathbf{r})\end{pmatrix},\quad \bar{\Psi}^{(\tau)}_{\sigma}(\mathbf{r})=\Psi^{(\tau)\dagger}_{\sigma}(\mathbf{r})\gamma^0, \tag{1}$$

where the following representation of the Dirac matrices is chosen:

$$\gamma^0=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},\quad \gamma^1=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix},$$

$$\gamma^2=\begin{pmatrix}0&-\imath&0&0\\-\imath&0&0&0\\0&0&0&\imath\\0&0&\imath&0\end{pmatrix}. \tag{2}$$

In continuum approximation the noninteracting quasiparticles in the layers are described by the Hamiltonian

$$H_0=\sum_{\sigma,\tau}\int d^2\mathbf{r}\bar{\Psi}^{(\tau)}_{\sigma}(\mathbf{r})\hat{H}^{(\tau)}\Psi^{(\tau)}_{\sigma}(\mathbf{r}), \tag{3}$$

where

$$\hat{H}^{(\tau)}=v_F(\gamma^1\hat{p}_x+\gamma^2\hat{p}_y),\quad \hat{p}_x=-\imath\hbar\frac{\partial}{\partial x},\hat{p}_y=-\imath\hbar\frac{\partial}{\partial y}.$$

The action that describes the noninteracting quasiparticles in a layer τ is

$$S^{(\tau)}_0=\int d^2\mathbf{r}dt\bar{\Psi}^{(\tau)}_{\sigma}(\mathbf{r},t)\left[\gamma^0\imath\hbar\frac{\partial}{\partial t}-v_F(\gamma^1\hat{p}_x+\gamma^2\hat{p}_y)\right]\times\Psi^{(\tau)}_{\sigma}(\mathbf{r},t). \tag{4}$$

In the presence of a perpendicular magnetic field $\mathbf{B}=(0,0,B)$ and a potential difference $\pm V_g/2$ (gate voltage) applied to each of the two layers, action (4) assumes the form

$$S^{(\tau)}_0=\int d^2\mathbf{r}dt\bar{\Psi}^{(\tau)}_{\sigma}(\mathbf{r},t)\times\left[\gamma^0\left(\imath\hbar\frac{\partial}{\partial t}-V^{(\tau)}_g\right)-v_F(\gamma^1\hat{\pi}_x+\gamma^2\hat{\pi}_y)\right]\Psi^{(\tau)}_{\sigma}(\mathbf{r},t), \tag{5}$$

where $\hat{\pi}_{x(y)}=\hat{p}_{x(y)}\mp(e/c)\mathbf{A}_{x(y)}(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})=(1/2)\mathbf{B}\times\mathbf{r}$ is the vector potential in a symmetric gauge.

In what follows we assume that the interaction between an electron with a position vector $\mathbf{r}_1$ from the top layer ($\tau=1$) and a hole with a position vector $\mathbf{r}_2$ from the bottom layer ($\tau=2$) is described by the Coulomb potential $V(\mathbf{r}_1-\mathbf{r}_2)=e^2/\varepsilon_0\sqrt{|\mathbf{r}_1-\mathbf{r}_2|^2+d^2}$. Instead of two position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, we present the center-of-mass $\mathbf{R}=\alpha(\mathbf{r}_1+\mathbf{r}_2)$ and the relative $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ coordinates ($\alpha=1/2$).

The basic assumption in our BS formalism is that the electron-hole bound states are described by the BS wave function (BS amplitude). This function determines the probability amplitude to find the electron at the point $\mathbf{r}_1$ at the moment t_1 and the hole at the point $\mathbf{r}_2$ at the moment t_2. The BS amplitude depends on the relative internal time $t-t'$ and on the "center-of-mass" time

$$\Phi^{\mathbf{Q}}(\mathbf{r},\mathbf{R};t,t')=\exp\left(-\frac{\imath E(\mathbf{Q})\alpha}{\hbar}(t+t')\right)\phi^{\mathbf{Q}}(\mathbf{r},\mathbf{R};t-t'), \tag{6}$$

where $E(\mathbf{Q})$ is the exciton dispersion. The BS equation for the equal-time BS amplitude in the center-of-mass and reduced coordinates is[14]

$$\Phi^{\mathbf{Q}}(\mathbf{r},\mathbf{R};t,t)=\int d^2\mathbf{r}'d^2\mathbf{R}'dt'G^{(1)}(\mathbf{R}+\alpha\mathbf{r},\mathbf{R}'+\alpha\mathbf{r}';t-t')\gamma^0\times G^{(2)}(\mathbf{R}'-\alpha\mathbf{r}',\mathbf{R}-\alpha\mathbf{r};t'-t)\times\gamma^0V(\mathbf{r}')\Phi^{\mathbf{Q}}(\mathbf{r}',\mathbf{R}';t',t'). \tag{7}$$

The Fourier transforms of the electron and hole propagators $G^{(\tau)}(\mathbf{r},\mathbf{r}';t)$ are defined in terms of the Dirac four-component spinors $\psi^{\kappa}(\mathbf{r})$ and the corresponding eigenvalues $E_n=\hbar v_F\sqrt{2n}/R$,[14]

$$G^{(\tau)}(\mathbf{r},\mathbf{r}';\omega)=\sum_{\kappa}\frac{\psi^{\kappa}(\mathbf{r})\bar{\psi}^{\kappa}(\mathbf{r}')}{\hbar\omega-E_n\pm\imath 0^+}. \tag{8}$$

Here we keep only the positive-energy pole contributions, $n=0,1,2,\ldots$, and $\kappa=(n,j_z,\sigma)$, where j_z is the z component of the total angular momentum.

When the translation symmetry is broken by the magnetic field, the Green's functions can be written as a product of phase factors and translation invariant parts. The phase factor depends on the gauge. In the symmetric gauge the Green's functions are

$$G^{(\tau)}(\mathbf{r},\mathbf{r}';\omega)=\exp\left[\imath\frac{e}{\hbar c}\mathbf{r}\cdot\mathbf{A}(\mathbf{r}')\right]\tilde{G}^{(\tau)}(\mathbf{r}-\mathbf{r}';\omega). \tag{9}$$

The broken translation symmetry requires a phase factor for the BS amplitude

$$\phi^{\mathbf{Q}}(\mathbf{r},\mathbf{R};\Omega)=\exp\left[\imath\frac{e}{\hbar c}\mathbf{r}\cdot\mathbf{A}(\mathbf{R})\right]\chi^{\mathbf{Q}}(\mathbf{r},\mathbf{R};\Omega). \quad (10)$$

The BS equation (7) admits translation invariant solution of the form

$$\chi^{\mathbf{Q}}(\mathbf{r},\mathbf{R};\omega)=\exp[-\imath(\mathbf{Q}\cdot\mathbf{R})]\tilde{\chi}^{\mathbf{Q}}(\mathbf{r};\omega). \quad (11)$$

The Fourier transform of the function $\tilde{\chi}^{\mathbf{Q}}(\mathbf{r};\omega)$ satisfies the following BS equation:

$$\begin{aligned}\tilde{\chi}^{\mathbf{Q}}(\mathbf{k};\omega)=&\int\frac{d^2\mathbf{q}}{(2\pi)^2}\frac{d^2\mathbf{p}}{(2\pi)^2}d^2\mathbf{R}\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi}e^{-\imath(\mathbf{q}+\mathbf{Q})\cdot\mathbf{R}}\\&\times\tilde{G}^{(1)}\left(\frac{1}{2}\mathbf{q}+\mathbf{k}-\frac{e}{\hbar c}\mathbf{A}(\mathbf{R});\hbar\omega+\alpha(E-V_g)\right)\gamma^0\\&\times\tilde{G}^{(2)}\left(-\frac{1}{2}\mathbf{q}+\mathbf{k}-\frac{e}{\hbar c}\mathbf{A}(\mathbf{R});\hbar\omega-\alpha(E-V_g)\right)\gamma^0\\&\times V\left(\mathbf{p}-\left[\mathbf{k}-\frac{2e}{\hbar c}\mathbf{A}(\mathbf{R})\right]\right)\tilde{\chi}_{\mathbf{Q}}(\mathbf{p};\Omega), \quad (12)\end{aligned}$$

where $\tilde{G}^{(\tau)}(\mathbf{k};\hbar\omega)$ are the Fourier transforms of $\tilde{G}^{(\tau)}(\mathbf{r};\hbar\omega)$.

In the effective-mass approximation the exact fermion Green's functions $G^{(\tau)}$ are replaced by the corresponding propagator of the free fermions. The translation invariant parts of the free fermion propagators can be decomposed over the Landau-level poles[15]

$$\begin{aligned}\tilde{G}^{(\tau)}(\mathbf{k};\hbar\omega)=&2\imath\sum_{n=0}^{\infty}(-1)^n e^{-R^2\mathbf{k}^2}\frac{\hbar\omega\gamma^0 f_1(k)+f_2(\mathbf{k})}{\hbar^2\omega^2-2n\hbar v_F^2 eB/c},f_1(k)\\=&\frac{1}{2}(1-\imath\gamma^1\gamma^2)L_n(2R^2k^2)\\&-\frac{1}{2}(1+\imath\gamma^1\gamma^2)L_{n-1}(2R^2k^2),\end{aligned}$$

$$\begin{aligned}f_1(k)=&\frac{1}{2}(1-\imath\gamma^1\gamma^2)L_n(2R^2k^2)\\&-\frac{1}{2}(1+\imath\gamma^1\gamma^2)L_{n-1}(2R^2k^2),\end{aligned}$$

$$f_2(\mathbf{k})=2v_F\hbar(k_x\gamma^1+k_y\gamma^2)L_{n-1}^1(2R^2k^2).$$

Here $L_n^1(x)$ are the generalized Laguerre polynomials, $L_{-1}^1(x)=L_{-1}(x)=0$, and $L_n(x)$ are the Laguerre polynomials. In strong magnetic fields the probability for transitions to the excited Landau levels due to the Coulomb interaction is small. Thus, the contributions to the Green's functions from the excited Landau levels is negligible, and therefore, one can apply the LLL approximation, where we keep only the $n=0$ term

$$\tilde{G}^{(1)}(\mathbf{k};\hbar\omega)\approx\imath\exp(-R^2\mathbf{k}^2)\frac{\gamma^0(1-\imath\gamma^1\gamma^2)}{\hbar\omega+\imath0^+},$$

$$\tilde{G}^{(2)}(\mathbf{k};\hbar\omega)\approx\imath\exp(-R^2\mathbf{k}^2)\frac{\gamma^0(1-\imath\gamma^1\gamma^2)}{\hbar\omega-\imath0^+}. \quad (13)$$

The infinitesimal imaginary parts in our case reflect the fact that there are holes in layer 2 (in electron-hole representation poles of the holes are above the real axis) and electrons in layer 1.

The solution of the BS equation (12) in the LLL approximation can be written in the following form:

$$\tilde{\chi}^{\mathbf{Q}}(\mathbf{k};\omega)=\exp[-R^2\mathbf{k}^2-\imath\mathbf{R}_0\cdot\mathbf{k}]\Phi_E(\omega). \quad (14)$$

Here $\Phi_E(\omega)$ is a 4×4 matrix. Thus, the LLL approximation reduces the problem from 2+1 dimensions to 0+1-dimension problem. The matrix $\Phi_E(\omega)$ and the magnetoexciton dispersion $E(\mathbf{Q})$ are determined by the solutions of the following equation:

$$\begin{aligned}\Phi_E(\omega)=&-I(|\mathbf{Q}|)\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi}\\&\times\frac{\gamma^0(1-\imath\gamma^1\gamma^2)\gamma^0\Phi_E(\Omega)\gamma^0(1-\imath\gamma^1\gamma^2)\gamma^0}{[\hbar\omega+\alpha(E-V_g)+\imath0^+][\hbar\omega-\alpha(E-V_g)-\imath0^+]}.\end{aligned} \quad (15)$$

The solution of Eq. (15) is given by

$$\begin{aligned}\Phi_E(\omega)=&\begin{pmatrix}0&0&0&0\\0&1&0&1\\0&0&0&0\\0&1&0&1\end{pmatrix}\\&\times\frac{1}{[\hbar\omega+\alpha(E-V_g)+\imath0^+][\hbar\omega-\alpha(E-V_g)-\imath0^+]},\end{aligned}$$

$$E(\mathbf{Q})=V_g-4I(\mathbf{Q}). \quad (16)$$

Thus, in the LLL approximation, the magnetoexciton dispersion is determined by the Coulomb interaction term $I(\mathbf{Q})=\int d^2\mathbf{r}\varphi_{00}^2(r)V(\mathbf{r}+\mathbf{R}_0)$, where $\varphi_{00}(r)=(\sqrt{2\pi}R)^{-1}\exp(-r^2/4R^2)$ is the ground-state wave function of an electron in a magnetic field. For small wave vectors we calculate

$$E(\mathbf{Q})\approx V_g-4E_{\mathrm{CQW}}+\frac{\hbar^2Q^2}{2M(B)},\quad\frac{M(B)}{M_{\mathrm{CQW}}}=\frac{1}{4}. \quad (17)$$

In graphene bilayer structures the magnetoexciton mass (binding energy) is four times lower (higher) than the corresponding magnetoexciton mass (binding energy) in coupled quantum wells with parabolic dispersion and the same d, ε_0, and B. In the limit of very small interlayer separation $d\ll R$ the asymptotical values of the binding energy and the effective magnetic mass of the magnetoexciton in bilayer graphene are $4E_b$ and $M_{\mathrm{small}}(B)=M_{2\mathrm{D}}/4\propto B^{1/2}$, respectively. In the limit of large interlayer separation $d\gg R$ the asymptotical value of the magnetic mass is $M_{\mathrm{large}}(B)=M_{2\mathrm{D}}\pi^{1/2}d^3/(2^{7/2}R^3)\propto B^2$. As we mentioned above, under the certain critical temperature T_c a Bose-Einstein condensation might be expected to occur. The condensate of magnetoexcitons should have superfluid properties under the Kosterlitz-Thouless (KT) critical temperature T_{KT}.[16] A pos-

sible verification of our predictions could be based on the fact that at a fixed superfluid density the phase stiffness and the KT critical temperature are both inversely proportional to the magnetoexciton mass, i.e., $T_{KT} \propto M^{-1}(B)$. Since the effective mass increases as a function of the magnetic field, one should expect that at a fixed superfluid density the KT critical temperature decreases in the limit of large interlayer separation as $T_{KT} \propto B^{-2}$ (as $T_{KT} \propto B^{-1/2}$ in the limit of small interlayer separation).

III. CONCLUSION

We have applied the BS formalism to the magnetoexcitons in graphene structures. The LLL approximation greatly simplifies the calculations, but we may ask whether the magnetoexciton dispersion will be significantly affected by the contributions from the *infinity number* of Landau levels with indexes $n \geq 1$ neglected in the LLL approximation.

Turning our attention to the parabolic band quantum-well structures we find that beyond the LLL approximation, the BS equation contains an extra term (BS term).[17] This term takes into account the transitions to the Landau levels with indexes $n \geq 1$. The contributions to the magnetoexciton binding energy and mass can be obtained by applying a variational procedure. The results are as follows. In a strong magnetic field, the ground-state energy is very close to that obtained by means of the Schrödinger equation, but the magnetoexciton dispersion is determined by the BS term rather than the electron-hole Coulomb term in the Schrödinger equation. In the relativistic case, going beyond the LLL approximation is an ambitious task (see, e.g., Ref. 18) which will be left as a subject of our future research.

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