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Spectral properties of excitons in the bilayer graphene

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A B S T R A C T

In this paper, we consider the spectral properties of the bilayer graphene with the local excitonic pairing interaction between the electrons and holes. We consider the generalized Hubbard model, which includes both intralayer and interlayer Coulomb interaction parameters. The solution of the excitonic gap parameter is used to calculate the electronic band structure, single-particle spectral functions, the hybridization gap, and the excitonic coherence length in the bilayer graphene. We show that the local interlayer Coulomb interaction is responsible for the semimetal-semiconductor transition in the double layer system, and we calculate the hybridization gap in the band structure above the critical interaction value. The formation of the excitonic band gap is reported as the threshold process and the momentum distribution functions have been calculated numerically. We show that in the weak coupling limit the system is governed by the Bardeen-Cooper-Schrieffer (BCS)-like pairing state. Contrary, in the strong coupling limit the excitonic condensate states appear in the semiconducting phase, by forming the Dirac's pockets in the reciprocal space.

1. Introduction

The electronic band gap of semiconductors and insulators largely determines their optical, transport properties and governs the operation of semiconductor based devices such as p-n junctions, transistors, photodiodes and lasers [1]. Opening up a band gap in the bilayer graphene (BLG), by applying the external electric field and finding a suitable substrate are two challenges for constituting the modern nanoelectronic equipment [2,3]. The imposition of external electrical field can tune the bilayer graphene from the semimetal to the semiconducting state [2]. On the other hand, the possibility of formation of the excitonic insulator state and the excitonic condensation in the bilayer graphene structures remains controversial in the modern solid state physics [4–14]. In difference with the quasi two-dimensional (2D) semiconducting systems, where those two states have been observed experimentally and well discussed theoretically [15–27], the formation of the excitonic condensate states in the BLG system, from the original electron-hole pairing states, is much more obscure because of the complicated nature of the single-particle correlations in these systems [6,8,10,13,14]. The weak correlation diagrammatic mechanism, discussed in the Refs.[13,14], is restricted only to the closed loop expansion in the diagrammatic series, and in this case, only the density fluctuation effects could affect the formation of the excitonic condensate states. Meanwhile, it has been shown [28–30] that even the undoped graphene can provide a variety of electron-hole type pairing chiral symmetry breaking orders especially for the strong Coulomb coupling case, which renders the treatments in Refs.[13,14] to be nontrivial. As the monolayer graphene, bilayer graphene has a semimetallic band structure with the zero bandgap, which is unsuitable for many electronic device applications, as routinely done with semiconducting devices. In 2007, Allan H. MacDonald and his colleagues have predicted that the electric displacement field, applied to the two layers of the BLG could introduce a tunable bandgap in the electronic band structure of the BLG [31], which has been proved later on, experimentally [32–34].

In this paper, we show the band gap formation in the bilayer graphene's band structure, mediated by the local interlayer Coulomb interaction parameter and without the external electric field. Particularly, we show how the interlayer Coulomb interaction tunes the BLG from the semimetallic state into the semiconducting one (or a possible insulator state, for large interaction limit), for a fixed value of the interlayer hopping amplitude. We will show that the formation of the band gap in the BLG is a threshold process in our case. We calculate the excitonic hybridization gap for different values of the interaction parameter. Furthermore, by using the exact solutions for the excitonic gap parameter and chemical potential, we calculate the single-particle spectral functions and the momentum distribution functions in the BLG for different values of the local interlayer interaction parameter. We will show that the system is governed by the weak-coupling Bardeen-Cooper-Schrieffer (BCS)-like pairing states for the small and intermediate values of the interlayer coupling parameter, and the behavior of the excitonic coherence length agrees well with the BCS

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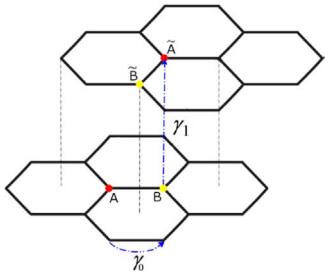

Fig. 1. The bilayer graphene structure. Two different sublattice site positions are shown (A,B, and $\widetilde{A}$, $\widetilde{B}$) in two different layers of the bilayer graphene structure.

type relation $\xi_c \sim \overline{\mu}/(k_{\mathcal{F}}\Delta)$, with Δ, being the excitonic pairing gap parameter. Contrary, in strong coupling limit the coherence length becomes proportional to Δ ($\xi_c \sim \Delta$), and the system is in the excitonic condensate regime.

In the Section 2, we introduce the bilayer Hubbard model for the BLG system. In the Section 3, we give the action of the bilayer graphene system and we obtain the coupled self-consistent equations for the excitonic gap parameter and chemical potential. The excitonic dispersion relations are also given there. Next, in the Section 4, we discuss the single-particle spectral properties and momentum distribution functions for different interlayer interaction limits and we calculate the interlayer excitonic coherence length in the bilayer graphene. In the Section 5, we give a conclusion to our paper.

2. The method

The BLG system, considered here, is composed of two coupled honeycomb layers with sublattices A, B and $\widetilde{A}$, $\widetilde{B}$, in the bottom and top layers respectively (see in Fig. Fig. 1). In the z-direction the layers are arranged according to Bernal Stacking (BS) order [35], i.e. the atoms on the sites $\widetilde{A}$ in the top layer lie just above the atoms on the sites B in the bottom layer graphene, and each layer is composed of two interpenetrating triangular lattices. For a simple treatment at equilibrium, we initially suppose the balanced BLG structure, i.e., with the equal chemical potentials in the both layers. When switching the local Coulomb potential W between the layers, we keep the charge neutrality equilibrium through the BLG, by imposing the half-filling condition in each layer of the BLG. Next, we will pass to the Grassmann representation for the fermionic variables, and we write the partition function of the system, in the imaginary time fermion path integral formalism [36]. For this, we introduce the imaginary-time variables τ, at each lattice site $\mathbf{r}$. The time variables τ vary in the interval $(0, \beta)$, where $\beta = 1/T$ with T being the temperature. Then, the Hamiltonian of the bilayer graphene, with the local interlayer interaction, has the following form

$$\begin{aligned} H = &-\gamma_0 \sum_{\langle \mathbf{r}\mathbf{r}'\rangle} \sum_{\sigma} (a^{\dagger}_{\sigma}(\mathbf{r}) b_{\sigma}(\mathbf{r}') + h.\,c.) \\ &-\gamma_0 \sum_{\langle \mathbf{r}\mathbf{r}'\rangle} \sum_{\sigma} (\widetilde{b}^{\dagger}_{\sigma}(\mathbf{r}) \widetilde{b}_{\sigma}(\mathbf{r}') + h.\,c.) \\ &-\gamma_1 \sum_{\mathbf{r}\sigma} (b^{\dagger}_{\sigma}(\mathbf{r}) \widetilde{a}_{\sigma}(\mathbf{r}) + h.\,c.) - \sum_{\mathbf{r}\sigma} \sum_{\ell=1,2} \mu_{\ell} n_{\ell\sigma}(\mathbf{r}) \\ &+U \sum_{\mathbf{r}} \sum_{\ell\eta} [(n_{\ell\eta\uparrow} - 1/2)(n_{\ell\eta\downarrow} - 1/2) - 1/4] \\ &+W \sum_{\mathbf{r}\sigma\sigma'} [(n_{1b\sigma}(\mathbf{r}) - 1/2)(n_{2\widetilde{a}\sigma'}(\mathbf{r}) - 1/2) - 1/4]. \end{aligned} \tag{1}$$

Here, we have used the graphite nomenclature notations [35] for the hopping amplitudes γ_0 and γ_1. Namely, the parameter γ_0 is the intraplane hopping amplitude, and γ_1 is the interlayer hopping amplitude in the BLG (see also in Fig. 1). The summation $\langle \mathbf{r}\mathbf{r}'\rangle$, in the first term, in Eq. (1), denotes the sum over the nearest neighbors lattice sites in the separated honeycomb layers in the bilayer graphene structure. We keep the small letters a, b and $\widetilde{a}$, $\widetilde{b}$ for the electron operators on the lattice sites A, B and $\widetilde{A}$, $\widetilde{B}$ respectively (see in Fig. 1). The index $\ell = 1, 2$ denotes the number of single layers in the BLG. Particularly, we use $\ell = 1$ for the bottom layer, and $\ell = 2$ for the top layer. Furthermore, we have $\eta = a, b$ for $\ell = 1$, and $\eta = \widetilde{a}, \widetilde{b}$, for $\ell = 2$. The symbol σ denotes the spin variables with two possible directions ($\sigma = \uparrow, \downarrow$). Next, $n_{\ell\sigma}(\mathbf{r})$ is the total electron density operator for the layer ℓ with a given spin direction σ

$$n_{\ell\sigma}(\mathbf{r}) = \sum_{\eta} n_{\ell\eta\sigma}(\mathbf{r}), \tag{2}$$

and $n_{\ell\eta\sigma}(\mathbf{r}) = \eta^{\dagger}_{\ell\sigma}(\mathbf{r})\eta_{\ell\sigma}(\mathbf{r})$ is the electron density operator for the η-type fermions with the spin σ. We consider the BLG structure with pure electronic layers without initial dopping in the system. The condition of half-filling in each layer reads as $\langle n_{\ell}\rangle = 1$, for $\ell = 1, 2$, where n_{ℓ} is the total electron density operator for the layer ℓ summed over the spin index σ: $n_{\ell}(\mathbf{r}) = \sum_{\sigma} n_{\ell\sigma}(\mathbf{r})$. Furthermore, U, in the Hubbard term in Eq. (1), parametrizes the intralayer Coulomb interaction. The parameter W, in the last term in Eq. (1), describes the local interlayer Coulomb repulsion between the electrons located on the B and $\widetilde{A}$ type of sites in the different layers of the BLG. We will put $\gamma_0 = 1$, as the unit of energy in the system, and we set $k_B = 1$, $\hbar = 1$ throughout the paper.

3. The Green's function matrix

The pairing between the electron and holes results in a gap in the excitation energy spectrum of the system. The pairing gap parameter between the particles with the same spin orientations is $\Delta_{\sigma\sigma'} = \Delta_{\sigma\sigma}\delta_{\sigma\sigma'}$, and we can also assume that the pairing gap is real $\Delta_{\sigma\sigma} = \Delta^{\dagger}_{\sigma\sigma} \equiv \Delta$. Then the excitonic pairing gap parameter will be defined as

$$\Delta_{\sigma\sigma} = W\langle b^{\dagger}_{\sigma}(\mathbf{r}\tau)\widetilde{a}_{\sigma}(\mathbf{r}\tau)\rangle. \tag{3}$$

In order to find the momentum dependence of the excitonic gap parameter, we will pass to the Fourier space representation, given by the transformation

$$\eta_{\sigma}(\mathbf{r},\,\tau) = \frac{1}{\beta N} \sum_{\mathbf{k}\nu_n} \eta_{\sigma\mathbf{k}}(\nu_n) e^{i(\mathbf{k}\mathbf{r} - \nu_n\tau)}, \tag{4}$$

where N is the total number of sites on the η-type sublattice, in the layer ℓ, and we write the partition function of the bilayer graphene system in the form

$$\mathcal{S}[\psi^{\dagger},\,\psi] = \frac{1}{\beta N} \sum_{\mathbf{k}\nu_n} \sum_{\sigma} \psi^{\dagger}_{\sigma\mathbf{k}}(\nu_n) \widehat{\mathcal{G}}^{-1}_{\sigma\mathbf{k}}(\nu_n) \psi_{\sigma\mathbf{k}}(\nu_n). \tag{5}$$

Here, $\nu_n = \pi(2n + 1)/\beta$ with $n = 0, \pm 1, \pm 2, \ldots$, are the fermionic Matsubara frequencies [37]. The four component Dirac spinors $\psi_{\sigma\mathbf{k}}(\nu_n)$, in Eq. (5), have been introduced at each discrete state $\mathbf{k}$ in the reciprocal space and for each spin direction $\sigma = \uparrow, \downarrow$. Being the generalized Weyl spinors, they are defined as

$$\psi_{\sigma\mathbf{k}}(\nu_n) = [a_{\sigma\mathbf{k}}(\nu_n),\, b_{\sigma\mathbf{k}}(\nu_n),\, \widetilde{a}_{\sigma\mathbf{k}}(\nu_n),\, \widetilde{b}_{\sigma\mathbf{k}}(\nu_n)]^{T}. \tag{6}$$

The matrix $\widehat{\mathcal{G}}^{-1}_{\sigma\mathbf{k}}(\nu_n)$, in Eq. (5), is the inverse Green's function matrix, of size 4×4. It is defined as

$$\widehat{\mathcal{G}}^{-1}_{\sigma\mathbf{k}}(\nu_n) = \begin{pmatrix} E_1(\nu_n) & -\widetilde{\gamma}_{1\mathbf{k}} & 0 & 0 \\ -\widetilde{\gamma}^{*}_{1\mathbf{k}} & E_2(\nu_n) & -\gamma_1 - \Delta^{\dagger}_{\sigma} & 0 \\ 0 & -\gamma_1 - \Delta_{\sigma} & E_2(\nu_n) & -\widetilde{\gamma}_{2\mathbf{k}} \\ 0 & 0 & -\widetilde{\gamma}^{*}_{2\mathbf{k}} & E_1(\nu_n) \end{pmatrix}. \tag{7}$$

Indeed, the structure of the matrix does not changes when inverting the spin direction, i.e., $\widehat{\mathcal{G}}^{-1}_{\downarrow\mathbf{k}}(\nu_n) \equiv \widehat{\mathcal{G}}^{-1}_{\uparrow\mathbf{k}}(\nu_n)$. The diagonal elements of the matrix, in Eq. (7), are the single-particle quasienergies

$$E_{\ell}(\nu_n) = -i\nu_n - \mu^{\mathrm{eff}}_{\ell}, \tag{8}$$

where the effectve chemical potentials $\mu^{\mathrm{eff}}_{\ell}$ with $\ell = 1, 2$ have been introduced as $\mu^{\mathrm{eff}}_{1} = \mu + U/4$ and $\mu^{\mathrm{eff}}_{2} = \mu + U/4 + W$. The parameters