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Superfluid phase transition in two-dimensional excitonic systems

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ABSTRACT

We study the superfluid phase transition in the two-dimensional (2D) excitonic system. Employing the extended Falicov–Kimball model (EFKM) and considering the local quantum correlations in the system composed of conduction band electrons and valence band holes we demonstrate the existence of the excitonic insulator (EI) state in the system. We show that at very low temperatures, the particle phase stiffness in the pure-2D excitonic system, governed by the non-local cross correlations, is responsible for the vortex–antivortex binding phase-field state, known as the Berezinskii–Kosterlitz–Thouless (BKT) superfluid state. We demonstrate that the existence of excitonic insulator phase is a necessary prerequisite, leading to quasi-long-range order in the 2D excitonic system.

1. Introduction

The interesting quasiparticles, excitons, play the fundamental role in the physics related to the recent revelations on the excitonic insulator (EI) state, [1–4] excitonic Bose–Einstein condensation (BEC) [3–6] and the excitonic superfluidity, [7–13]. In analogy with Cooper pair condensate [14], one can naturally expect that the electron–hole pairs (excitons), being the bosons with neutral charges, should eventually undergo BEC or the Bose-superfluid Berezinskii–Kosterlitz–Thouless (BKT) transition [15,16] (in the case of negligible quantum dissipations) at the very low temperatures. The first one is typical for the three-dimensional (3D) system, where it is the dominant phase transition, whereas, the second type of transition is typical for two-dimensional (2D) systems, where the long-range order is absent [17,18]. As in the case of the usual Bose gases, there should be a relation between these two excitonic phase transitions as it is reported recently [11]. It is well known that the BEC in the interacting uniform systems occurs only for $D > 2$. However, the absence of BEC does not necessarily imply the lack of a superfluid phase transition in $D = 2$, assuming that the well-defined conditions are satisfied by the system [7,12]. In sharp contrast to the 3D case, interactions in 2D Bose system cannot be treated as a minor correction to the BEC picture of the ideal Bose gas and they qualitatively change the behavior of the system. In fact, the excitonic superfluidity requires the interacting Bose gas, [19] on the contrary, BEC does not. The BEC is always superfluid and the existence of the critical Landau velocity [19] in a Bose–Einstein condensed gas is well known [20]. On the other hand, the ideal Bose gas could exhibit the phase transition to the BEC state being absolutely not superfluid.

Despite the continuous attempts, using the ultra-high quality materials, to observe superfluidity in bilayer electron–hole systems, such as the double wells in the GaAs–AlGaAs heterostructures [21–23] and graphene bilayers (in the case of graphene, barriers as thin as 1 nm), the superfluid phase has not been observed yet, except of quantum Hall regime in the presence of the external magnetic field, where the physics is quite different [9]. Accordingly, it may seem that the electron–hole superfluidity at the vanishing external magnetic field will never occur in a solid state system, however, it has been shown [24] that a double bilayer graphene system, separated by barrier of thickness 1 nm, should generate an excitonic superfluid at experimentally attainable temperatures, and in the case of the absence of the external magnetic field. One of the key reasons why the excitonic superfluidity is so hard to observe experimentally in 2D case is in fact related to the dominant role of quantum fluctuations at low dimensions and at low temperatures, when the very large zero-point oscillations are present. This peculiarity is due to the absence of any real heavy particle in the electron–hole (e–h) system.

In the present paper, we address the role of the particle phase coupling in the purely 2D in-plane interacting excitonic system. We explore the low-temperature quantum collective behavior of the excitons and we extend the theoretical works mentioned above, by showing that the formation of the excitonic superfluid state is governed by the non-local cross correlations between nearest neighbors (n.n.) excitonic pairs in contrast to the formation of the EI state, where the local on-site correlations are important. We derive the BKT transition lines, and we discuss the values of the physical parameters entering in the system.

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2. The model

For the study of the EI state and the excitonic superfluidity in 2D, we have chosen the two-band extended Falicov–Kimball model (EFKM), [3,4] due to its large applicability for treatment of the electronic correlations. The Hamiltonian of the EFKM model is given by

$$\mathcal{H} = -t_c \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \left[\bar{c}(\mathbf{r}) c(\mathbf{r}') + h.c.\right] - \bar{\mu} \sum_{\mathbf{r}} n(\mathbf{r}) - t_f \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \left[\bar{f}(\mathbf{r}) f(\mathbf{r}') + h.c.\right] + \frac{\epsilon_c - \epsilon_f}{2} \sum_{\mathbf{r}} \tilde{n}(\mathbf{r}) + U \sum_{\mathbf{r}} \frac{1}{4}\left[n^2(\mathbf{r}) - \tilde{n}^2(\mathbf{r})\right]. \quad (1)$$

Here $\bar{f}(\mathbf{r})$ ($\bar{c}(\mathbf{r})$) creates an f (c) electron at the lattice position $\mathbf{r}$, the summation $\langle \mathbf{r}, \mathbf{r}'\rangle$ runs over pairs of n.n. sites of 2D square lattice. The density type shorthand notation is introduced: $n(\mathbf{r}) = n_c(\mathbf{r}) + n_f(\mathbf{r})$ and $\tilde{n}(\mathbf{r}) = n_c(\mathbf{r}) - n_f(\mathbf{r})$. Next, t_c is the hopping amplitude for c-electrons and ϵ_c is the corresponding on-site energy level. Similarly, t_f is the hopping amplitude for f-electrons and ϵ_f is the on-site energy level for f-orbital. The sign of the product $t_c t_f$ determines the type of semiconductor, for $t_c t_f < 0$ ($t_c t_f > 0$) we have a direct (indirect) band gap semiconductor. The on-site (local) Coulomb interaction U in the last term of the Hamiltonian in Eq. (1) plays the coupling role between the electrons in the f and c sub-systems. The chemical potential $\bar{\mu}$ is $\bar{\mu} = \mu - \bar{\epsilon}$, where $\bar{\epsilon} = (\epsilon_c + \epsilon_f)/2$. We will use $t_c = 1$ as the unit of energy and we fix the band parameter values $\epsilon_c = 0$ and $\epsilon_f = -1$. For the f-band hopping amplitude t_f we consider the values $t_f = -0.3$ and $t_f = -0.1$. Throughout the paper, we set $k_B = 1$ and $\hbar = 1$ and lattice constant $a = 1$.

3. The EI state discussion

The Hamiltonian in Eq. (1) is containing two separate quadratic terms and is suitable for decoupling by functional path integration method [25]. We use imaginary-time fermionic path integral techniques, and we introduce the fermionic Grassmann variables $f(\mathbf{r}\tau)$ and $c(\mathbf{r}\tau)$ at each site $\mathbf{r}$ and for each time τ, which varies in the interval $0 \leqslant \tau \leqslant \beta$, where $\beta = 1/T$ with T being the thermodynamic temperature. The time-dependent variables $c(\mathbf{r}\tau)$ and $f(\mathbf{r}\tau)$ are satisfying the anti-periodic boundary conditions $x(\mathbf{r}\tau) = -x(\mathbf{r}\tau + \beta)$, where $x = f$ or c. After decoupling the last interaction term in the Hamiltonian in Eq. (1) we will have for the grand canonical partition function of the system

$$\mathcal{Z}_{\mathrm{GC}} = \int [\mathcal{D}\bar{c}\,\mathcal{D}c][\mathcal{D}\bar{f}\,\mathcal{D}f][\mathcal{D}V][\mathcal{D}\varrho] e^{-\mathcal{S}[\bar{c},c,\bar{f},f,V,\varrho]}, \quad (2)$$

where the action in the exponential is given by

$$\mathcal{S}[\bar{c}, c, \bar{f}, f, V, \varrho] = \sum_{\mathbf{r}} \int_0^\beta d\tau \left[\frac{V^2(\mathbf{r}\tau)}{U} + \frac{\varrho^2(\mathbf{r}\tau)}{U} - iV(\mathbf{r}\tau) n(\mathbf{r}\tau) - \varrho(\mathbf{r}\tau)\tilde{n}(\mathbf{r}\tau)\right] + \sum_{x=f,c} \mathcal{S}_B[\bar{x}, x] + \int_0^\beta d\tau \mathcal{H}(\tau). \quad (3)$$

The new variables $V(\mathbf{r}\tau)$ and $\varrho(\mathbf{r}\tau)$ in the action are the decoupling fields for quadratic terms in the Hamiltonian, in Eq. (1), proportional to $n^2(\mathbf{r}\tau)$ and $\tilde{n}^2(\mathbf{r}\tau)$ respectively. Next, $\mathcal{S}_B[\bar{f}, f]$ and $\mathcal{S}_B[\bar{c}, c]$ are Berry actions for f and c-electrons and they are defined as follows: $\mathcal{S}_B[\bar{x}, x] = \sum_{\mathbf{r}} \int_0^\beta d\tau\, \bar{x}(\mathbf{r}\tau)\dot{x}(\mathbf{r}\tau)$, where $\dot{x}(\mathbf{r}\tau) = \partial_\tau x(\mathbf{r}\tau)$ is the time derivative. Next, we will factorize usual electron operators f and c in terms of new fermionic variables $\tilde{f}$ and $\tilde{c}$ coupled to the unitary charge-carrying U(1) rotor. To this end we write the potential $V(\mathbf{r}\tau)$ as the sum of a static and periodic part $V(\mathbf{r}\tau) = V_0 + \tilde{V}(\mathbf{r}\tau)$. Then, for the periodic part, we introduce the $U(1)$ phase field $\varphi(\mathbf{r}\tau)$ via the "Faraday"-type relation [26]

$$\tilde{V}(\mathbf{r}\tau) = \frac{\partial \varphi(\mathbf{r}\tau)}{\partial \tau}. \quad (4)$$

For the static part V_0 and $\varrho(\mathbf{r}\tau)$-field, the saddle-point evaluations give $V_0^{\mathrm{s.p.}} = i\frac{Un}{2} - i\bar{\mu}$ and $\varrho^{\mathrm{s.p.}} = \frac{U\tilde{n}}{2} - \frac{\epsilon_c - \epsilon_f}{2}$. Here n is the average total particle density $n = \langle n_c(\mathbf{r}\tau)\rangle + \langle n_f(\mathbf{r}\tau)\rangle$ (furthermore, we will fix $n = 1$, corresponding to the case of half-filling [3,4]) and $\tilde{n}$ is the average of the difference of particle densities $\tilde{n} = \langle \tilde{n}(\mathbf{r}\tau)\rangle$. Then the partition function of the system becomes

$$\mathcal{Z}_{\mathrm{GC}} = \int [\mathcal{D}\bar{c}\,\mathcal{D}c][\mathcal{D}\bar{f}\,\mathcal{D}f][\mathcal{D}\varphi] e^{-\mathcal{S}[\bar{c},c,\bar{f},f,\varphi]} \quad (5)$$

and the total action in Eq. (3) reduces to

$$\mathcal{S}[\bar{c}, c, \bar{f}, f, \varphi] = \mathcal{S}_{\mathrm{eff}}[\varphi] + \mathcal{S}_B[\bar{c}, c] + \mathcal{S}_B[\bar{f}, f] - t_c \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \int_0^\beta d\tau \left[\bar{c}(\mathbf{r}\tau) c(\mathbf{r}'\tau) + h.c.\right] - t_f \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \int_0^\beta d\tau \left[\bar{f}(\mathbf{r}\tau) f(\mathbf{r}'\tau) + h.c.\right] + \sum_{\mathbf{r}} \int_0^\beta d\tau \left[\mu_n n(\mathbf{r}\tau) + \mu_{\tilde{n}} \tilde{n}(\mathbf{r}\tau)\right]. \quad (6)$$

Here

$$\mathcal{S}_{\mathrm{eff}}[\varphi] = \sum_{\mathbf{r}} \int_0^\beta d\tau \left[\frac{\dot{\varphi}^2(\mathbf{r}\tau)}{U} - \frac{2\bar{\mu}}{iU}\dot{\varphi}(\mathbf{r}\tau) - i\dot{\varphi}(\mathbf{r}\tau) n(\mathbf{r}\tau)\right] \quad (7)$$

is the phase-only action, which contains fluctuating imaginary term $i\dot{\varphi}(\mathbf{r}\tau)n(\mathbf{r}\tau)$. The chemical potentials μ_n and $\mu_{\tilde{n}}$ are defined as $\mu_n = \frac{Un}{2} - \bar{\mu}$ and $\mu_{\tilde{n}} = \frac{\epsilon_c - \epsilon_f}{2} - \frac{U\tilde{n}}{2}$.

Next, we perform the local gauge transformation to new fermionic variables $\tilde{f}(\mathbf{r}\tau)$ and $\tilde{c}(\mathbf{r}\tau)$. For the electrons of f and c orbitals, the U(1) gauge transformation could be written as

$$\begin{bmatrix} x(\mathbf{r}\tau) \\ \bar{x}(\mathbf{r}\tau) \end{bmatrix} = \hat{\mathcal{U}}(\varphi) \cdot \begin{bmatrix} \tilde{x}(\mathbf{r}\tau) \\ \bar{\tilde{x}}(\mathbf{r}\tau) \end{bmatrix}, \quad (8)$$

where $\hat{\mathcal{U}}(\varphi)$ is the U(1) transformation matrix $\hat{\mathcal{U}}(\varphi) = \hat{I} \cdot \cos\varphi(\mathbf{r}\tau) + i\hat{\sigma}_z \cdot \sin\varphi(\mathbf{r}\tau)$ with the unit matrix $\hat{I}$ and $\hat{\sigma}_z$ being the Pauli matrix.

After those transformations we can write the total action of the system in the Fourier-space representation introducing the vector-space notations and, furthermore, we will derive gap equation for the excitonic order parameter Δ. The effective phase averaged action of the system in the Fourier space takes the following form:

$$\mathcal{S}_{\mathrm{eff}}[\bar{\tilde{c}}, \tilde{c}, \bar{\tilde{f}}, \tilde{f}] = \frac{1}{\beta N} \sum_{\mathbf{k}\nu_n} \left[\bar{\tilde{c}}_{\mathbf{k}}(\nu_n), \bar{\tilde{f}}_{\mathbf{k}}(\nu_n)\right] \mathcal{G}^{-1}(\mathbf{k}, \nu_n) \begin{bmatrix} \tilde{c}_{\mathbf{k}}(\nu_n) \\ \tilde{f}_{\mathbf{k}}(\nu_n) \end{bmatrix}. \quad (9)$$

Here $\mathcal{G}^{-1}(\mathbf{k}, \nu_n)$ is the inverse of the Green function matrix, given by