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Phase coherence and spectral functions in the two-dimensional excitonic systems

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ABSTRACT

The nonlocal correlation mechanism between excitonic pairs is considered for a two dimensional exciton system. On the base of the unitary decomposition of the usual electron operator, we include the electron phase degrees of freedom into the problem of interacting excitons. Applying the path integral formalism, we treat the excitonic insulator state (EI) and the Bose–Einstein condensation (BEC) of preformed excitonic pairs as two independent problems. For the BEC of excitons the phase field variables play a crucial role. We derive the expression of the local EI order parameter by integrating out the phase variables. Then, considering the zero temperature limit, we obtain the excitonic BEC transition probability function, by integrating out the fermions. We calculate the normal excitonic Green functions for the conduction and valence band electrons and we derive the excitonic spectral functions, both analytically and numerically. Different values of the Coulomb interaction parameter are considered.

1. Introduction

The Coulomb interaction between the electrons and holes gives rise to a very rich physics related to the excitonic systems. The excitons, as composite objects [1] with a total zero spin, have a tendency to condense at the very low temperatures, and this is shown for the first time in the sixties of the past millennium [2–4]. In general, the Bose–Einstein condensation (BEC) of excitons and the formation of the excitonic insulator (EI) state are considered as the same in the existing literature [5–13]. The EI state is a new phase, which develops in the scenario of semimetal (SM)–semiconductor (SC) phase transition, when approaching the transition from the SC side [4,14]. As it is shown in Refs. [5–7], the EI order parameter is non-null for a given interval of the Coulomb interaction parameter and for a given value of the valence band hopping amplitude. From the interpretation of the results given there, it follows that in the small interaction region, the system is in the Bardeen–Cooper–Schrieffer (BCS) state [15] with a very weak binding energies of electron–hole pairs, contrary, when approaching from the SC side of the EI state, the system shows BEC behavior with tightly bound excitons [8,16], thus exhibiting a BCS-BEC type crossover [5–7,17]. As we mentioned above, in all cited works here, the exciton condensation occurs at the same temperature, as the EI phase transition. It is worth to indicate that the coherence is discussed there in the sense of the direct binding between electrons and holes, without dealing with the phase variables of the quasiparticles.

However, a series of recent theoretical works suggest the importance of the phase correlations on the phase transition scenario in the excitonic systems [18–23]. Particularly, in Refs. [18,19], it is shown theoretically that the EI state and the excitonic BEC are not exactly the same. The importance of the phase coherence in the excitonic pair plasma is discussed there, with a classification of two distinct phase transitions in the excitonic plasma and the discussion about the exciton BEC is provided. It is shown [18–20,22,23] that in the low density limit of the excitonic pairs, the critical temperature of excitonic BEC should be much smaller than the temperature of the pair formation.

In the high $e-h$ density limit we have the convergence of theories, since in this case the transition lines of excitonic condensation and of that of the pair formation are coinciding. Indeed, where the mean distance between the particles is shorter than the excitonic Bohr radius, the weakly bound $e-h$ pairs behave like the Cooper pairs in the conventional superconductors at sufficiently low temperatures [3,4,24]. In this case, the condensation is of the BCS type. In Ref. [20], the authors employ the two-band Hubbard model within the self-consistent t-matrix approximation to show that in the low density limit the gas of free excitons undergoes the BEC phase transition at the very low temperatures, and the BEC temperature transition line is not coinciding with that of the pair

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formation. In fact, the BEC of the excitonic pairs is possible only when the macroscopic phase coherence is present in the system [18]. The EI state is an excitonium state, where the incoherent $e-h$ bound pairs are formed and furthermore, at the lower temperatures, the BEC of excitons appears in consequence of reconfiguration and coherent condensation of preformed excitonic pairs.

In the weak-coupling limit, the transition to $e-h$ condensed phase is related to the relative motion between electrons and holes [20], which implies the BCS-like regime and is in contrast to the case of strong-coupling, when the BEC state is related to the motion of the center of mass of excitons. The $e-h$ mass difference in the BCS-BEC transition scenario leads to a large suppression of the BEC transition temperature, which is proved to not be the same as the excitonic pair formation temperature [20,22,23]. This is in contrast with the previous treatments [5–13], where the EI state is associated with the BEC state of excitons, as to be identical. We treat the $e-h$ system in the frames of (spinless) two-dimensional (2D) extended Falicov–Kimball model (EFKM), as a purposeful model, to include the *f*–*f* hopping mechanism that could be also responsible for the exciton formation [9]. Using the electron operator representation, we address the role of the phase factor in the context of the interacting excitons. As a first step of the theory, we obtain the EI order parameter by employing the functional integration technique and we discuss the stability region (in the *T*-*U* plan) of the exciton pair formation. Furthermore, at the zero temperature limit, we integrate out the fermions and we discuss the obtained phase action and the phase stiffness. We show that the phase stiffness in the system is directly related to the exciton condensation in the 2D excitonic system at zero temperature. We calculate the phase stiffness parameter for different values of the *f*-band hopping amplitude.

Then, turning to the phase sector, we employ the Bogoliubov mean field displacement approximation, for the bosonic charge variables and, hence, we separate the excitonic condensate part in the $e-h$ paired plasma (excitonium). Furthermore, we calculate the exciton BEC transition probability, as a function of the attractive Coulomb interaction parameter U/t, which is normalized to the hopping integral of the conduction band electrons. By using the Fourier space representation, we give the expressions of the total normal Green functions for the *f* and *c*-band electrons and we emphasize on the phase dependence of those functions. As a consequence, we obtain the frequency dependent normal spectral functions, at the zero temperature case and, furthermore, the phase-coherent density of states (DOS). The numerical evaluations of normal DOS functions, for the *f* and *c* band electrons, show a gapless character of the spectrum of excitations, in contrast to the traditionally admitted incoherent DOS behavior. We show that the hybridization-gap is totally absent for all frequency modes and for all values of the Coulomb interaction parameter. We argue that the gapless behavior in the DOS spectra is a result of competition of two independent excitations in the system: the phase fluctuations and strong quantum coherence effects at zero temperature limit. Note that a similar gapless character in the DOS spectrum of cold excitons is observed recently in Ref. [25], where this effect is associated with metallic charge-density-wave phase and it is driven by the strong electron correlations.

The paper is organized as follows. In Section 2, we introduce the model Hamiltonian. The electron factorization and resulting phase action are presented in Section 3. In Section 4, we get the effective fermionic action for the EI state in the system. The numerical results are presented there. In Section 5 we integrate out the fermions and we obtain the phase stiffness parameter, both analytically and numerically. In Section 6 we discuss the 2D excitonic BEC at $T=0$ and we calculate the ecxitonic BEC transition probability function. Section 7 is devoted to the calculation of the single particle spectral functions and density of states. At the end of Section 7 we give the numerical evaluations for DOS functions and we discuss the obtained results. Meanwhile, an experimental technique is proposed to prove directly the DOS behavior. Finally, in Section 8 we give a conclusion of our results. The theoretical calculation of the phase action is given in the Appendix.

2. The method

2.1. EFKM Hamiltonian

The Hamiltonian of the spinless EFKM model is given by

$$\mathcal{H} = -\sum_{\mathrm{x=f,c}}\left\{\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} t_{\mathrm{x}}[\bar{x}(\mathbf{r})x(\mathbf{r}') + h.c.] + (\mu_{\mathrm{x}} - \epsilon_{\mathrm{x}})\sum_{\mathbf{r}} n_{\mathrm{x}}(\mathbf{r}) - \frac{U}{2}\sum_{\mathbf{r}} n_{\mathrm{x}}(\mathbf{r})n_{\tilde{\mathrm{x}}}(\mathbf{r})\right\}. \quad (1)$$

Here, the operator $\bar{x}(\mathbf{r})$ ($x(\mathbf{r})$) creates (annihilates) an *f* or *c* electron at the lattice position $\mathbf{r}$, the notation $\tilde{x}$ in the last term in Eq. (1) means the orbital opposite to x, the summation $\langle \mathbf{r}, \mathbf{r}'\rangle$ runs over pairs of nearest neighbor (n.n.) sites on the 2D square lattice. The spin degrees of freedom have been ignored for simplicity. Next, t_x is the hopping amplitude for *x*-electrons and ϵ_{x} is the corresponding on-site energy level. The sign of the product $t_{\mathrm{x}}t_{\tilde{\mathrm{x}}}$ determines the type of semiconductor, for $t_{\mathrm{x}}t_{\tilde{\mathrm{x}}} < 0$ ($t_{\mathrm{x}}t_{\tilde{\mathrm{x}}} > 0$) we have the direct (indirect) band gap semiconductor. The case $t_f \equiv 0$ corresponds to that of the dispersionless *f* band and usual Falicov–Kimball model [26] (FKM) could be derived (in this case, the local *f*-electron number is conserved).

The on-site (local) interaction parameter *U*, in the last term of the Hamiltonian in Eq. (1), is the Coulomb repulsion parameter (interorbital) between the electrons in the *f* and *c* orbitals. As we will see later on, the strength of the local Coulomb interaction will tune the SM–SC transition in the system and the formation of the local EI state in the excitonic system. In the case of the degenerated *f* and *c* bands, i.e. when $\epsilon_{\mathrm{x}} = \epsilon_{\tilde{\mathrm{x}}}$ and $t_{\mathrm{x}} = t_{\tilde{\mathrm{x}}}$, the EFKM model reduces to the standard Hubbard model [27]. Furthermore, we adjust the chemical potentials μ_{x} and $\mu_{\tilde{\mathrm{x}}}$ in order to maintain separate the number of electrons in *f* and *c* orbitals. Then, the equilibrium value of chemical potential $\mu \equiv \mu_{\mathrm{x}} = \mu_{\tilde{\mathrm{x}}}$ in Eq. (1) will be determined from the half-filling condition, i.e. we suppose that $\langle n_{\mathrm{x}}(\mathbf{r})\rangle + \langle n_{\tilde{\mathrm{x}}}(\mathbf{r})\rangle = 1$. In what follows, we assume a band structure with a direct band gap, i.e. $t_{\mathrm{x}}t_{\tilde{\mathrm{x}}} < 0$ and without the loss of generality the *c* electrons are considered to be "light", while the *f* electrons are "heavy", i.e. $t_f < 1$, and the hopping integral for *c* electrons is taken to be the unit of the energy scale $t_c = 1$. Throughout the paper, we set $k_B = 1$ and $\hbar = 1$, and, the lattice constant, $d=1$. For frequency notations, we keep the symbol ν for fermions and ω for bosons. We set also $\epsilon_c = 0$.

The genuine feature of the EFKM Hamiltonian in Eq. (1) is that it is equivalent to the asymmetric Hubbard model, if we associate for orbitals *c* and *f* the spin variables, thus replacing the fermionic Hilbert space with the pseudo-fermionic one, and then by linearizing the interaction term via the bosonic states (see in Ref. [6]).

2.2. Hubbard–Stratanovich linearisation

It is more convenient to write the EFKM Hamiltonian given in Eq. (1) in more symmetric form, suitable for the mean-field decoupling