Non-local-cross-correlations and macroscopic phase coherence in excitonic systems

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We present an alternative mechanism for the excitonic Bose Einstein condensation (BEC) in the three dimensional electronic system. The quantum physics of the effective cold bosons formed from the electrons and holes is explored using the phase coherence mechanism. We proposed a microscopic description of the exciton condensation in a three dimensional (3D) system in terms of the effective actions. The path integral formalism is applied for the electronic system and the equation for the exciton order parameter is obtained. We derive the excitonic insulator (EI) state and the excitonic pair (EP) formation critical temperature in a self-consistent way and we solve the equations numerically. In order to consider the non-local pair correlations, we evaluate the series of the cumulant expansion of the effective fermionic action and we consider the second order term with respect to the interband hopping amplitude $t$. We obtain the analytical expression for the phase coupling parameter and we evaluate it numerically. A new emergent critical temperature for the excitonic BEC is derived within the proposed calculation scheme and it is found to be much smaller than usually admitted EP transition temperature. Excitonic correlation functions are discussed and the BEC transition amplitude is derived numerically for different values of the Coulomb interaction parameter. Analytical expression of the excitonic spectral function is given and the shapes of excitonic density of states (DOS) are presented.

I. INTRODUCTION

The physics of the excitonic insulator state as a bound state of the conduction band electrons and valence band holes has a long history. It is examined in the pioneering works of Jerome and Halperin.12 Despite intensive study on the subject, the first experimental observation of the EI phase has a history of about two decades.13 when such a state is observed in ZnSe/Zn_{0.75}Cd_{0.25}Se type of quantum well structures. It is interesting to mention that coherent excitonic lasing is demonstrated there and the BCS state is refered as “coherent exciton” state.4 Mainly, the “coherent” exciton state becomes important at the characteristic high density $n_c$ typical to the BCS regime.4 A series of experimental investigations,25 in the compound TmSe$_{0.45}$Te$_{0.55}$ suggest the existence of the EI state in such a material. The angle resolved photoemission spectra (ARPES) on these compounds,5 demonstrate that the ground state therein is a well defined excitonic insulator. The evidence in favor of the EI state is proved also in the transition-metal dichalcogenid layered compound 1T-TiSe$_2$, where the EI scenario is responsible for the charge-density-wave transition in such a material.16 Despite the important number of the papers published on the subject, there is neither a theoretical work nor the experimental one, in which the EI state is proved to be identical with the Bose-Einstein condensate state of the excitons.17

First possible evidence for the BEC state in the system of excitons is discussed by Keldysh and Kozlov in Ref. 17. The authors have considered the low density system of excitons and the stability condition of the Bose-condensed ground state is given in the case of the weak attraction between the particles. Contrary, at high e-h density, 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 conventional superconductors at sufficiently low temperatures, i.e., the BCS state of e-h pairs.1,21,22 Therefore, an expected BCS-BEC crossover represents actually a fascinating problem typical to the excitonic systems. Especially, it is interesting from the viewpoint of the difference from the similar crossover in superconductors or trapped atomic Fermi gases.22-24 The transition to the e-h pair condensate phase, in the weak-coupling limit, is related to the relative motion between electrons and holes,25 implying the BCS regime and is in contrast to the case of the strong-coupling regime, when the BEC state is related to the motion of the center of mass of excitons. In the whole BCS-BEC transition region the e-h mass difference leads to a large suppression of the BEC transition temperature, which is proved to not be same as EP formation temperature.25

The recent theoretical investigations,26-28 concerning the excitonic BEC and the EI state, are generally based on the Hartree-Fock (HF) approximation for the mean-field theory and on the scalar slave-boson (SB) scheme, which reproduces the Gutzwiller solution of the Hubbard model as a saddle point.29 Particularly, Zenker et al. in Ref. 28 have elaborated a slave-boson calculation techniques and the EI state is derived there for the initially non-degenerated orbitals of conduction band $c$ and the valence band $f$. Moreover, in their work, a good agreement with the previous mean-field-based result,31 is achieved for the excitonic gap parameter, but the excitonic condensation temperature $T_c$ has been reduced significantly. However, the excitonic insulator state and excitonic condensation are spontaneously found the same.32-34 Although, this is not affecting the general physical picture of the excitonic insulator,35 apart of the
discussion about the excitonic condensation critical temperature. The phase boundary of the EI region typifies therein either a BEC or a BCS condensate state corresponding respectively to the strong and weak limits of the Coulomb interaction and a BEC-BSC type of crossover is expected for the general case.\textsuperscript{22,29} Recently, it is shown theoretically that the excitonic insulator and the excitonic condensate are not exactly the same\textsuperscript{34,35} The author in Refs. \textsuperscript{24} and \textsuperscript{25} shows from general considerations that in the low density limit of the excitonic pairs, the critical temperature $T_c$ of excitonic condensate transition should be much smaller than the temperature $T_{EI}$ of EP formation, in contrast to the previous treatments\textsuperscript{26–29} where the EI state is associated with the BEC state of excitons. Similarly, in Ref. \textsuperscript{25} it is shown that 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 the reconfiguration and coherent condensation of preformed excitonic pairs. Obviously, 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 EP formation. The Bose condensation of the excitonic pairs is possible only when the macroscopic phase coherence is present in the system.\textsuperscript{31} The experimental proof of spontaneous phase coherence, between the pairs in the excitonic bosonic gas and the possible BEC transition at the low-energy state, is given in Ref. \textsuperscript{36} concerning the GaAs/AlGaAs, quasi two dimensional coupled quantum well structures. Mainly, the phase coherence is found in the region of macroscopically ordered excitonic state.\textsuperscript{37} However, the experimental evidence of the existence of two distinct transition temperatures, for the general case of three dimensional bulk system, is yet lacking in the literature. In fact, the question whether a true “coherent” BEC transition is present in the system of excitons (in the case of high exciton density limit) still ambiguous. The experimental proof of it, is a very cumbersome problem, because of dominant role of quantum fluctuations at low temperatures $T \lesssim E_{Ry}^{eh}$, when the very large zero-point oscillations are present. This peculiarity is related to the absence of any real heavy particles in the e-h system. The electrons and holes have the masses of about the same order of magnitude $m_e \sim m_h$.

The continued confusion, regarding EI state and condensation for excitonic system, motivates us to re-examine the problem of BEC of the excitonic gas, based on phase coherence scheme in the extended Falicov-Kimball model (EFKM).

First, within the path integral formalism\textsuperscript{33} relevant to the fermions, we get the analytical solution for the EI state in the form of coupled self-consistent-equations (SCE), which we solve numerically. Furthermore, supposing the macroscopic phase coherence at the very low temperatures and considering all possible direct on-site and NLCC correlations between nearest neighbors (n.n.) excitonic pairs, we obtain the expression for the exchange coupling interaction parameter $J_{ex}$ between pairs and we evaluate the four-point fermionic correlators arising from theory. The form of $J_{ex}$ (see in Section \textsuperscript{VI} of the present paper) indicates that the macroscopic phase coherence in the system is characterized by an energy scale $J_{ex} \sim (\Delta t_e t_h)/(t_e + t_h)$ for all values of the Coulomb interaction parameter $U$ (details are given in the Section \textsuperscript{VI} and it is related to the motion of the center of mass of e-h composed particle, because $(t_e + t_h)/(t_e + t_h) \approx (m_e + m_h)^{-1}$. Namely, for the large-$U$ limit, our model maps into the hard core Boson model with the kinetic energy proportional to $\Delta t_e t_h/U$ ($\Delta$ being the local excitonic order parameter) and the potential energy $(t_e^2 + t_h^2)/U$, applying that the exchange coupling parameter becomes proportional to the BEC critical temperature. We show namely, that NLCC between the electrons and holes of different n.n. excitonic pairs, are relevant for the excitonic condensation.

Furthermore, we get the self-consistent solution of the BEC transition temperature in the general case including both, strong and weak coupling limits and complementing the achievements in Ref. \textsuperscript{25}.

The BEC transition amplitude is given also, treating the non-local gauge bosonic sector, and its temperature dependence is found. We complete our results by calculating analytically the excitonic spectral functions and we evaluate numerically the density of states.

The paper is organized as follows. In Sec. II, the general phenomenology concerning the excitonic system is given. In Sec. III, the model Hamiltonian, electron factorization and analytical calculation schemes are introduced. The total effective action of the system is obtained by the saddle-point approximation method and the partition function of the system is given. The Section IV is devoted to the SCE derivation within the path integral formalism. The numerical solution of SCE is given in Section V. The pair correlations and resulting excitonic condensation is discussed in the Section VI. Fur-
thermore, in Section VII, we evaluate on the form of the excitonic spectral functions and we get the form of density of states. In Section VIII we sort out the principal achievements of our paper.

II. THE PHENOMENOLOGY

We discuss the coherence in the EFKM model not in the sense usually admitted till now. Particularly, it is well-known that the hybridization between the $c$ and $f$ band electrons leads to the non-vanishing expectation value $(\bar{c}f)$ in the EI region and the spontaneous pairing of $c$ electrons with $f$ holes mediated by the electrostatic Coulomb interaction is responsible for the formations of the EI state in the system.\textsuperscript{26–29} But it is always not obvious that the hybridization and the coherence are the same (in the sense discussed in Ref. 27).

The fundamental is that the coherence between the electrons and holes in the single EI will not lead to the macroscopic condensation for an ensemble of excitons.

In our case, we derive the EI state supposing the spontaneous pairing interaction between the electrons and holes in the single pair, mediated by the tunable Coulomb interaction. Furthermore, by lowering the temperature, we consider the macroscopic phase coherent state between the preformed excitonic pairs mediated by the fermion-averaged exchange interaction between them. In this case, we have the phase coherence between “exciton” quasiparticles and the subsequent Bose-condensation of the excitonic pairs. We will show also that the EI state is a necessary prerequisite for the macroscopic phase coherent state of the ensemble of excitons. The general schematics of purposed strategy is given in Fig. 1. In the left panel in Fig. 1 the EI state formation is presented as a cumulative from the partial contributions of local excitonic order parameters $\Delta_i = (\bar{c}_i f_i)$, where the index $i$ is the lattice site position. Thus, the left panel in Fig. 1 represents the excitonic plasma formation, and the transition temperature $T_{EI}$ is the temperature at which the EP formation begins (see in Sections IVB and V). Above this transition temperature, the system constitutes of the free e-h particles plasma, i.e. the normal band insulator (BI) regime. In the right panel in Fig. 1 we have presented schematically the possible cross-correlations between n.n. excitonic particles, coupled via the non-local exchange interaction parameter $J_{ex}$, which is related (see the Section VIIB) to the motion of the center of masses of excitons, hence assuring the BEC condensation of pre-formed (see in Fig. 1) excitonic plasma. As we will see later-on, the non-local phase dependent constituent of the parameter $J$, contributing to BEC of excitons, is a sum of cross-correlations between n.n. excitonic pairs.

In this perspective, we factorize usual electron operator $c$ in terms of the fermionic variables $\hat{c}$ coupled to unitary gauge bosonic $U(1)$ variables $z = e^{i\varphi}$. Thus the transformation is: $c = \hat{c}e^{i\varphi}$. As a result, the electron appears in the theory like a composite object of that of the fermion with the attached $U(1)$ phase-“flux-tube” (we presented it schematically in Fig. 2a and Fig. 2b like the bosonic clouds, surrounding fermionic particles). The flows of phase flux (see dashed arrows in Fig. 2a, and Fig. 2b) are independent of spin of the fermions, but depend on the particle type. For the electrons and holes, the superflow has the opposite direction, thus no of supercurrent could traverse across system (see in Fig. 2a no Meissner effect happens in this case). This is in contrast to the usual BCS picture, where the pairing is between the electrons and the superflow of the phase-flux tubes has the same direction (in Fig. 2b). The electron factorization in terms of two variables has an unprecedented impact on the whole theory. Especially, the emergent bosonic gauge field, related to the phase variables, leads to a Bose-type of band renormalization factor and, furthermore, is crucial for the BEC of excitons, derived in the frame of the quantum rotor model (see in the Section VI).

FIG. 2: The gauge representation of the exciton and Cooper pair.

It is worthwhile to mention that the obtained EI region is formed principally of the local on-site electron correlations (see the image on the left-hand side in Fig. 1), when the interaction between excitonic pairs is neglected, i.e. EI state is a cumulative from the individual local excitons. Contrary, for the condensate state, we have considered also non-local-cross-correlations (NLCC) between the electrons and holes of different n.n. pairs (image in the right-hand side of Fig. 1). The term of second order

% Diagram for Fig. 1
% (a) The gauge representation of exciton. The dashed-arrows represent the direction of the bosonic phase flux around the fermionic particles. The solid arrows represent the spin of the electron or hole.
% (b) The gauge representation of Cooper pair. The dashed-arrows represent the direction of the bosonic phase flux around the fermionic particles. The solid arrows represent the spins of the electrons.
in the series of the cumulant distribution for the effective fermionic action will be a good approximation for the non-local pair correlation treatment (for details see the Section VI).

III. THE METHOD

A. The model Hamiltonian

As the model for study the EI state and the excitonic condensation at low temperatures we have chosen the two-band extended Falicov-Kimball model (EFKM)\textsuperscript{23,33,39–43}, due to its large applicability for treatment of the electronic correlations. The Hamiltonian of the EFKM model is

\[
H = -t_c \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} [\bar{c}(\mathbf{r})c(\mathbf{r}') + \text{h.c.}] - (\mu_c - \epsilon_c) \sum_{\mathbf{r}} n_c(\mathbf{r}) - t_f \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} [\bar{f}(\mathbf{r})f(\mathbf{r}') + \text{h.c.}] - (\mu_f - \epsilon_f) \sum_{\mathbf{r}} n_f(\mathbf{r}) + U \sum_{\mathbf{r}} n_c(\mathbf{r})n_f(\mathbf{r}).
\]

(1)

Here \( \bar{f}(\mathbf{r}) \) (\( c(\mathbf{r}) \)) creates an \( f \) (\( c \)) electron at the lattice site position \( \mathbf{r} \), the summation \( \langle \mathbf{r}, \mathbf{r}' \rangle \) runs over pairs of nearest neighbor sites of the three-dimensional cubic lattice. For \( t_c, t_f < 0 \) (\( t_c, t_f > 0 \)) we may have a direct (indirect) band gap. The case \( t_f \equiv 0 \) corresponds to that of the dispersionless \( f \) band and the usual Falicov-Kimball model (FKM)\textsuperscript{23} could be derived (the local \( f \)-electron number is conserved). Next, \( t_c \) is the hopping integral for \( c \)-electrons and \( \epsilon_c \) is the corresponding on-site energy level. Similarly, \( t_f \) is the hopping integral for \( f \)-electrons and \( \epsilon_f \) is the on-site energy level for \( f \)-orbital. On-site (local) Coulomb interaction \( U \) in the last term of the Hamiltonian in Eq. (1) determines the distribution of the electrons between \( f \) and \( c \) sub-systems. As we will see later on, the strength of the local Coulomb interaction will tune the metal-insulator transition in the system. In the case of degenerated \( f \) and \( c \) bands, i.e. when \( \epsilon_f = \epsilon_c \) and \( t_f = t_c \), the EFKM model reduces to the standard Hubbard model\textsuperscript{39} Furthermore, we adjust the chemical potentials \( \mu_f \) and \( \mu_c \) in order to maintain the number of electrons in \( f \) and \( c \) orbitals separately. Then, the equilibrium value of the chemical potential \( \mu \equiv \mu_f = \mu_c \) in Eq. (1) will be determined from the half-filling condition, i.e. we suppose that \( \langle n_c(\mathbf{r}) \rangle + \langle n_f(\mathbf{r}) \rangle = 1 \). In what follows, we assume a band structure with a direct band gap, i.e. \( t_c, t_f < 0 \) 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: \( t_c = 1 \), and \( \epsilon_c = 0 \). Throughout the paper, we set also \( k_B = 1 \) and \( \hbar = 1 \).

In fact, the EFKM Hamiltonian in Eq. (1) is equivalent to the asymmetric Hubbard model, if we associate to the orbitals \( c \) and \( f \) the spin variables, by replacing the fermionic Hilbert space with the pseudo-fermionic one and then linearizing the interaction term via the bosonic states (see in Ref. 39). The principal advantage of the EFKM, in comparison with the genuine FKM, is that it is taking into account the direct nearest-neighbors \( f \) electron hoppings\textsuperscript{27} \( (t_f) \) and it can be shown\textsuperscript{18} that the EI state is unstable when the pure FKM is approached.

B. Functional integral formalism and effective phase action: decoupling of interactions

To proceed further, we transform the last four-fermionic interaction term in the Hamiltonian Eq. (1) by rewriting it as

\[
U \sum_{\mathbf{r}} n_c(\mathbf{r})n_f(\mathbf{r}) = \frac{U}{4} \sum_{\mathbf{r}} \left[ n^2(\mathbf{r}) - \bar{n}^2(\mathbf{r}) \right], \tag{2}
\]

where we introduced the short-hand notations\textsuperscript{27} \( n(\mathbf{r}) = n_c(\mathbf{r}) + n_f(\mathbf{r}) \) and \( \bar{n}(\mathbf{r}) = n_c(\mathbf{r}) - n_f(\mathbf{r}) \), after which the Hamiltonian in Eq. (1) takes the form

\[
H = -t_c \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} [\bar{c}(\mathbf{r})c(\mathbf{r}') + \text{h.c.}] - \bar{\mu} \sum_{\mathbf{r}} n(\mathbf{r}) - t_f \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} [\bar{f}(\mathbf{r})f(\mathbf{r}') + \text{h.c.}] + \frac{\epsilon_c - \epsilon_f}{2} \sum_{\mathbf{r}} \bar{n}(\mathbf{r}) + U \sum_{\mathbf{r}} \frac{1}{4} \left[ n^2(\mathbf{r}) - \bar{n}^2(\mathbf{r}) \right]. \tag{3}
\]

Moreover, \( n(\mathbf{r}) \) is the total particle density in the system, and \( \bar{n}(\mathbf{r}) \) is the particle density difference function between the conduction band and valence band. Here we have putted \( \bar{\mu} = \mu - \bar{\epsilon} \), where \( \bar{\epsilon} = (\epsilon_c + \epsilon_f)/2 \) is the average energy level parameter. The Hamiltonian in Eq. (3) is containing two separate quadratic terms and is suitable for decoupling by functional path integration method\textsuperscript{38,59}

1. The partition function and decoupling fields

We employ the imaginary-time, fermionic path integral method and we introduce the fermionic Grassmann variable\textsuperscript{38} \( \bar{f}(\mathbf{r}, \tau) \) and \( c(\mathbf{r}, \tau) \) at each site \( \mathbf{r} \) and each time \( \tau \) varying in the interval \( 0 \leq \tau \leq \beta \), with \( \beta = 1/T \) with \( T \) being the thermodynamic temperature. The time-dependent variables \( c(\mathbf{r}, \tau) \) and \( \bar{f}(\mathbf{r}, \tau) \) are satisfying the anti-periodic boundary conditions \( x(\mathbf{r}, \tau) = -x(\mathbf{r} + T, \beta) \), where \( x = f \) or \( c \).

The grand canonical partition function of system of fermions written as a functional integral over the Grassmann fields is

\[
Z_{\text{GC}} = \int [D\bar{c}Dc][D\bar{f}Df] e^{-S[\bar{c},c,\bar{f},f]}, \tag{4}
\]
where the action in exponential is given in the path integral formulation in the form of

\[ S[c, f, \tilde{c}, \tilde{f}] = S_B[c, \tilde{c}] + S_B[f, \tilde{f}] + \int_0^\beta d\tau H(\tau). \]  

(5)

Here \( S_B[c, \tilde{c}] \) and \( S_B[f, \tilde{f}] \) are fermionic Berry terms for \( c \) and \( f \)-electrons respectively. They are defined as

\[ S_B[x, x] = \sum_r \int_0^\beta d\tau \bar{x}(rr) \dot{x}(rr) \]

(6)

and \( \dot{x}(rr) = \partial_\tau x(rr) \) is the usual time derivative.

2. Decoupling of term proportional to \( n^2 \)

Next, we will decouple the quadratic density terms in Eq.(3) using Hubbard-Stratonovich linearisation procedure \(^{15} \) by introducing the new variables \( V(rr) \) and \( \varphi(rr) \) conjugated respectively to the density terms \( n(rr) \) and \( \tilde{n}(rr) \). For quadratic term, proportional to \( n^2(rr) \) in the exponential of the partition function in Eq.(4), we have

\[ \exp \left[ -\frac{U}{4} \sum_r \int_0^\beta d\tau n^2(rr) \right] = \int [DV] e^{-\sum_r \int_0^\beta d\tau \left[ \frac{\varphi^2(rr)}{2} - iV(rr)n(rr) \right]} . \]

(7)

Furthermore, we combine the exponential in Eq.(7) with the effective chemical potential term, linear in total electron density \( n(r) \) (see the second term in Eq.(3)). Then, we decompose the variables \( V(rr) \) into a static and the periodic part

\[ V(rr) = V_0(r) + \tilde{V}(rr), \]

(8)

where \( \int_0^\beta d\tau \tilde{V}(rr) = 0 \). As a result, the integration over variables \( V(rr) \) becomes the integration over the scalar static variables \( V_0(r) \) and the integration over the periodic field \( \tilde{V}(rr) \):

\[ \int [DV] ... \rightarrow \int [DV_0] \int [D\tilde{V}] ... . \]

(9)

For the periodic part in Eq.(8), we introduce the emergent phase variables \( \varphi(rr) \) according to the following "Faraday"-type relation (see in Ref. \(^{50} \) for details)

\[ \tilde{V}(rr) = \partial_\tau \varphi(rr) \equiv \dot{\varphi}(rr). \]

(10)

Thus, for the dynamic part, we transform the functional integration over decoupling variables \( \tilde{V}(rr) \), into integration over the generic phase variables \( \varphi(rr) \) as

\[ \int [D\tilde{V}] ... \rightarrow \int [D\varphi] ... . \]

(11)

In performing integration over the phase field one should take into account that

\[ \varphi(r\beta) - \varphi(r0) = 2\pi m(r), \]

(12)

where \( m(r) = 0, \pm 1, \pm 2, \ldots \) are topological integer winding numbers. Therefore, the integration measure in Eq.(11) is defined in our theory as

\[ \int [D\varphi] ... \equiv \sum_{|m(r)|} \int_0^{2\pi} \prod_r d\varphi(r) \times \int_{\varphi(r0) = \varphi(r)} \prod_r d\varphi(r) ... \]

(13)

and includes the summations over winding numbers defined by Eq.(12).

For the scalar static part \( V_0(r) \), we get the following functional integral

\[ \int [DV_0] e^{\sum_r \int_0^\beta d\tau \left[ \frac{\varphi^2(rr)}{2} + V_0(r)n(rr) - \frac{\mu}{iU} \varphi(rr)n(rr) \right]} . \]

(14)

The saddle-point value of \( V_0(r) \) is given by

\[ V_0 = i\frac{U\mu}{2} - \mu, \]

(15)

where \( n \) is total average particle density \( n = n_c + n_f \) (furthermore, we will fix \( n \) as equal to 1 corresponding to the case of half-filling). Thereby, after decoupling the quadratic term proportional to \( n^2 \) in the Hamiltonian in Eq.(6), we get the following contribution to the total partition function in Eq.(4)

\[ \exp \left[ -S_{\text{eff}}[\varphi] - \sum_r \int_0^\beta d\tau \mu_p n(rr) \right] , \]

(16)

where the emergent phase-only action \( S_{\text{eff}}[\varphi] \) is given as

\[ S_{\text{eff}}[\varphi] = \sum_r \int_0^\beta d\tau \left[ \frac{\varphi^2(rr)}{U} - \frac{2\mu}{iU} \varphi(rr) - i\varphi(rr)n(rr) \right] \]

(17)

and effective chemical potential \( \mu_p \), attached to the total density operator in Eq.(16), is given in the form \( \mu_p = \frac{U\mu}{2} - \mu \).

3. Decoupling of term proportional to \( \tilde{n}^2 \)

The decoupling of the quadratic term proportional to \( \tilde{n}^2(rr) \) in the exponential of the partition function in Eq.(4) is also straightforward. We obtain

\[ \exp \left[ \sum_r \int_0^\beta d\tau \frac{U}{4} \tilde{n}^2(rr) \right] = \int [D\bar{n}] e^{-\sum_r \int_0^\beta d\tau \left[ \frac{\varphi^2(rr)}{2} - \varphi(rr)\tilde{n}(rr) \right]} , \]

(18)
Combining the expression in the exponential in Eq.(18) with the similar linear term in the expression of the Hamiltonian in Eq.(3), we have

\[ \int [D\tilde{\theta}] e^{\sum_{t} \int_{0}^{\beta} dt - \frac{\epsilon_{c} - \epsilon_{f}}{2} \left[ \tilde{\nu}(\tau t) - \frac{\epsilon_{c} - \epsilon_{f}}{2} \right]}. \]

The saddle-point evaluation for \( g \) gives

\[ g_{0} = \frac{U\tilde{\nu}}{2} - \frac{\epsilon_{c} - \epsilon_{f}}{2}, \]

where \( \tilde{\nu} = \langle \tilde{\nu}(\tau t) \rangle \) is the average of the particle density difference function. As a result of the decoupling, we obtain “Zeeman”-like contribution to the partition function

\[ \exp \left[ - \sum_{r} \int_{0}^{\beta} d\tau \mu_{c}\tilde{\nu}(\tau t) \right] \]

with the attached effective chemical potential \( \mu_{c} = \frac{\epsilon_{c} - \epsilon_{f}}{2} - \frac{U\tilde{\nu}}{2}. \)

4. Linearized action with the phase-field contribution

To summarize, the grand canonical partition function of the system, after of both procedures of decoupling, is

\[ Z_{GC} = \int [D\tilde{\theta}] [D\tilde{\phi}] [D\varphi] e^{-S[\tilde{c}, \tilde{f}, \tilde{\phi}, \varphi]}, \]

where the action \( S[\tilde{c}, \tilde{f}, \tilde{\phi}, \varphi] \) in the exponential is already linear in terms of the particle densities and is given by

\[ S[\tilde{c}, \tilde{f}, \tilde{\phi}, \varphi] = S[\varphi] + S_{B}[\tilde{c}, \tilde{c}] + S_{B}[\tilde{f}, \tilde{f}] \]

\[ -t_{c} \sum_{(r,r')} \int_{0}^{\beta} d\tau [\tilde{c}(r \tau t)\tilde{c}(r' \tau t) + h.c.] \]

\[ -t_{f} \sum_{(r,r')} \int_{0}^{\beta} d\tau [\tilde{f}(r \tau t)\tilde{f}(r' \tau t) + h.c.] \]

\[ + \sum_{r} \int_{0}^{\beta} d\tau [\mu_{c}\tilde{\nu}(r \tau t) + \mu_{c}\tilde{\nu}(r \tau t)]. \]

After Hubbard-Stratanovich lienarisation, we got the total action of the system that is linear in terms of fermion density and contains in addition a term, depending purely of the phase variables of the particles, and also the terms, proportional to the effective chemical potentials \( \mu_{p} \) and \( \mu_{c} \) which are setting the limits of the Coulomb interaction parameter \( U \).

C. The U(1) gauge transformation

To proceed, we perform the local gauge transformation to new fermionic Grassmann variables \( \tilde{f}(r \tau t) \) and \( \tilde{c}(r \tau t) \) in order to eliminate the last imaginary term appearing in the expression of the phase action in Eq.(17). For the electrons of \( f \)-orbital, the U(1) transformation is

\[ \begin{bmatrix} c(r \tau t) \\ f(r \tau t) \end{bmatrix} = \begin{bmatrix} \tilde{c}(r \tau t) \\ \tilde{f}(r \tau t) \end{bmatrix} e^{i\varphi(r \tau t)}, \]

where we used the bosonic phase variables \( \varphi \) introduced in Eq.(10). For the complex conjugate variables, we have

\[ \begin{bmatrix} \tilde{c}(r \tau t) \\ \tilde{f}(r \tau t) \end{bmatrix} = \begin{bmatrix} c(r \tau t) \\ f(r \tau t) \end{bmatrix} e^{-i\varphi(r \tau t)}. \]

As a result, the electron appears in the theory like a composite object composed of fermion with the attached U(1) phase “flux-tube” \( e^{i\varphi(r \tau t)} \) (see Figs.(2a, 2b)). After transformations given in Eqs.(24) and (25) we obtain the total action of the system in the form (for comparison see the action in Eq.(23) before transformations)

\[ S[\tilde{c}, \tilde{f}, \tilde{\phi}, \varphi] = S_{0}[\varphi] + S_{B}[\tilde{c}, \tilde{c}] + S_{B}[\tilde{f}, \tilde{f}] \]

\[ -t \sum_{(r,r')} \int_{0}^{\beta} d\tau [\tilde{c}(r \tau t)\tilde{c}(r' \tau t)e^{-[\varphi(r \tau t) - \varphi(r' \tau t)]} + h.c.] \]

\[ -t \sum_{(r,r')} \int_{0}^{\beta} d\tau [\tilde{f}(r \tau t)\tilde{f}(r' \tau t)e^{-[\varphi(r \tau t) - \varphi(r' \tau t)]} + h.c.] \]

\[ + \sum_{r} \int_{0}^{\beta} d\tau [\mu_{c}\tilde{\nu}(r \tau t) + \mu_{c}\tilde{\nu}(r \tau t)]. \]

Now, \( t \) and \( \tilde{t} \) in Eq.(26) are respectively \( \tilde{c} \)-band and \( \tilde{f} \)-band fermion hopping integrals. We get in Eq.(26) a new emergent quadratic phase-action \( S_{0}[\varphi] \)

\[ S_{0}[\varphi] = \sum_{r} \int_{0}^{\beta} d\tau \left[ \tilde{\varphi}^{2}(r \tau t) - \frac{2\tilde{\nu}}{i\tilde{t}\varphi(r \tau t)} \right]. \]

We will see in the Section VI that the phase action in Eq.(27) is very important for deriving the low temperature expression of the non-local gauge bosonic correlator and then to obtain self-consistently the BEC transition temperature in the frames of the spherical model.

The partition function of the system in the new variables \( \tilde{c} \) and \( \tilde{f} \) is

\[ Z_{GC} = \int [D\tilde{c}] [D\tilde{f}] [D\varphi] e^{-S[\tilde{c}, \tilde{f}, \tilde{\phi}, \varphi]}. \]

From this form of the partition function we will generate the effective actions for fermions and for bosonic phase sector (see Sections IV and VI, see also the general procedure presented in Fig. 3).
S[\bar{c}, c, \tilde{f}, \tilde{f}]

U(1) gauge transformation

μ

\[ S[\bar{c}, c, \tilde{f}, \tilde{f}, \varphi] \]

\[ \varphi \text{ integration} \]

Fermion integration

\[ S\text{ eff}[\bar{c}, c, \tilde{f}, \tilde{f}, \varphi] \]

Gap, EI transition: \( T_{EI} \)

Exchange corr. J

Excitonic-condensate: \( T_e \)

\[ S\text{ eff}[\varphi] \]

FIG. 3: (Color online) Functional integration procedure.

IV. SELF-CONSISTENT SOLUTION FOR THE EI STATE

A. Phase-averaged action

In this Section of our paper we apply the U(1) gauge transformations given in Eqs. (24), and (25) to the fermionic variables in the initial Hamiltonian of the system in Eq. (1), and then we will decouple the four fermionic interaction term within the HF approach by applying Bogoliubov mean-field approximation. The mean-field decoupling scheme of the interaction term is

\[ n_\nu(\mathbf{r}\tau)n_{\nu}(\mathbf{r}\tau) \approx \langle n_\nu(\mathbf{r}\tau) \rangle n_{\nu}(\mathbf{r}\tau) + \langle n_{\nu}(\mathbf{r}\tau) \rangle n_\nu(\mathbf{r}\tau) - \frac{1}{2} \Delta c(\mathbf{r}\tau) f(\mathbf{r}\tau) - \frac{1}{2} \Delta f(\mathbf{r}\tau) c(\mathbf{r}\tau) \]

where \( n_\nu(\mathbf{r}\tau) \) and \( n_{\nu}(\mathbf{r}\tau) \) are fermion densities after U(1) transformations. The general strategy of calculations is presented in Fig. 3.

Furthermore, we will average the phase variables with the partition function given in Eq. (22) and we obtain

\[ Z_{GC} = \int [D\tilde{c}D\tilde{f}] e^{-S_{\text{eff}}[\tilde{c}, \tilde{f}, \tilde{f}, \tilde{f}]} , \]

where the effective action in the exponential in Eq. (29) is given by the relation

\[ e^{-S_{\text{eff}}[\tilde{c}, \tilde{f}, \tilde{f}, \tilde{f}]} = \int [D\varphi] e^{-S[\bar{c}, c, \tilde{f}, \tilde{f}, \varphi]} . \]

The Fourier transformation of fermionic variables \( \tilde{f}(\mathbf{r}\tau) \) and \( \tilde{c}(\mathbf{r}\tau) \) is given by

\[ \tilde{x}(\mathbf{r}\tau) = \frac{1}{\beta N} \sum_{k\nu_n} \tilde{x}_k(\nu_n) e^{i(\mathbf{k}\mathbf{r}\nu_n\tau)} \]

with \( \tilde{x} = \tilde{f}, \tilde{c} \) for \( \tilde{f} \) and \( \tilde{c} \) type of fermions. \( N \) is the number of lattice sites for a given orbital and \( \nu_n = \pi(2n + 1)/\beta \) are the Fermi-Matsubara frequencies with \( n = 0, \pm 1, \pm 2, \ldots \). The effective action

\[ S_{\text{eff}}[\tilde{c}, \tilde{f}, \tilde{f}, \tilde{f}] = \frac{1}{\beta N} \sum_{k\nu_n} \tilde{x}_k(\nu_n) (\tilde{c}_\nu - i\nu_n - t_k) \tilde{c}_k(\nu_n) + \frac{1}{\beta N} \sum_{k\nu_n} \tilde{f}_k(\nu_n) (\tilde{c}_\nu - i\nu_n - \tilde{f}_k(\nu_n) - \frac{\Delta}{\beta N} \sum_{k\nu_n} \tilde{c}_k(\nu_n) \tilde{f}_k(\nu_n) . \]

We have obtained in Eq. (32) the Hartree quasiparticle-energies \( \epsilon_{\tilde{f}} \) and \( \epsilon_{\tilde{c}} \) as

\[ \epsilon_{\tilde{c}} = \epsilon_c - \mu + Un_{\tilde{f}} + i \langle \dot{\varphi}(\mathbf{r}r') \rangle , \]

\[ \epsilon_{\tilde{f}} = \epsilon_f - \mu + Un_{\tilde{c}} + i \langle \dot{\varphi}(\mathbf{r}r') \rangle . \]

Note, that we kept naturally the same notations for quasiparticle band energy parameters \( \epsilon_c, \epsilon_f \). Furthermore, \( n_{\tilde{f}} \) and \( n_{\tilde{c}} \) in Eqs. (33) and (34) are \( \tilde{f} \) and \( \tilde{c} \) fermion average densities \( n_{\tilde{f}} = \langle n_{\tilde{f}}(\mathbf{r}\tau) \rangle = \langle \tilde{c}(\mathbf{r}\tau) \tilde{f}(\mathbf{r}\tau) \rangle \). In addition to the usual Hartree shift, given by the term \( Un_{\tilde{c}} \) in Eqs. (33) and (34), we have also a gauge bosonic imaginary term of the form \( i \langle \dot{\varphi}(\mathbf{r}r') \rangle \) and from the symmetry reasons we are omitting this term for the first treatment. Next, \( t_k \) and \( t_k \) in Eq. (32) are band-renormalized hopping amplitudes \( t_k = 2ig(\mathbf{k}) \) and \( t_k = 2ig(\mathbf{k}) \), where \( g \) stands for the gauge boson bandwidth renormalization factor

\[ g = \left. \langle e^{-i\varphi(\mathbf{r}r') - \varphi(\mathbf{r}'r')} \rangle \right|_{|\mathbf{r} - \mathbf{r}'| = d} \]

and \( \epsilon(\mathbf{k}) \) is the three-dimensional lattice dispersion \( \epsilon(\mathbf{k}) = \cos(d_xk_x) + \cos(d_yk_y) + \cos(d_zk_z) \) with \( d_\alpha (\alpha = x, y, z) \), being the components of the lattice spacing vector \( \mathbf{d} = \mathbf{r} - \mathbf{r}' \) with \( \mathbf{r} \) and \( \mathbf{r}' \) nearest neighbors site positions. For the simple cubic geometry we have \( d_\alpha = 3 \).

Employing the vector-space notations, we can rewrite the action in Eq. (32) in more compact form

\[ S_{\text{eff}}[\tilde{c}, \tilde{f}, \tilde{f}, \tilde{f}] = \frac{1}{\beta N} \sum_{k\nu_n} \left[ \tilde{c}_k(\nu_n), \tilde{f}_k(\nu_n) \right] G^{-1}(\mathbf{k}, \nu_n) \times \left[ \tilde{c}_k(\nu_n), \tilde{f}_k(\nu_n) \right] . \]

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

\[ G^{-1}(\mathbf{k}, \nu_n) = \left( \begin{array}{c} E^c_k(\nu_n) & -\Delta \\ -\Delta & E^f_k(\nu_n) \end{array} \right) . \]
where the single-particle quasienergies \( E^c_k(\nu_n) \) and \( E^f_k(\nu_n) \) are given after Eq.\((32)\)

\[
E^c_k(\nu_n) = \tilde{\epsilon}_c - i\nu_n - t_k, \tag{38}
\]

\[
E^f_k(\nu_n) = \tilde{\epsilon}_f - i\nu_n - \tilde{t}_k. \tag{39}
\]

**B. EI state analytics**

The EI low-temperature phase is characterized by local excitonic order parameter \( \Delta = U \langle \tilde{\epsilon}(rr)\tilde{f}(rr) \rangle \). As we mentioned in the Section II, the EI state is the cumulative of local on-site electron-hole correlations (see the left picture in Fig. 1). The average in the expression of the local EI order parameter and also fermion density averages \( n_{\tilde{\epsilon}} = \langle \tilde{\epsilon}(rr)\tilde{\epsilon}(rr) \rangle \), representing the average occupancies of the respective band levels, could be calculated in the frame of path integral method. Namely, using Eqs.\((29)\) and \((37)\) we get a set of SC equations for the EI order parameter \( \Delta \), the single-particle fermion density averages \( n_{\tilde{\epsilon}}, n_{\tilde{f}} \) and the EI chemical potential \( \mu \) (note that we have a Hartree-band for the chemical potential, which collapses when approaching to the EI transition line). The EI low-temperature phase is characterized by local excitonic order parameter \( \Delta = U \langle \tilde{\epsilon}(rr)\tilde{f}(rr) \rangle \). As we mentioned in the Section II, the EI state is the cumulative of local on-site electron-hole correlations (see the left picture in Fig. 1). The expectation value given in the expression of the local EI order parameter could be calculated in the frame of path integral method as well as the fermion density averages \( n_{\tilde{\epsilon}} = \langle \tilde{\epsilon}(rr)\tilde{\epsilon}(rr) \rangle \), which are the average occupancies of the respective band levels. Namely, using Eqs.\((29)\) and \((37)\) we get a set of SC equations for the EI order parameter \( \Delta \), single-particle fermion densities \( n_{\tilde{\epsilon}}, n_{\tilde{f}} \) and the EI chemical potential \( \mu \) (note that we have a Hartree-band for the chemical potential, which collapses when approaching to the EI transition line from the SM side of the transition scenario).

\[
\frac{1}{N} \sum_k \left[ \tilde{f}(E^c_k) + \tilde{f}(E^f_k) \right] = 1, \tag{40}
\]

\[
\bar{n} = \frac{1}{N} \sum_k \xi_k \frac{\tilde{f}(E^c_k) - \tilde{f}(E^f_k)}{\sqrt{\xi_k^2 + 4\Delta^2}}, \tag{41}
\]

\[
\Delta = -\frac{U\Delta}{N} \sum_k \frac{f(E^c_k) - f(E^f_k)}{\sqrt{\xi_k^2 + 4\Delta^2}}. \tag{42}
\]

Here \( \xi_k = -t_k + \tilde{\epsilon}_c + \tilde{t}_k - \tilde{\epsilon}_f \) is the quasiparticle dispersion and energy parameters \( E^{\pm}_k \) and \( E^c_k \) are

\[
E^{\pm}_k = \frac{1}{2} \left( -t_k + \tilde{\epsilon}_c - \tilde{t}_k \pm \sqrt{\xi_k^2 + 4\Delta^2} \right). \tag{43}
\]

In Fig. 4 we have presented schematically the SC cycle-

**FIG. 4:** (Color online) The schematic diagram for SCE solution procedure of the local EI order parameter \( \Delta \).

procedure for the excitonic order parameter \( \Delta \). The difference between the energy parameters in Eq.\((43)\) defines the charge transfer gap in the system \( \Delta_c = E^c_k - E^{-}_k \) (see the left-panel 1 at the top in Fig. 4). The Eq.\((40)\) defines the equilibrium values of the chemical potential. Furthermore, \( f(\epsilon) \) denotes the Fermi-Dirac distribution function \( f(\epsilon) = 1/\left[ e^{\beta \epsilon} + 1 \right] \).

We define also the frequency-summed normal and anomalous momentum dependent functions \( n_{\tilde{\epsilon}}(k) \) and \( F_{\tilde{\epsilon}f}(k) \)

\[
n_{\tilde{\epsilon}}(k) = \frac{1}{\beta} \sum_{\nu_n} G_{\tilde{\epsilon}f}^{\nu}(k, \nu_n), \tag{44}
\]

\[
n_{\tilde{f}}(k) = \frac{1}{\beta} \sum_{\nu_n} G_{\tilde{f}f}^{\nu}(k, \nu_n), \tag{45}
\]

\[
F_{\tilde{\epsilon}f}(k) = \frac{1}{\beta} \sum_{\nu_n} F_{\tilde{\epsilon}f}^{\nu}(k, \nu_n), \tag{46}
\]

where \( G_{\tilde{\epsilon}f}^{\nu}(k, \nu_n) \), \( G_{\tilde{f}f}^{\nu}(k, \nu_n) \) and \( F_{\tilde{\epsilon}f}^{\nu}(k, \nu_n) \) are Fourier transformations of the normal and anomalous Green functions. We have

\[
n_{\tilde{\epsilon}}(k) = \frac{1}{\beta} \sum_{\nu_n} \frac{\tilde{\epsilon}_c - i\nu_n - \tilde{t}_k}{E^c_k(\nu_n)E^c_f(\nu_n) - |\Delta|^2}, \tag{47}
\]

\[
n_{\tilde{f}}(k) = \frac{1}{\beta} \sum_{\nu_n} \frac{\tilde{\epsilon}_f - i\nu_n - \tilde{t}_k}{E^f_k(\nu_n)E^f_f(\nu_n) - |\Delta|^2}, \tag{48}
\]

\[
F_{\tilde{\epsilon}f}(k) = \frac{1}{\beta} \sum_{\nu_n} \frac{\Delta}{E^c_k(\nu_n)E^c_f(\nu_n) - |\Delta|^2}. \tag{49}
\]

Summing over fermionic Matsubara frequencies, we get

\[
n_{\tilde{\epsilon}}(k) = -u_k^2 f(E^c_k) - u_k f(E^c_k), \tag{50}
\]

\[
n_{\tilde{f}}(k) = -u_k^2 f(E^f_k) - u_k f(E^f_k), \tag{51}
\]

\[
F_{\tilde{\epsilon}f}(k) = u_k u_k f(E^c_k) - f(E^f_k). \tag{42}
\]

For the coefficients \( u_k \) and \( v_k \) appearing in Eq.\((42)\) we have

\[
u_k^2 = \frac{1}{2} \left( 1 - \frac{\xi_k}{\sqrt{\xi_k^2 + 4\Delta^2}} \right), \tag{54}
\]

\[
u_k^2 = \frac{1}{2} \left( 1 + \frac{\xi_k}{\sqrt{\xi_k^2 + 4\Delta^2}} \right), \tag{55}
\]

\[
u_k u_k = \frac{\Delta}{\sqrt{\xi_k^2 + 4\Delta^2}}. \tag{55}
\]
In complete analogy, with the HF approximation\textsuperscript{30,31} we will assume, that at the Fermi momentum $|F_{\epsilon f}(k_F)| = 1$ i.e. $n_F(k_F) = n_F(k_F) = 0.5$.

The spatial coherence of a bosonic system is encoded in its one-body density matrix, therefore, the anomalous momentum function is directly related to the excitonic coherence length. Hence, we can associate the characteristic decay of $F_{\epsilon f}(k)$ with the coherence length defined by the relation

$$\xi_{coh}^2 = \sum_k |\nabla_k F_{\epsilon f}(k)|^2 / \sum_k |F_{\epsilon f}(k)|^2. \quad (56)$$

V. NUMERICAL OUTCOMES AND DISCUSSION

The numerical solution of the system of SC equations\textsuperscript{40,41} is performed for the fixed value of the total particle density $n = n_F + n_N = 1$ and $k$-summations were performed with the $(100 \times 100 \times 100)$ $k$-points in the First Brillouin Zone (FBZ). The finite difference approximation method is used within the HYBRJ algorithm\textsuperscript{50} which is retaining the fast convergence of Newton’s method\textsuperscript{52}. The accuracy of convergence for numerical solutions is achieved with a relative error of order $10^{-7}$.

The picture in the left-panel 1 in Fig. 5 shows the charge transfer gap function $\Delta_c$, discussed in Section IV B, for $t = -0.3$. For small values of Coulomb interaction $U$, the charge transfer gap is nearly zero, which is the manifestation of the semimetallic (SM) limit. In augmenting the interaction parameter $U$, the gap $\Delta_c$ is gradually increasing and remains open for the large values of $U$, indicating the Hartree limit. In this case we pass to semiconductor (SC) side of the phase diagram. Thus, we have a SC-SM transition scenario or a BCS-BEC crossover at much lower temperatures, not coinciding with EP formation temperature (see in the Section VI for details)\textsuperscript{25,29}.

The EI formation region at the SM-SC transition\textsuperscript{25,30,31} (when $\Delta(T_{EI}, U) = 0$) for different values of the hopping integral $t$ is shown in the left-panel 2 in Fig. 5. We see that the stability region of the EI phase is larger in the cases of the large hopping amplitudes. We observe a very good agreement with the previously done HF and SB results\textsuperscript{20,27}. The exact SCE solutions for the chemical potential at the boundary of EI transition (i.e. when $\Delta$ vanishes) is presented in the left-panel 3 in Fig. 5.

The solution for density difference function $\tilde{n}$ between the bands is given in the right panel 4 at the top in Fig. 5. Particularly, $\tilde{n}$ is plotted for two different values of the hopping amplitude $t$ and for two different cases, that of the EI transition critical region ($\Delta(T_{EI}, U) = 0$) and below of it, i.e. the EI state ($T < T_{EI}$) with $\Delta \neq 0$. We see that for a given value of the interaction parameter $U$, when approaching to the boundary of the EI stability region from the EI side ($T < T_{EI}$), the $f$-band occupation becomes higher and, naturally, the SC phase is reached more rapidly.

In the right-panel 5 in Fig. 5 we have presented the numerical outcomes for the chemical potential in the EI state of the system. Notably, at very small Coulomb interaction parameter, the chemical potential is coinciding with $\mu_{EI}$ of the transition region (when $T \sim T_{EI}$), thus, collapsing into the single valued case $\mu \to \mu_{EI}$. Contrary, for higher values of $U$ we have a generous degeneracy related to $\mu$ and a Hartree-type gap ($\Delta_H \sim \mu_{max} - \mu_{min}$) is continuously opening indicating the SM-SC passage in the system. The chemical potential bands for, different values of $t$, are plotted in the right-panel 6 in Fig. 5.

FIG. 5:
(Color online) Numerical solution for excitonic stability region and the EI state. The following physical quantities are presented: the charge gap function $\Delta_c$ (left-panel 1), temperature of EP formation $T_{EI}$ (left-panel 2), the critical values of the chemical potential $\mu_{EI}$ (left-panel 3), the band-occupation difference function $\tilde{n}$ (right-panel 4), the chemical potential $\mu$ in the EI regime (right-panel 5), the local excitonic gap parameter $\Delta$ (right-panel 6).
different colors.

The right-panel 6 in Fig. 6 shows the numerical solutions of local excitonic order parameter $\Delta$ for the Ef state ($T < T_{E Ef}$). Different values of $\tilde{t}$ are considered.

In Fig. 7 we show the results for the normal and anomalous momentum distribution functions given in Eqs. (50) and (52). The $k$-dependencies of the $\tilde{c}$-band normal momentum function $n_{\tilde{c}}(k)$, and the anomalous function $F_{\tilde{c}f}(k)$ are presented for $T = 0$, along the direction $(0, 0, 0) \rightarrow (\pi, \pi, \pi)$ of the momentum space and their $U$-dependence is shown. Two different values of the hopping integral $f$ are considered. The normal $f$-band momentum function is not considered here, because $n_{\tilde{c}}(k) = 1 - n_{\tilde{f}}(k)$. In the weak coupling regime the normal distribution function $n_{\tilde{f}}(k)$ drops at $k = k_F$ (see the left-panel 1 and right-panel 4 in Fig. 6) and anomalous momentum function $F_{\tilde{c}f}(k)$ is picked at the Fermi momentum (see the left-panel 2 and right-panel 5 in Fig. 6). With increasing of $U$, $n_{\tilde{f}}(k)$ spread out in $k$-space and also $F_{\tilde{c}f}(k)$ becomes broad indicating the small value of the e-h pair radius. In the strong coupling limit the anomalous function decreases for all momenta of the reciprocal space, which is consistent with the behavior of the excitonic order parameter $\Delta$ (see the right-panel 6 in Fig. 5). We can see also (see the left-panel 2 and right-panel 4 in Fig. 6) that in the strong coupling regime, $k_F$ approaches to $(0, 0, 0)$, thus performing the momentum transfer of the e-h composed particle. This is also related to the apparent signature of BEC of excitons (see discussion in the introduction of the present paper and the Section III).

In Fig. 7 we show the temperature dependence of the anomalous momentum function $F_{\tilde{c}f}(k)$ for different values of the Coulomb interaction $U$ and for $\tilde{t} = 0.3$. In the left panel 1 in Fig. 7 the temperature dependence of the momentum function is presented for $U = 1.2$. The chemical potential in this case is of single valued $\mu_0 = -0.265$. In the left panels 2 and 3 $U = 2.0$ and both (the upper and lowest) limits of the chemical potential are considered. At the upper band we have $\mu_{\text{max}} = 0.221$ and at the lower band $\mu_{\text{min}} = -0.04$. The right panels 4 and 5 shows temperature dependence of $F_{\tilde{c}f}(k)$ for $U = 9.0$. We see in all pictures, that the temperature has a destructive influence on the amplitude of $F_{\tilde{c}f}(k)$ leading to its total suppression at high temperatures. And in the right panel 6 in Fig. 7 tight-binding density of states $\rho_{\text{TB}}$ is presented for the simple cubic lattice structure.

The $k$-summations in the analytical expression of the coherence length $\xi_{\text{coh}}$ given in Eq. (50) were done with the $(100 \times 100 \times 100)$ $k$-points in the FBZ. Obtained curves are presented in the left-panel 3 and right-panel 6 in Fig. 6. The rapid growth of the coherence length for small values of $U$ is anticipated as the excitons cooled down below the temperature of their quantum degeneracy. On the other hand, opposite to this, the coherence length decreases rapidly with increasing $U$, which physically means that with increasing the interaction parameter we are destroying the spatial correlations between electrons and holes. Furthermore, we find that the coherence length has a shallow minimum in the crossover regime ($U \sim 4$ for $\tilde{t} = -0.01$ and $U \sim 7$ for $\tilde{t} = -0.3$) and then $\xi_{\text{coh}}$ again increases with a small gain, with increasing further $U$.

At the end of this Section we should note, that reducing the dimensionality 3D$\rightarrow$2D doesn’t affect the general behavior of momentum functions and excitonic coherence length $\xi_{\text{coh}}$ which is not the case for the excitonic condensate transition critical temperature (see the Section VI).
VI. MACROSCOPIC PHASE COHERENCE AND CONDENSATION

A. Fermion integration

In this section we will follow the right-lowest root presented in Fig. 5 in the Section IV. Namely, we will integrate out fermions in Eq. (28) and, furthermore, we will derive the expression of the phase-only action by employing the non-zero-temperature Wick averaging method and quantum spherical model (QSM) for the bosonic sector. We will show, how the non-local fermionic (in the fermionic sector) and gauge-bosonic (in the QSM) correlations lead to the macroscopic phase coherent state of the ensemble of excitons. Furthermore, considering the QSM, we obtain the excitonic BEC critical temperature $T_c$ and we find it much lower (about two orders of magnitude) in comparison with the excitonic pair formation transition temperature $T_{EL}$.

The integration over fermions in the expression in Eq. (28) of the total partition function of the system gives the effective action for the phase sector in our model. The partition function in Eq. (28) could be rewritten as

$$Z_{GC} = \int [D\phi] e^{-S_{eff}[\phi]},$$

where the effective phase action in the exponential is

$$S_{eff}[\phi] = -\ln \int [D\tilde{c}D\tilde{e}] \left[ D\tilde{f} D\tilde{f} \right] e^{-S}. \tag{57}$$

Expanding the logarithm in the right hand side in Eq. (58) we will have

$$S_{eff}[\phi] = \bar{S}_0 + \langle S \rangle_{\tilde{\phi} \tilde{f}} - \frac{1}{2} \left[ \langle S^2 \rangle_{\tilde{\phi} \tilde{f}} - \langle S \rangle_{\tilde{\phi} \tilde{f}}^2 \right]. \tag{59}$$

Here $\langle ... \rangle_{\tilde{\phi} \tilde{f}}$ is

$$\langle ... \rangle_{\tilde{\phi} \tilde{f}} = \frac{\int [D\tilde{c}D\tilde{e}] \left[ D\tilde{f} D\tilde{f} \right] ... e^{-S}}{\int [D\tilde{c}D\tilde{e}] \left[ D\tilde{f} D\tilde{f} \right] e^{-S}}. \tag{60}$$

The phase averaging in Eq. (60) can be considered as the quantum statistical averaging with an effective phase field action $S_{eff}$. This consideration is sometimes called like the Bogoliubov-mean-field self-consistency condition. Thus, we replace

$$\langle ... \rangle_{\tilde{\phi} \tilde{f}} \rightarrow \langle ... \rangle_{S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]} \tag{61}$$

and for the effective phase action we find

$$S_{eff}[\phi] = \bar{S}_0 + \langle S \rangle_{S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]} - \frac{1}{2} \left[ \langle S^2 \rangle_{S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]} - \langle S \rangle_{S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]}^2 \right]. \tag{62}$$

After self-consistency assumption in Eq. (61), the average in Eq. (60) will be

$$\langle ... \rangle_{S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]} = \frac{\int [D\tilde{c}D\tilde{e}] \left[ D\tilde{f} D\tilde{f} \right] ... e^{-S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]}}{\int [D\tilde{c}D\tilde{e}] \left[ D\tilde{f} D\tilde{f} \right] e^{-S_{eff}[\tilde{c},\tilde{e},\tilde{f},\tilde{f}]}}. \tag{63}$$

The relations in Eq. (61) and (63) are principal for the theory. Using them together, we resolve the problem of interacting fermions as a self-consistently coupled problem of the noninteracting fermions and the gauge-bosonic phase field. The bosonic sector plays the role of a suitable background (the glue), on which the collective excitations and correlations of the fermionic sector appear.
B. NLCC in the excitonic system

In this Section we show how the macroscopic phase coherence in the excitonic system is responsible for the excitonic BEC in 3D EFKM. We will examine the form of the effective phase action $S_{\text{eff}}[\varphi]$ obtained in a self-consistent way in Eq. (62) considering only the four-fermionic terms therein, thereby treating relevant non-local fermionic correlations. Therefore, the important part of the effective phase action is

$$
S_{\text{eff}}[\varphi] = S_0[\varphi] + S_{J\lambda}[\varphi],
$$

where $S_{J\lambda}[\varphi] = -\frac{1}{2} \left\langle \mathcal{S}^2 \right\rangle_{S_{\text{eff}}[\tilde{c},\tilde{c},\tilde{f},\tilde{f}]}$. We present here, the evaluation of the second term in Eq. (64), proportional to the product $t(\mathbf{r}_1, \mathbf{r}_2)\tilde{t}(\mathbf{r}_2, \mathbf{r}_2')$ (we kept formally the lattice site notations in the hopping integrals for the $\tilde{f}$ and $\tilde{c}$-bands). Derivation of the similar term proportional to $\tilde{t}(\mathbf{r}_1, \mathbf{r}_2)'t(\mathbf{r}_2, \mathbf{r}_2')$ is very similar and we will push it out, to not complicate the manuscript. Taking the form of the action in Eq. (26), as reference for further evaluations, we have

$$
\frac{1}{2} \left\langle \mathcal{S}^2 \right\rangle_{S_{\text{eff}}[\tilde{c},\tilde{c},\tilde{f},\tilde{f}]} = 
\frac{1}{2} \sum_{(\mathbf{r}_1, \mathbf{r}_1')} \sum_{(\mathbf{r}_2, \mathbf{r}_2')} \int d\tau d\tau' \left[ t(\mathbf{r}_1, \mathbf{r}_1') \tilde{t}(\mathbf{r}_2, \mathbf{r}_2) \times
\right.
\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle \times
$$

$$
\left. \times e^{-i[\varphi(\mathbf{r}_1, \tau) - \varphi(\mathbf{r}_1', \tau)]} e^{-i[\varphi(\mathbf{r}_2, \tau') - \varphi(\mathbf{r}_2', \tau')]} + t(\mathbf{r}_1, \mathbf{r}_1') \tilde{t}(\mathbf{r}_2, \mathbf{r}_2) \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle \times
\right.
\left. \times e^{-i[\varphi(\mathbf{r}_1, \tau) - \varphi(\mathbf{r}_1', \tau)]} e^{-i[\varphi(\mathbf{r}_2, \tau') - \varphi(\mathbf{r}_2', \tau')]} + t(\mathbf{r}_1', \mathbf{r}_1) \tilde{t}(\mathbf{r}_2', \mathbf{r}_2) \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2', \tau') \tilde{f}(\mathbf{r}_2, \tau') \rangle \times
\right.
\left. \times e^{i[\varphi(\mathbf{r}_1, \tau) - \varphi(\mathbf{r}_1', \tau)]} e^{-i[\varphi(\mathbf{r}_2, \tau') - \varphi(\mathbf{r}_2', \tau')]} \right].
$$

Dialing with the path integral formalism, we have the imaginary-time dependent fermionic variables. Thus, we use the many-body Wick averaging root for that case. For example, the fermionic average of type $\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle$ is transforming then into a sum of products of two-particle-like Green functions. Next, the thersms of the type $\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \rangle$ will vanish due to the symmetry of the fermionic action in Eq. (26). Contributions, proportional to the average $\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \rangle$ will be negleted, since they are not contributing to the excitonic correlations.

Hence

$$
\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle = 
= \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \rangle \langle \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle 
- \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2, \tau') \rangle \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2', \tau') \rangle 
+ \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2', \tau') \rangle \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \rangle 
= G_{\tilde{c}\tilde{c}}(\mathbf{r}_1 - \mathbf{r}_1', 0) G_{\tilde{f}\tilde{f}}(\mathbf{r}_2 - \mathbf{r}_2, 0) 
- F_{\tilde{c}\tilde{f}}(\mathbf{r}_1 - \mathbf{r}_2, \tau - \tau') F_{\tilde{f}\tilde{c}}(\mathbf{r}_2 - \mathbf{r}_1', \tau' - \tau). \quad (66)
$$

The calculation of other terms is also straightforward

$$
\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle = 
= \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \rangle \langle \tilde{f}(\mathbf{r}_2, \tau') \tilde{f}(\mathbf{r}_2', \tau') \rangle 
- \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2, \tau') \rangle \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2', \tau') \rangle 
+ \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2', \tau') \rangle \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \rangle 
= G_{\tilde{c}\tilde{c}}(\mathbf{r}_1' - \mathbf{r}_1, 0) G_{\tilde{f}\tilde{f}}(\mathbf{r}_2' - \mathbf{r}_2', 0) 
- F_{\tilde{c}\tilde{f}}(\mathbf{r}_1' - \mathbf{r}_2', \tau - \tau') F_{\tilde{f}\tilde{c}}(\mathbf{r}_2' - \mathbf{r}_1', \tau' - \tau). \quad (67)
$$

and

$$
\langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2', \tau') \tilde{f}(\mathbf{r}_2, \tau') \rangle = 
= \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{c}(\mathbf{r}_1', \tau) \rangle \langle \tilde{f}(\mathbf{r}_2', \tau') \tilde{f}(\mathbf{r}_2, \tau') \rangle 
- \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2', \tau') \rangle \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2, \tau') \rangle 
+ \langle \tilde{c}(\mathbf{r}_1', \tau) \tilde{f}(\mathbf{r}_2, \tau') \rangle \langle \tilde{c}(\mathbf{r}_1, \tau) \tilde{f}(\mathbf{r}_2', \tau') \rangle 
= G_{\tilde{c}\tilde{c}}(\mathbf{r}_1' - \mathbf{r}_1, 0) G_{\tilde{f}\tilde{f}}(\mathbf{r}_2' - \mathbf{r}_2, 0) 
- F_{\tilde{c}\tilde{f}}(\mathbf{r}_1' - \mathbf{r}_2, \tau - \tau') F_{\tilde{f}\tilde{c}}(\mathbf{r}_2' - \mathbf{r}_1, \tau' - \tau). \quad (68)
$$

After calculating all averages in Eqs. (66)-(69), we recombine them with similar terms from the component proportional to $\tilde{t}(\mathbf{r}_1, \mathbf{r}_1')t(\mathbf{r}_2, \mathbf{r}_2')$, hence, we obtain the relevant portion of the effective excitonic phase action $S_{\text{exc}}[\varphi]$ in the form
Here, the summations run over all sites of 3D lattice space. The second term in Eq. (70) gives the constant contribution to the phase action and we neglect it for the first treatment. Furthermore, in order to simplify the non-local (in time variables) effective phase action in Eq. (70) we resort on the gradient expansion for the phase field in the form

\[
\phi(r, t') = \phi(r, t) + (t' - t) \partial_t \phi(r, t) + O \left( (t' - t)^2 \right). \tag{71}
\]

The variation of the product of the anomalous Green functions \( \tilde{F}(t' - t') \tilde{F}(t' - t) \) in Eq. (70) with the time difference \( |t - t'| \) in the first term of the action in Eq. (70) is much faster than in the arguments of the trigonometric functions multiplied to it. For this reason we will put \( t' = t \) in all arguments of the trigonometric functions corresponding to the zero order term in the Taylor series expansion of the phase variables in Eq. (71). At this stage, we define the non-local excitonic phase coupling parameter \( J_{\text{ex}} \) as usual

\[
J_{\text{ex}} = -4t \int_0^\beta d\tau' F_{\text{ex}}(r, r', t - t') F_{\text{ex}}(r, r', t - t'). \tag{72}
\]

For the product of the anomalous propagators in Eq. (72) we have

\[
F_{\text{ex}}(t' - t') F_{\text{ex}}(t' - t) = \frac{4\Delta^2 U^2}{2z(\beta N)^2} \sum_{k,v_n} \sum_{k',v_{n'}} \frac{\epsilon(k)\epsilon(k') e^{-\nu_{n'} - \nu_n}}{E_{k}(v_n)E_{k'}(v_{n'}) - |\Delta|^2} \left[ E_{k}(v_n)E_{k'}(v_{n'}) - |\Delta|^2 \right]. \tag{73}
\]

After the integration over imaginary time \( t' \) in Eq. (73), we perform Matsubara frequency summation in Eq. (74) and we obtain the excitonic phase coupling parameter \( J_{\text{ex}} \) in the form

\[
J_{\text{ex}} = \frac{16\Delta^2 t}{zN^2} \sum_{k,k'} \frac{\epsilon(k)\epsilon(k')}{\sqrt{\xi_k^2 + 4\Delta^2}} \left[ \Lambda_1(k,k') \tanh \left( \frac{\beta E^+_k}{2} \right) - \Lambda_2(k,k') \tanh \left( \frac{\beta E^-_k}{2} \right) \right]. \tag{75}
\]

The parameters \( \Lambda_1(k,k') \) and \( \Lambda_2(k,k') \) in Eq. (75) are given by

\[
\Lambda_1(k,k') = \frac{1}{E^+_k - E^-_{k'}} \cdot \frac{1}{E^+_k - E^-_{k'}}, \tag{76}
\]

\[
\Lambda_2(k,k') = \frac{1}{E^-_{k'} - E^-_k} \cdot \frac{1}{E^-_{k'} - E^-_k}. \tag{77}
\]
In numerical evaluation of the phase coupling parameter $J_{\text{ex}}$, given in Eq. (75), it is pivotal to transform the $k$-summations into energy integrals, introducing tight-binding density of states for the simple cubic lattice (see right panel 6 in Fig. 7). The reason of it is encoded in the expression of denominators in Eqs. (76) and (77). In fact, the energy parameters $E^+_k$ and $E^+_k$ (and $E^-_k$, $E^-_k$) in denominators in Eqs. (76) and (77), are very close when $k$ vary continuously, thus leading to a very strong divergent character of the parameters $\Lambda_i(k,k')$ ($i = 1, 2$). The use of density of states and subsequent integration lead to the smoothing of those singularities, assuring the effective finite solution of the excitonic phase coupling parameter $J_{\text{ex}}$. As we see, Eq. (75) relates phase coupling parameter $J_{\text{ex}}$ with the local pairing order parameter $\Delta$. Thereby, the exciton pair formation (not the condensation) is a necessary prerequisite for the appearance of phase coupling between the n.n. excitonic pairs. For low-temperatures, the macroscopic phase coherence of preformed excitonic pairs is leading to the excitonic BEC in the system. The numerical evaluations of $J_{\text{ex}}$ in Eq. (75) for $T = 0$ K are shown in the left panel in Figs. 8 and 9.

At the end of this Section we would like to emphasize on the form of the phase coupling parameter $J_{\text{ex}}$. Especially, it follows from Eq. (75) that the macroscopic phase coherence in the system is characterized by an energy scale $J_{\text{ex}} \sim (\Delta t_e t_h)/(t_c + t_h)$ for all values of the Coulomb interaction parameter $U$, which is related to the motion of the center of mass of e-h composed particle, because $(t_e t_h)/(t_c + t_h) \approx (m_e + m_h)^{-1}$. For the strong interaction limit we are converging with the hard core Boson model with the kinetic energy proportional to $\Delta t_e t_h/U$ ($\Delta$ being the local excitonic order parameter). Thereby, we have shown that NLCC between the electrons and holes of different n.n. excitonic pairs, are relevant for the excitonic condensation.

C. Condensate transition amplitude

1. Excitonic correlation function

As discussed in Ref. [60], the luminescence line-shapes in the excitonic system can be analyzed in terms of spectral density function $A_{\text{cf}}(k,\omega)$ of the interacting excitonic gas, which also determines the excitonic center-of-mass distribution related to the condensation in the low-temperature limit. Within our theoretical approach we can access a variety of correlation functions for the system. We concentrate now on the excitonic propagator in terms of the initial fermionic variables $c$ and $f$ defined in general as

$$G_{\text{cf}}(r, r'; \tau) = \langle \bar{c}(r) f(r') \rangle.$$  \hspace{1cm} (78)

After introducing the $U(1)$ transformations defined in Eqs. (24) and (25), we will have the decomposition of

![FIG. 8: (Color online) Left panel in the figure: non-local excitonic phase coherence parameter $J_{\text{ex}}$ as a function of Coulomb interaction $U$. Right panel in the figure: exciton BEC transition critical temperature as a function of the Coulomb interaction $U$. The numerical calculations are done for $\tilde{t} = -0.1$.](image)

![FIG. 9: (Color online) Left panel in the figure: non-local excitonic phase coherence parameter $J_{\text{ex}}$ as a function of Coulomb interaction $U$. Right panel in the figure: exciton BEC transition critical temperature as a function of the Coulomb interaction $U$. The numerical calculations are done for $\tilde{t} = -0.3$.](image)
Green function

\[ F_{\text{cl}}(r, r') = F_{\text{cl}}(r, r')G_z(r, r'), \] (79)

where we introduced the fermionic \( G_{\text{cl}}(r, r') \) and bosonic phase-phase propagator \( G_z(r, r') \), defined as follows

\[ F_{\text{cl}}(r, r') = \langle \hat{\chi}(r) \hat{\bar{\chi}}(r') \rangle, \]
\[ G_z(r, r') = \langle e^{-i[\varphi(r) - \varphi(r')]} \rangle. \] (80)

Then we pass to the Fourier space representation for the Green functions

\[ F_{\text{cl}}(k, \nu_n) = \frac{1}{\beta N} \sum_{k, \nu_n} F^{\text{cl}}(k, \nu_n) e^{i[k(r-r') - \nu_n(\tau-\tau')]}, \] (81)

\[ G_z(k, \omega_n) = \frac{1}{\beta N} \sum_{k, \omega_n} G_z(k, \omega_n) e^{i[k(r-r') - \omega_n(\tau-\tau')]} \] (82)

Furthermore, the Fourier transformation of the function in Eq. (80) will be written as a convolution in the reciprocal space

\[ F_{\text{cl}}(k, \nu_n) = \frac{1}{\beta N} \sum_{q, \omega_n} G_z(q, \omega_n) F_{\text{cl}}(k - q, \nu_n - \omega_n). \] (83)

Next, we introduce the unitary bosonic complex variables \( z(r) = e^{i\varphi(r)} \) and the phase-phase propagator \( G_z(r, r') \) will be rewritten as

\[ G_z(r, r') = \langle z(r) \tilde{z}(r') \rangle. \] (84)

Furthermore, the variables \( z(r) \) play the role of the phase-flux attached to the fermions (see discussion in Section I and Section III, see also the pictures in Fig. 2a and 2b).

In general case, the local expression of the phase-phase correlation function in Eq. (84) is equal to unity, but at very low temperatures, especially at \( T = 0 \) this low breaks down, because we consider the symmetry breaking related to the Bosonic sector, thus, critically, we have the fluctuation form \( z(r) = \langle e^{i\varphi(r)} \rangle + \tilde{z}(r) \) and the unimodularity constraint is broken. In the very low temperature limit, considering the BEC of excitons, we have the spontaneous breaking of local U(1) gauge-symmetry related to the phase field, leading to the non-vanishing expectation value of \( z(r) \). In order to demonstrate this, we separate the single particle state \( k = 0 \) by using Bogoliubov displacement operation (see for details in Refs. [39, 83]). Then, we write for the complex variables \( z(k, \omega_n) \)

\[ z(k, \omega_n) = \beta N \psi_0 \delta_{k, 0} \delta_{\omega_n, 0} + \tilde{z}(k, \omega_n)(1 - \delta_{k, 0}) \times (1 - \delta_{\omega_n, 0}), \] (85)

where \( \psi_0 \) is the condensate transition amplitude \( \langle z(k, \omega_n) \rangle \) of the bosonic field. Next \( \tilde{z}(k, \omega_n) \) is the non-condensate part of effective Bose-field. The Fourier transformation of the phase-phase propagator \( G_z(k, \omega_n) \) in Eq. (82) is

\[ G_z(k, \omega_n) = \frac{1}{\beta N} \sum_{k, \omega_n} \langle z(k, \omega_n) \tilde{z}(k, \omega_n) \rangle e^{-i[kd - \omega_n \delta]} \] (86)

We consider the expectation value \( \langle z(k, \omega_n) \tilde{z}(k, \omega_n) \rangle \) in the local limit, i.e. when \( d = r' - r = 0 \) and \( \delta = \tau' - \tau = 0 \) and we should draw the condensate part by applying the transformation in Eq. (85). Hence, we have

\[ G_z(k, \omega_n) = \frac{1}{\beta N} \sum_{k, \omega_n} \langle z(k, \omega_n) \tilde{z}(k, \omega_n) \rangle \]
\[ = \beta N |\psi_0|^2 \delta_{k, 0} \delta_{\omega_n, 0} + \tilde{G}_z(k, \omega_n). \] (87)

Thereby, Eq. (87) defines the coherent macroscopic state for the excitonic system and the excitonic BEC is expected in the next. Furthermore, we separate the condensate mode \( \{q = 0, \omega_n = 0\} \) in Eq. (83). We have

\[ F_{\text{cl}}(k, \nu_n) = |\psi_0|^2 F_{\text{cl}}(k, \nu_n) + \]
\[ + \frac{1}{\beta N} \sum_{q \neq 0} \tilde{G}_z(q, \omega_n) F_{\text{cl}}(k - q, \nu_n - \omega_n). \] (88)

As we see, the excitonic propagator composes of two parts, one, responsible for the excitonic condensate and the other, non-condensate excitation part. Note also that first term in Eq. (88) is a product of condensate transition probability \( |\psi_0|^2 \) with the fermionic propagator \( F_{\text{cl}}(k, \nu_n) \).

2. Quantum spherical model, \( T \sim T_c \)

In the Section VI A above, we derived the effective phase-only action \( S_{\text{eff}}[\varphi] = S_0[\varphi] + S_{\text{loc}}[\varphi] \). In the following, we cast the \( S_{\text{eff}}[\varphi] \) into quantum rotor representation \( \tilde{S} \) which enables the study of the spontaneous U(1) symmetry breaking resulting in global phase coherent state among electron-hole pairs. We introduce the new variables \( z(r) \) (see the Section V.A. into the partition function in Eq. (84)) using the following identity

\[ \int [DzD\bar{z}] \delta \left( \sum_r |z(r)|^2 - N \right) \times \]
\[ \times \delta \left( z - e^{i\varphi(r)} \right) \delta \left( \bar{z} - e^{-i\varphi(r)} \right) = 1. \] (89)

The inherent unimodular constraint on the complex variables \( z(r) \) (\( |z(r)|^2 = 1 \)) implies that on average the following condition holds

\[ \frac{1}{N} \sum_r |z(r)|^2 = 1 \] (90)
which forms a spherical constraint on a set of unimodular variables $z(\mathbf{r})$ which can be resolved by introducing the Lagrange multiplier $\lambda$ resulting from the Laplace transform of the functional delta representation

$$
\delta \left( \sum_r |z(\mathbf{r})|^2 - N \right) = \int_{-\infty}^{+\infty} \left[ \frac{DL\lambda}{2\pi i} \right] \times e^{-i\int_0^\beta d\tau \sum_r \lambda (|z(\mathbf{r})|^2 - 1)}.
$$

(91)

This adds a quadratic term in the $z$-field to the phase action $S_{\text{eff}}[\varphi]$. Next, we rewrite the action in Eq. (91) in a more convenient form, using the trigonometric half-angle transformation rule

$$
\cos 2(\varphi(\mathbf{r}) - \varphi(\mathbf{r}')) = 2 \cos^2(\varphi(\mathbf{r}) - \varphi(\mathbf{r}')) - 1.
$$

(92)

Then, in terms of the complex variables $z(\mathbf{r})$, the transformation in Eq. (92) leads to a biquadratic form of the phase action in Eq. (91). We have

$$
S_{\text{ex}}[\varphi] = S_{\text{ex}}[\bar{z}, \bar{z}]
$$

$$
= -\frac{J_{\text{ex}}}{2} \int_0^\beta d\tau \sum_{(r,r')} \left[ \bar{z}(\mathbf{r})z(\mathbf{r'}) + c.c. \right]^2.
$$

(93)

Furthermore, the fourth-order bosonic action in Eq. (93) could be decoupled with the help of boson-Hubbard-Stratonovich transformation by introducing the complex variables $w(\mathbf{r}, \mathbf{r'})$ at each site of the 3D cubic lattice

$$
e^{-\frac{J_{\text{ex}}}{2} \int_0^\beta d\tau \sum_{(r,r')} \left[ \bar{w}(\mathbf{r})w(\mathbf{r'}) + c.c. \right]^2} = \int [Dw] e^{-\frac{J_{\text{ex}}}{2} \int_0^\beta d\tau \sum_{(r,r')} \left[ \bar{w}(\mathbf{r})w(\mathbf{r'}) + c.c. \right]^2} \times e^{\int_0^\beta d\tau \sum_{(r,r')} w(\mathbf{r}, \mathbf{r'}) \bar{w}(\mathbf{r})z(\mathbf{r'}) + c.c.}.
$$

(94)

The integral in Eq. (94) over the $w(\mathbf{r}, \mathbf{r'})$ field could be calculated using saddle-point method, which amounts by replacing $w(\mathbf{r}, \mathbf{r'})$ variables by their saddle-point value

$$
w_0 = J_{\text{ex}} \left( \langle \bar{z}(\mathbf{r})z(\mathbf{r'}) + c.c. \rangle \right) \equiv 2J_{\text{ex}} g,
$$

(95)

where we used the expression of bandwidth renormalization factor $g$ given in the Eq. (95). Substituting the value of $w_0$ back into the Eq. (94), we obtain a part of the effective phase action $S_{\text{ex}}[\bar{z}, \bar{z}]$ in the form

$$
S_{\text{ex}}[\bar{z}, \bar{z}] = -4gJ_{\text{ex}} \int_0^\beta d\tau \sum_{(r,r')} \bar{z}(\mathbf{r})z(\mathbf{r'}). \langle
$$

(96)

Finally, after the integration out the phase variables, in the partition function, we get

$$
Z = Z_0 \int [D\lambda] \int [D\bar{z}] e^{-S_{\lambda}[\bar{z}, \bar{z}]},
$$

(97)

where $Z_0$ is the statistical sum of a set of non-interacting quantum rotors

$$
Z_0 = \int [D\varphi] e^{-S_0[\varphi]},
$$

(98)

while the action $S_{\lambda}[\bar{z}, \bar{z}]$ is

$$
S_{\lambda}[\bar{z}, \bar{z}] = \frac{1}{\beta N} \sum_{\mathbf{k}, \omega_n} \bar{z}(\mathbf{k}, \omega_n)G_z^{-1}(\mathbf{k}, \omega_n)z(\mathbf{k}, \omega_n) - \lambda,
$$

(99)

where $G_z^{-1}(\mathbf{k}, \omega_n)$, is the inverse of the bosonic Green function calculated for our QSM

$$
G_z^{-1}(\mathbf{k}, \omega_n) = \lambda - 8gJ_{\text{ex}} \langle \psi(\mathbf{k}) \rangle + \gamma^{-1}(\omega_n).
$$

(100)

$\omega_n$ in Eq. (100) are Bose-Matsubara frequencies, $\omega_n = \frac{2\pi n}{\beta}$ with $(n = 0, \pm 1, \pm 2, ...)$, given by the Fourier transformation of bosonic variables $z(\mathbf{r}) = \frac{1}{\beta N} \sum_{\mathbf{k}, \omega_n} z(\mathbf{k}, \omega_n) e^{i(\mathbf{k} - \omega_n) \mathbf{r}}$. Furthermore, $\gamma^{-1}(\omega_n)$ is the inverse of the Fourier transformation of two-point phase correlation function

$$
\gamma(\mathbf{r}, \mathbf{r'}) = \frac{1}{Z_0} \int [D\varphi] e^{-S_0[\varphi]} e^{i[\varphi(\mathbf{r}) - \varphi(\mathbf{r'})]}, \langle
$$

(101)

The calculation of the Fourier transformation of the correlation function in Eq. (101) is straightforward

$$
\gamma(\omega_n) = \frac{8}{UZ_0} \sum_{m=-\infty}^{+\infty} \frac{e^{-\frac{U\beta}{2}(m - \frac{\omega_n}{\beta})^2}}{1 - 16 \left( \frac{\omega_n}{\beta} - \frac{1}{2} \left( m - \frac{2\omega_n}{\beta} \right) \right)^2},
$$

(102)

where $Z_0$ is the partition function of the non-interacting Bose sector

$$
Z_0 = \sum_{m=-\infty}^{+\infty} e^{-\frac{U\beta}{2}(m - \frac{\omega_n}{\beta})^2}.
$$

(103)

The summations in Eqs. (102) and (103) run over topological winding numbers $m$ of the group $U(1)$ (see also the Section III).

**D. Exciton BEC, $T \lesssim T_c$**

In the thermodynamic limit $N \to \infty$ the integration over $\lambda$-field in Eq. (97) can be performed exactly using the saddle-point method by introducing the complex variables $\bar{z}(\mathbf{r})$ to the phase action $S_{\text{ex}}[\bar{z}, \bar{z}]$ in the form of our QSM

$$
1 = \frac{1}{(\beta N)^2} \sum_{\mathbf{k}, \omega_n} \langle z(\mathbf{k}, \omega_n) \bar{z}(\mathbf{k}, \omega_n) \rangle \equiv \frac{1}{\beta N} \sum_{\mathbf{k}, \omega_n} G_z(\mathbf{k}, \omega_n),
$$

(104)
where the average is defined with the help of the QSM action in Eq. (98) given at the saddle-point value of λ = λ0

\[ (...) = \frac{\int [D\bar{n}Dz] e^{-S_{\bar{n}}[\bar{n},z]} }{\int [D\bar{n}Dz] e^{-S_{\bar{n}}[\bar{n},z]} }. \] (105)

Next, substituting \( G_z(k,\omega_n) \) from Eq. (87) into the expression of Eq. (104) we get after some algebra

\[ 1 - |\psi_0|^2 = \frac{1}{\beta N} \sum_{k\neq 0,\omega_n\neq 0} G_z(k,\omega_n), \] (106)

which is the equation for the critical BEC temperature derived from QSM. At the critical temperature, where \( \psi_0 = 0 \), the uniform static order parameter susceptibility diverges (see the Thouless criterion, discussed in the Section II in Ref. 25), thus \( G_z^{-1}(k = 0,\omega_n = 0) = 0 \) from which we can derive the critical value of the Lagrange multiplier \( \lambda_c^0 \)

\[ \lambda_c^0 - 8gJ_{ex}c(0) + \gamma^{-1}(\omega_n = 0) = 0. \] (107)

Furthermore, we find

\[ \lambda_0 = -\frac{U}{8} + 24gJ_{ex} + \frac{2\mu^2}{U}. \] (108)

Then, Eq. (106) takes the form

\[ 1 - |\psi_0|^2 = \frac{1}{\beta N} \sum_{k\neq 0,\omega_n\neq 0} \lambda_0^0 - 8gJ_{ex}c(k) + \gamma^{-1}(\omega_n). \] (109)

The solution for the BEC transition amplitude \( \psi_0 \) is given in Fig. 10.

Furthermore, after the Bose-Matsubara frequency summations in Eq. (109), and considering the case when \( T \sim T_c \), we obtain the following equation for the excitonic BEC critical temperature

\[ \frac{U}{4N} \sum_k \frac{n[\kappa_1(k)] - n[\kappa_2(k)]}{\sqrt{\mu^2 + 4gUJ_{ex}[\epsilon(0) - \epsilon(k)]}} = 1, \] (110)

where \( n[\epsilon] \) is the Bose-Einstein distribution function \( n[\epsilon] = 1/(e^{\beta \epsilon} - 1) \) and the variables \( \kappa_{1k} \) and \( \kappa_{2k} \) are given by

\[ \kappa_{1,2}(k) = -\mu \pm \sqrt{\mu^2 + 4gUJ_{ex}[\epsilon(0) - \epsilon(k)]}, \] (111)

The solution of equation Eq. (110) gives the critical temperature \( T_c(U, J_f, g, J_{ex}) \) of transition to the phase coherent excitonic condensate state (see the right panels in Fig. 9 and Fig. 10). We see also, that at the fundamental state with \( \k = 0 \) there is a residual gap \( \Delta W = \kappa_1(0) - \kappa_2(0) = -2\mu \) related to the condensate, which equals the binding energy of a molecule in the BEC limit \( E_{bind} \approx (2\mu) \) [64-66]

**E. Excitonic density of states**

Now, we are ready to calculate the analytical form of the excitonic spectral function \( A_{clos}(k, \omega) \) and, later on, the profiles of the excitonic density of states (DOS) for the condensate and the non-condensate states in the system. We introduce here the excitonic spectral function \( A_{clos}(k, \nu_n) \) that carries the same physical information as the correlation function \( F_{clos}(k, \nu_n) \) itself. We have

\[ F_{clos}(k, \nu_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega A_{clos}(k, \omega) \frac{\nu_n - \omega}{\nu_n - \omega}. \] (112)

The integration here, is over continuous frequencies \( \omega \). In the same way we can introduce the spectral functions \( A_{clos}(k, \omega) \) and \( A_{clos}(k, \omega) \) associated to the bosonic and the pure fermionic parts and corresponding respectively to the correlation functions \( G_z(k, \omega_n) \) and \( F_{clos}(k, \nu_n) \)

\[ G_z(k, \omega_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega A_z(k, \omega) \frac{\omega_n - \omega}{\nu_n - \omega}. \] (113)

and

\[ F_{clos}(k, \nu_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega A_{clos}(k, \omega) \frac{\omega_n - \omega}{\nu_n - \omega}. \] (114)

Furthermore, using Eq. (68), we can write for the total excitonic spectral function \( A_{clos}(k, \omega) \)

\[ A_{clos}(k, \omega) = |\psi_0|^2 A_{clos}(k, \omega) + \frac{1}{N} \sum_{q \neq 0} \int d\omega A_z(q, \omega) \times A_{clos}(k - q, \omega - \omega') |n(-\omega') + f(\omega - \omega')|. \] (115)
From the spectral functions we can obtain excitonic DOS by summing over the reciprocal wave vectors $k$ with appropriate normalization factor, hence, the total excitonic density of states is $\rho_{ct}(\omega) = -\frac{1}{\pi} \sum_k A_{ct}(k, \omega)$.

Hence, using the expression for $A_{ct}(k, \omega)$ in Eq. (115), we get

$$\rho_{ct}(\omega) = |\psi_0|^2 \rho_{\tilde{c} \bar{f}}(\omega) + \tilde{\rho}_{ct}(\omega), \quad (116)$$

where $\tilde{\rho}_{ct}(\omega)$ is the density of states corresponding to the non-condensate part of the system and is given as a convolution in terms of continuous frequency modes

$$\tilde{\rho}_{ct}(\omega) = \int_{-\infty}^{+\infty} d\omega' \rho_c(\omega') \rho_{\tilde{f}}(\omega - \omega') \times [n(-\omega') + f(\omega - \omega')]. \quad (117)$$

A key feature of the result in Eq. (116), is that we have separated DOS contribution from the condensate.

Then, we calculate explicitly, the density of states related to the bosonic and fermionic parts in Eq. (116), i.e. $\rho_z(\omega)$ and $\rho_{\tilde{c}}(\omega)$. Density of states are related to the imaginary parts of the corresponding retarded Green functions which can be evaluated as the analytical continued functions, i.e.

$$\rho_z(\omega) = -\frac{1}{\pi} \sum_{\mathbf{k}} \Im G_{z}^R(\mathbf{k}, \omega) =$$

$$= -\frac{1}{\pi} \sum_{\mathbf{k}} \Im G_z(\mathbf{k}, \omega_n) |_{\omega_n \rightarrow \omega + i\eta},$$

$$\rho_{\tilde{c}}(\omega) = -\frac{1}{\pi} \sum_{\mathbf{k}} \Im F_{\tilde{c}}^R(\mathbf{k}, \omega) =$$

$$= -\frac{1}{\pi} \sum_{\mathbf{k}} \Im F_{\tilde{c}}(\mathbf{k}, \omega_n) |_{\omega_n \rightarrow \omega + i\eta} \quad (118)$$

and the functions $\chi_{i} [\Lambda_{i}(\omega)]$ in the denominators of the right-hand side in Eq. (120) are given by

$$\Lambda_1(\omega) = \sqrt{\left[\left(t + \bar{t}\right)\omega - \varepsilon_{i\bar{f}} + \varepsilon_{j\bar{f}}\right]^2 + 4\bar{t} t |\Delta|^2}, \quad (121)$$

$$\Lambda_2(\omega) = \sqrt{\left[\left(t + \bar{t}\right)\omega - \varepsilon_{i\bar{f}} + \varepsilon_{j\bar{f}}\right]^2 + 4\bar{t} t |\Delta|^2}, \quad (122)$$

Then, we use the Cauchy relation $\lim_{\omega \rightarrow 0} \frac{1}{\omega \mp \mu} = P(1/\omega) \pm i\pi \delta(\omega)$, where the symbol $P$ denotes the Cauchy principal value. We obtain

$$\rho_z(\omega) = \frac{U}{4} \int_{-\infty}^{+\infty} dx \rho_{\square}(x) \left[ \frac{\delta (\omega - \kappa_{1}(x))}{\sqrt{\mu^2 + 4gUJ_{ex} (3 - x)}} + \frac{\delta (\omega - \kappa_{2}(x))}{\sqrt{\mu^2 + 4gUJ_{ex} (3 - x)}} \right], \quad (119)$$

where $\kappa_i(x)$ $i = 1, 2$ are continuous versions of functions given in Eq. (114), i.e. $\kappa_{1,2}(x) = -\mu + \sqrt{\mu^2 + 4gUJ_{ex} (3 - x)}$

$$\rho_{\tilde{c}}(\omega) = -\Delta \left\{\frac{\rho_{\square}[A_{1}(\omega)]}{|\chi_{1}[A_{1}(\omega)]|} + \frac{\rho_{\square}[A_{2}(\omega)]}{|\chi_{2}[A_{2}(\omega)]|}\right\}, \quad (120)$$

where the functions $\chi_{i} [\Lambda_{i}(\omega)]$ in the denominators of the right-hand side in Eq. (120) are given by

$$\chi_{1} [\Lambda_{1}(\omega)] = 2 \left( t + \bar{t} \right) \omega + 8\bar{t} t \Lambda_{1}(\omega) - 2 \left( \varepsilon_{i\bar{f}} + \varepsilon_{j\bar{f}} \right), \quad (123)$$

$$\chi_{2} [\Lambda_{2}(\omega)] = 2 \left( t + \bar{t} \right) \omega + 8\bar{t} t \Lambda_{2}(\omega) - 2 \left( \varepsilon_{i\bar{f}} + \varepsilon_{j\bar{f}} \right). \quad (124)$$
Next, we put the expressions in Eqs. (119) and (120) into the formula of the excitonic density of states given in Eq. (116) and we have

$$
\rho_{ci} = -U \Delta \cdot \int_{-\infty}^{\infty} dx \rho_{x} (x) \rho_{\bar{x}} \left[ A_{1} (\omega - \kappa_{1} (x)) \right]
$$

$$
-U \Delta \cdot \int_{-\infty}^{\infty} dx \rho_{x} (x) \rho_{\bar{x}} \left[ A_{2} (\omega - \kappa_{2} (x)) \right]
$$

$$
-U \Delta \cdot \int_{-\infty}^{\infty} dx \rho_{x} (x) \rho_{\bar{x}} \left[ A_{2} (\omega - \kappa_{2} (x)) \right]
$$

$$
-U \Delta \cdot \int_{-\infty}^{\infty} dx \rho_{x} (x) \rho_{\bar{x}} \left[ A_{2} (\omega - \kappa_{2} (x)) \right]
$$

The numerical evaluations of the density of states at $T = 0$ are given in Figs. 11, 12, and 13. Particularly, in Fig. 11, we have presented purely the fermionic density of states $\rho_{\bar{x}} (\omega)$ and we examine it over the entire BCS-BEC crossover region (i.e. for different values of the Coulomb interaction strength $U$). We see, that at the very small interaction limit, when $1 \leq U \leq 2$ (the BCS limit) DOS exhibits a BCS-like double-peak structure (see the left panel 1 and left panel 2 in Figs. 11) with a well defined pseudogap at zero frequency $\omega = 0$. For higher values of $U$ this structure is smoothing (see the left panel 3, left panel 4 in Fig. 11) and the pseudogap is gradually decreasing signaling the appearance of the BEC limit of the transition. In the BEC limit, when $U \geq 8$, the double-peak structure disappears totally with the pseudogap (vanishing totally at $U = 10.6$). In this region of the transition, we have DOS separation into two parts, corresponding respectively to negative-$\omega$ and positive-$\omega$ frequency regions (see the plots for $U = 9.0, 9.6, 10.6$ in Fig. 11) and, for the positive frequency region, we have sufficiently large broadening of DOS spectrum (see the region in right panels 5-8 in Fig. 11 for $0 \leq \omega \leq 12$). We observe also gradual decrease in the amplitude of DOS across the whole crossover region.

The same general behavior is observed for the non-condensate part of the DOS (the function $\rho_{\bar{x}} (\omega)$ in Figs. 12) given by Eq. (117). Moreover, we have a large separation between the DOS peaks and, for the positive frequencies, DOS becomes negative for all values of the Coulomb interaction $U$. It is remarkable also that there is no pseudogap observed in the DOS spectrum.

In Fig. 13 we have presented total excitonic DOS structure, i.e. the function $\rho_{ci} (\omega)$, given analytically by the Eq. (125). For positive frequencies, the behavior of $\rho_{ci} (\omega)$ is very similar with $\rho_{\bar{x}} (\omega)$, contrary, in the region of negative-$\omega$, a third peak appears in the DOS spectrum due to the pure fermionic part multiplied with the BEC transition probability $|\psi_{0}|^{2}$ (see in Eq. (116)). It is interesting to note that in the BCS limit at $U = 1.8$ (see the left panel 1 in Fig. 13) this peak is practically absent in the DOS spectrum of $\rho_{ci} (\omega)$. The reason of it, is the very small value of the condensate fraction (in this case the condensate fraction is totally absent, because for $0 \leq U \leq 1.8$ we have $|\psi_{0}|^{2} = 0$, see also, the curve in blue in Fig. 10).

VII. CONCLUSION

We have studied 3D system of conduction band electrons and valence band holes in the frame of the extended Falicov-Kimball model. We have implemented the path integral formalism, in which the Coulomb interaction term is expressed in terms of $U(1)$ quantum phase variables $\varphi$ conjugated to the local particle number, providing a useful interpretation of the problem. At low temperatures, the electron-hole system becomes unstable with respect to the formation of the excitons at $T = T_{EI}$, exhibits a local gap $\Delta$ in the excitation spectrum controlled by the parameter $U$, which gives the relevant energy scales for the excitonic insulator state. Furthermore, we have shown that for the large values of $U$ the excitons form the incoherent pairs uncorrelated with each other, until they undergo the excitonic BEC at lower temperature $T_{c} < T_{EI}$ controlled by the phase coupling mechanism between excitonic pairs with $J \ll U$. Here, as a result of the spontaneous symmetry breaking, an expectation value of $\langle e^{i\varphi} \rangle \neq 0$ appears, signaling of the presence of the phase coherence in the system. Therefore, pairing and condensation are not generally the same, however, in the weak coupling limit $U/t \ll 1$, the binding energy of excitonic pairs is small, thus the pair breaking controls the condensation. This is what happens in a standard BCS superconductor, where dynamics of the phase variables is unimportant. However, in the excitonic system with the strong pairing we have the situation, where the pairs are strongly bound, but can be mutually uncorrelated with each other, until they become phase coherent at $T \lesssim T_{c}$. Thereby, we have shown...
that the local excitonic order parameter is a necessary prerequisite for the macroscopic phase coherent state in the excitonic system and the last one is governed by the non-local-cross-correlations between the n.n. excitonic pairs. DOS spectrum, governed by the pure-fermionic part of the condensate, and non-condensate excitation spectrum, are determined both analytically and numerically. For the fermionic part of the DOS we found the strong evidence for the pseudogap in the excitation spectra, which is gradually decreasing with the increase of the Coulomb interaction and in accordance with general discussion in Ref. 65. The total density of states for the excitons is calculated numerically.

Although, the excitonic gap can be used to explain some experimental results (like tunneling data and resistivity measurements), $\Delta$, does not signifies the macroscopic coherence in the excitonic system. For example, the exciton phase coherence may be evidenced by coherence of their light emission, which can be studied by interferometry (see e.g., Ref. 36) and by the experiments on luminescence in the cuprous oxide excitonic system.\(^6\)

Now, it is interesting to relate the results of our calculations on the 3D excitonic system to the experimental results, e.g., for the compound TmSe\(_{0.45}\)Te\(_{0.55}\), which is an intermediate valent semiconductor\(^5\). The hopping parameter $\tilde{t}$ is estimated as $|\tilde{t}| = 0.3|t| = 5$ meV (see Ref. 28). Using these values, we find the maximum for excitonic pair transition temperature $T_\Delta^{\text{max}} = 186.6$ K at $U = 8|t|$. The maximum of the phase coherence transition temperature is found to be smaller of about two orders of magnitude at $T_c^{\text{max}} = 0.44$ K for $U = 4.8|t|$. We present also the values for the other important physical quantities: the maximum of the phase coupling parameter is of order of $J^{\text{max}} = 1.76 \times 10^{-6}$ eV at $U \simeq 5|t|$, while the charge-gap bandwidth was found to be $W = |\Delta_c^{\text{min}}| = 0.0682$ eV and the single particle excitation gap is of order $\Delta_g = 0.057$ eV at $U = 10.6|t|$. The obtained values fit into the experimental results on TmSe\(_{0.45}\)Te\(_{0.55}\), where $T_{E\text{I}}$ is found to be of order 250 K and below\(^5\). However, the fact that the excitonic gap $\Delta$ can be used to explain some experimental results, it is not the same as the macroscopic coherence in the excitonic system, as it was supposed previously\(^{26-29}\).\(^{26-29}\) In fact, the macroscopic phase coherence is not affecting the EI state and the vise versa is true.

The excitonic phase coherence may be evidenced by the coherence of their light emission, which can be studied by interferometry measurements\(^{36}\). Therefore, measurements of the intensity of the line-shape of the exciton decay (by emitting photons upon electron-hole recombination) may be a powerful probe of the DOS spectrum in the excitonic system\(^{60}\).
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FIG. 12: (Color online) Non-condensate density of states $\tilde{\rho}_{n,f}$ for $t = -0.3$ and for different values of the Coulomb interaction strength.
FIG. 13: (Color online) Total excitonic density of states for $\tilde{t} = -0.3$ and for different values of the Coulomb interaction strength.