Exciton condensation in a three-dimensional extended Falicov-Kimball model

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We study the excitonic phase transition in a system of conduction band electrons and valence band holes described by the three-dimensional extended Falicov-Kimball (EFKM) model with tunable Coulomb interaction $U$ between both species. By lowering the temperature the electron-hole system may become unstable with respect to the formation of the excitons i.e. electron-hole pairs at temperature $T = T_{\Delta}$, exhibiting a gap $\Delta$ in the particle excitation spectrum. We prove that for large values of $U$ the excitons form the incoherent pairs uncorrelated with each other until they undergo the excitonic Bose-Einstein condensation (BEC) at lower $T = T_c$ driven by the phase stiffness between the excitonic pairs. We found that the true condensate transition temperature $T_c$ appears to be much smaller than the exciton pair formation temperature $T_{\Delta}$. In this context a BEC to Bardeen-Cooper-Schrieffer (BCS) type crossover could be expected: in the strong interaction case the system is first driven into the gaped excitonic insulator (EI) state and subsequent condensation of incoherent exciton pairs at $T_c < T_{\Delta}$ driven by the phase stiffness, while in the small $U$ the temperature $T_c \sim T_{\Delta}$ implying that the excitonic condensate is governed by the pair formation as in the BCS-like regime. To this end we implement the functional integral formulation of the EFKM, where the Coulomb interaction term is expressed in terms of $U(1)$ quantum phase variables conjugate to the local particle number, providing a useful representation of strongly correlated system.

The effective action formalism allows us to formulate a problem in the phase only action in the form of the quantum rotor model and obtain analytical formula for the critical lines.

I. INTRODUCTION

The Coulomb interaction between the conduction band electrons and the valence band holes causes in some solid state materials the formation of the new bound states of these two quasiparticles called the excitons. These new formations lead to the various interesting physical phenomena in solid state materials and they are the subjects of the intensive experimental and theoretical researches. In the scenario of the semiconductor-metal phase transition a new phase develops approaching to the transition from the semiconductor side. This state is called as the “excitonic insulator” (EI) and is characterized by the strong binding between the conduction band electrons and valence band holes. For example, series of the recent experimental investigations in TmSe$_{0.45}$Te$_{0.55}$ suggested the existence of the EI state in that material. Another example of the material with a well defined EI state is the quasi-one-dimensional Ta$_2$NiSe$_5$ with highly polarizable Se. The angle-resolved photoemission spectra (ARPES) on these compounds demonstrate that the ground state therein is an excitonic insulator. The evidence in favor of the EI state is proved also in the transition metal layered compound 17-TISe$_2$ where the EI scenario is driving to the charge-density wave transition in such a material.

The importance of the phase coherence in the system of excitonic pair plasma is discussed recently where a classification of two distinct transitions of the excitonic plasma is given and discussion about the exciton condensation conditions is provided. It is well known that reducing the temperature leads to the quantum degeneracy of the exciton system and to Bose-Einstein condensation (BEC). The experimental proof of the spontaneous phase coherence in an excitonic bose gas and the possible BEC transition at the low-energy state is given recently concerning 2D GaAs/AlGaAs coupled quantum well structure. Mainly, the phase coherence is found in the region of macroscopically ordered excitonic states and also the BEC of the quasi-two-dimensional excitons at the bottom of the in-plane potential traps for the specially designed semiconductor heterostructure. In addition, the exciton temperature relaxation to that of the lattice is discussed and it is shown that for the realization of the true BEC state the critical temperature should be much lower (about six orders of magnitude) than the exciton formation temperature in the initial photo-generation.

Turning to the theory, there have been a number of works on the excitonic systems. Using the band structure calculation and the mean-field analysis for the EI state it was found that a structural phase transition driven by the BEC takes place in the layered chalcogenide material such as the recently corroborated sample of Ta$_2$NiSe$_5$. In the small interaction region the system is in the Bardeen-Cooper-Schrieffer (BCS) state with weakly bound electron-hole pairs, while approaching from the semiconductor side the system shows typical BEC behavior with tightly bound excitons thus exhibiting a BCS-BEC type crossover. This type of crossover mechanism is found in a study of the electron-hole plasma condensation in highly excited semiconductors. In another work, a BEC-BCS crossover was studied using the...
effective-mass model for valence and conduction band electrons.\textsuperscript{25} In this context, the three-dimensional extended spinless Falicov-Kimball model (EFKM) with the dispersive $f$-orbital electrons at half-filling has been analyzed recently.\textsuperscript{26,27} The spontaneous symmetry breaking for the EI state and the BCS-BEC like crossover for the two-dimensional extended Falicov-Kimball model is discussed also in Ref.\textsuperscript{28}. The spectrum of low-energy collective excitations in the EFKM is discussed recently.\textsuperscript{29} The mean field stability of the EI state observed within the EFKM model is attributed to the broken degeneracy due the presence of the finite $f$-band hopping. It is shown that the EI state is unstable when the case of the pure Falicov-Kimball model (FKM) (fully localized bands) is approached. Also the Bogoliubov-de Gennes equations were implemented using the exact diagonalization method and the Hartree-Fock type (HF) self-consistent equations for the ground state of the spinless EFKM model are derived in two and three dimensions.\textsuperscript{30} Based on the analysis of electron-hole pairing in the extended Falicov-Kimball model, the authors in Ref.\textsuperscript{31} show that tuning the Coulomb attraction between both species, a continuous BCS-BEC like crossover might be achieved. Moreover, it has been shown that the $f$-$f$ hopping mechanism could be also responsible for the exciton formation.\textsuperscript{32–34}

In the present paper we explore the quantum collective behavior of the excitons and extend the theoretical works mentioned above, by showing that the formation of the excitonic condensate is directly related to the \textit{phase stiffness} between the conduction band electrons and valence band holes. To this end we study the excitonic phase transition in a system of conduction band electrons and valence band holes described by the three-dimensional extended Falicov-Kimball\textsuperscript{35,36} model with tunable Coulomb interaction $U$ between both species. We found, in agreement with previous studies that by lowering the temperature the electron-hole system may become unstable with respect to the formation of excitons i.e. electron-hole pairs at temperature $T = T_\Delta$, exhibiting a gap $\Delta$ in the particle excitation spectrum. Moreover, we prove that for large values of $U$ the excitons form the incoherent pairs uncorrelated with each other until they undergo the excitonic Bose-Einstein condensation (BEC) at lower $T = T_c$ driven by the phase stiffness between the electrons and holes. We found that the true condensate transition temperature $T_c$ appears to be much smaller than the exciton pair formation temperature $T_\Delta$. In this context a BEC to Bardeen-Cooper-Schrieffer (BCS) type crossover could be expected: in the strong interaction case the system is first driven into the gaped excitonic insulator (EI) state and subsequent condensation of incoherent exciton pairs at $T_c < T_\Delta$ driven by the phase stiffness, while in the small $U$ the temperature $T_c \sim T_\Delta$ implying that the excitonic condensate is governed by the pair formation as in the BCS-like regime. To this end we implement the functional integral formulation of the EFKM model, where the Coulomb interaction term is expressed in terms of U(1) quantum phase variables conjugate to the local particle number, providing a useful representation of strongly correlated systems. As a result the electrons and holes emerge as composite particles involving flux tubes with the quantum phase variable dual to the particle number density. The effective action formalism allows us to formulate a problem in the phase only action in the form of the quantum rotor model and obtain analytical formula for the critical lines. Using the suitable symmetry of the EFKM Hamiltonian we employ a U(1) gauge transformation to the new fermionic and phase-bosonic variables. Then, integrating out the gauge fermions we obtain the effective phase stiffness action. Furthermore, we derive numerically the phase stiffness parameter for various values of the Coulomb interaction and we derive the phase stiffness action basing on the effective quantum rotor model to alternate the effective phase action.

The plan of the paper is as follows: in the Section II we provide the Hamiltonian of the model EFKM, then in the Section III we introduce the new decoupling potentials and we handle with the four fermion interaction term in the initial Hamiltonian. In Section IV we discuss the role of the phase stiffness for the exciton condensation. Furthermore, in the Section V we derive the excitonic gap parameter, excitonic pair formation transition temperature, excitonic coherence length and the charge transfer gap for different values of the $f$-band hopping integral. In Section VI we show how the phase stiffness parameter could be derived from the effective phase action and using the quantum rotor approach. At the end of the Section VI a self-consistent equation for the excitonic BEC critical temperature $T_c$ is derived and solved numerically. Conclusions are given in Section VII. A number of technical details is given in Appendices.

\section{II. The Hamiltonian}

We consider the Hamiltonian of the extended Falicov-Kimball model

$$
H = -i \sum_{\langle rr' \rangle} [\bar{c}(r)c(r') + h.c.] - (\mu - \epsilon_c) \sum_r n_c(r)
- i \sum_{\langle rr' \rangle} [\bar{f}(r)f(r') + h.c.] - (\mu - \epsilon_f) \sum_r n_f(r)
+ U \sum_r n_c(r)n_f(r),
$$

(1)

where $\bar{c}(r) (c(r))$ are the creation (annihilation) operators of the electron of the $c$-orbitals at the site with the position $r$ and $\langle rr' \rangle$ runs over pairs of nearest neighbor sites of the three-dimensional cubic lattice. Furthermore $t$ is the hopping integral for the $c$-electrons and $\epsilon_c$ is the on-site energy level. Similarly, $\bar{f}(r) (f(r))$ are the creation (annihilation) operators of the $f$-orbital electrons and $t$ is the hopping integral for the $f$-electrons. 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, thus replacing the fermion Hilbert space by the pseudo-fermionic one and linearizing the interaction term via the bosonic states. Furthermore, \( \epsilon_f \) is the on-site energy level of the \( f \)-orbital and \( \mu \) is the chemical potential. The equilibrium value of the chemical potential \( \mu \) will be determined from the half-filling condition, i.e., \( n_c = 1 - n_f \), where \( n_x \equiv \langle n_x(r) \rangle \) is the average particle density with \( x = c, f \) for the \( c \) and \( f \)-orbital electrons respectively. Furthermore, we suppose that the chemical potentials of both orbitals are the same as in the work in Ref. 28. Parameter \( U \), entering in the last term of the Hamiltonian, is the Coulomb repulsion between two types of electrons. Furthermore \( n_c(r) \) and \( n_f(r) \) are the \( c \)- and \( f \)-electron density operators and they are defined as usual by the relation \( n_x(r) = \bar{x}(r)x(r) \).

We consider also the following values for the band parameters \( \epsilon_c = 0 \) and \( \epsilon_f = -1 \). With this consideration the \( c \)-electrons are itinerant and the \( f \)-electrons are quasilocalized on the atomic sites. Throughout the paper, we set \( k_B = 1 \) and \( \hbar = 1 \).

### III. THE METHOD

In the first step, we transform the fermionic interaction term in the Hamiltonian by rewriting the density product in the last term in Eq. (1) in the equivalent form

\[
n_c(r)n_f(r) = \frac{n^2(r)}{4} - \frac{\bar{n}^2(r)}{4},
\]

where we introduced the short-hand notations

\[
n(r) = n_c(r) + n_f(r), \quad \bar{n}(r) = n_c(r) - n_f(r).
\]

With the new notations we can rewrite the Hamiltonian Eq. (1) of the system as

\[
H = -i \sum_{(rr')} [\bar{c}(r)c(r') + h.c.] - \bar{\mu} \sum_r n(r) - i \sum_{(rr')} [\bar{f}(r)f(r') + h.c.] + \frac{\epsilon_c - \epsilon_f}{2} \sum_r \bar{n}(r) + U \sum_r \frac{1}{4} \left[ n^2(r) - \bar{n}^2(r) \right].
\]

We put here \( \bar{\mu} = \mu - \bar{\epsilon} \) and \( \bar{\epsilon} = (\epsilon_c + \epsilon_f)/2 \) is the average energy level parameter. The Hamiltonian in Eq. (10) is now suitable for decoupling the quadratic density terms using the Gaussian path integral method.

#### A. Functional integral formalism: decoupling of interactions

Dealing with fermions within the path integral method requires introduction of the Grassmann variables \( c(r\tau) \) and \( f(r\tau) \) at each site \( r \) and imaginary time \( \tau \) varying in the interval \( 0 \leq \tau \leq \beta \), where \( \beta = 1/k_B T \) (with \( T \) being the thermodynamic temperature). The variables \( c(r\tau) \) and \( f(r\tau) \) satisfy the anti-periodic boundary conditions \( x(r\tau) = -x(r\tau + \beta) \). The partition function of the system of fermions written as a functional integral over the Grassmann field is

\[
Z = \int [DcD\bar{c}] \int [DfD\bar{f}] \ e^{-S[\bar{c},c,f,f]},
\]

where the action in the exponential is given in the path integral formulation as

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

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

\[
S_B[\bar{x},x] = \sum_r \int_0^\beta d\tau \bar{x}(r\tau) \frac{\partial}{\partial \tau} x(r\tau).
\]

Next, we decouple the quadratic density terms in Eq. (10) using the Hubbard-Stratonovich transformation by introducing the new variables \( V(r\tau) \) and \( \phi(r\tau) \) conjugated to the density terms \( n(r\tau) \) and \( \bar{n}(r\tau) \) respectively. For the quadratic term proportional to \( n^2(r\tau) \) in the exponential of the partition function in Eq. (11) we have

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

After combining the exponential in Eq. (11) with the effective \( \bar{\mu} \) chemical potential term proportional to the total electron density \( n(r) \) in Eq. (15), we can decompose the variables \( V(r\tau) \) into a static and the periodic parts

\[
V(r\tau) = V_0(r) + \bar{V}(r\tau),
\]

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

\[
\int [DV] ... = \int [DV_0] \int [D\bar{V}] ... .
\]

For the periodic part in Eq. (11), using Faraday-type relation we introduce the \( \text{U}(1) \) phase field \( \phi(r\tau) \) according to the relation

\[
\bar{V}(r\tau) = \frac{\partial \phi(r\tau)}{\partial \tau} \equiv \phi(r\tau).
\]
Thus, for the dynamic part, we transform the integration over the gauge variables $\tilde{V}(r\tau)$ into the integration over the generic phase variables $\varphi(r\tau)$

$$\int [D\tilde{V}] \rightarrow \int [D\varphi] \ldots$$  \hspace{1cm} (13)$$

In performing the integration over the phase field one should take into account that the field configurations satisfy the condition \cite{40.43}

$$\varphi(r\beta) - \varphi(r0) = 2\pi m(r),$$  \hspace{1cm} (14)$$

where $m(r) = 0, \pm 1, \pm 2, \ldots$ are the U(1) integer winding numbers. The integration measure in Eq.(13) over $\varphi$ variables is defined as

$$\int [D\varphi] \ldots = \sum_{[m(r)]} \int_0^{2\pi} \prod_r d\varphi_0(r) \times \int_{\varphi(\tau\beta) = \varphi(r) + 2\pi m(r)} \prod_r d\varphi(r\tau) \ldots$$  \hspace{1cm} (15)$$

and includes summation over winding numbers defined in Eq.(14). For the scalar static part $V_0(r)$ we have the following functional integral

$$\int [DV_0] e^{\sum_r \int_0^\beta d\tau - \frac{\tilde{V}^2(r\tau)}{4} + V_0(r)|n(r\tau) - \frac{\tilde{n}}{2}|}.$$  \hspace{1cm} (16)$$

The saddle-point value of $V_0(r)$ is given as $V_{0sp} = \frac{1}{\beta} \tilde{n} - \tilde{\mu}$, where $n$ is the total average particle density $\tilde{n} = n_c + n_f$. And we have the contribution to the partition function in Eq.(9) in the form

$$\exp \left[ -S[\varphi] - \sum_r \int_0^\beta d\tau \tilde{\mu} n(r\tau) \right],$$  \hspace{1cm} (17)$$

where the effective phase only action $S[\varphi]$ is given as

$$S[\varphi] = \sum_r \int_0^\beta d\tau \left[ \frac{\dot{\varphi}^2(r\tau)}{U} - \frac{2\tilde{\mu}}{iU} \varphi(r\tau) - i\dot{\varphi}(r\tau) n(r\tau) \right]$$  \hspace{1cm} (18)$$

and the effective chemical potential $\tilde{\mu}$ attached to the total density operator is introduced: $\tilde{\mu} = \frac{\tilde{n}}{2} - \tilde{\mu}$. The decoupling of the quadratic term proportional to $\tilde{n}^2(r\tau)$ in the exponential of the partition function in Eq.(16) is also straightforward. We obtain

$$\exp \left[ \sum_r \int_0^\beta d\tau \frac{U}{4} \tilde{n}^2(r\tau) \right] = \int [D\tilde{U}] \sqrt{\frac{\beta}{2}} = e^{\sum_r \int_0^\beta d\tau \left[ \frac{\tilde{n}^2(r\tau)}{2U} + \tilde{\varphi}(r\tau) \tilde{n}(r\tau) \right]}.$$  \hspace{1cm} (19)$$

Combining the expression in the exponential in Eq.(19) with the similar linear in $\tilde{n}$ term in the expression of the transformed Hamiltonian in Eq.(5), we have

$$\int [D\tilde{U}] e^{\sum_r \int_0^\beta d\tau \left[ \frac{\tilde{n}^2(r\tau)}{2U} + \tilde{\varphi}(r\tau) \tilde{n}(r\tau) \right]},$$  \hspace{1cm} (20)$$

The saddle-point evaluation gives for $\varphi$

$$\varphi_0 = \frac{\tilde{n}}{2} - \frac{\epsilon_c - \epsilon_f}{2},$$  \hspace{1cm} (21)$$

where $\tilde{n} = \langle \tilde{n}(r\tau) \rangle$. As the result of the decoupling we obtain the following “Zeeman-like” contribution in the partition function

$$\exp \left[ -\sum_r \int_0^\beta d\tau \mu_n \tilde{n}(r\tau) \right],$$  \hspace{1cm} (22)$$

with the attached effective chemical potential $\mu_n = \frac{\epsilon_c - \epsilon_f}{2} - \tilde{\mu}$. To summarize, the partition function of the system after decoupling procedures will be

$$Z = \int [D\tilde{c}D\tilde{f}] \left[ D\varphi \right] e^{-S[c,c,f,f,\varphi]},$$  \hspace{1cm} (23)$$

where the action $S[c,c,f,f,\varphi]$ in the exponential is

$$S[c,c,f,f,\varphi] = S[\varphi] + S_B [\tilde{c},c] + S_B [\tilde{f},f]$$

$$-i \sum_{(r\tau')} \int_0^\beta d\tau \left[ \tilde{c}(r\tau) c(r'\tau) + h.c. \right]$$

$$-i \sum_{(r\tau')} \int_0^\beta d\tau \left[ \tilde{f}(r\tau) f(r'\tau) + h.c. \right]$$

$$+ \sum_r \int_0^\beta d\tau \left[ \tilde{\mu} n(r\tau) + \mu_n \tilde{n}(r\tau) \right]$$  \hspace{1cm} (24)$$

suitable for derivation of the effective phase and fermionic actions.

**B. The U(1) gauge transformation**

To proceed, we perform the local gauge transformation to the new fermionic Grassmann variables $a(r\tau)$ and $b(r\tau)$ in order to eliminate the last imaginary term appearing in the expression of the phase action in Eq.(13). For the c-orbital electrons the U(1) transformation is

$$\left[ \begin{array}{c} c(r\tau) \\ \tilde{c}(r\tau) \end{array} \right] = \tilde{U}(\varphi) \left[ \begin{array}{c} a(r\tau) \\ \tilde{a}(r\tau) \end{array} \right],$$  \hspace{1cm} (25)$$

where $\tilde{U}(\varphi)$ is the U(1) transformation matrix $\tilde{U}(\varphi) = \tilde{I} \cos \varphi(r\tau) + i\tilde{\sigma}_z \sin \varphi(r\tau)$ with the unit matrix $\tilde{I}$ and $\sigma_z$ being the Pauli matrix. We used the bosonic
phase variables \( \varphi \) introduced in Eq. (12). For the \( f \)-orbital electrons the similar transformation is
\[
\begin{bmatrix}
f(\mathbf{r}\tau) \\
f(\mathbf{r}\tau)
\end{bmatrix} = \hat{U}(\varphi) \begin{bmatrix}
b(\mathbf{r}\tau) \\
b(\mathbf{r}\tau)
\end{bmatrix}.
\]
(26)

As a result, the electron appears in the theory like a composite object composed of fermion with the attached \( U(1) e^{i\varphi(\mathbf{r}\tau)} \) phase “flux-tube”. After those transformations the total action of the system reads
\[
S[\bar{a}, \bar{b}, \bar{a}, \bar{b}, \varphi] = S_B[\bar{a}, \bar{a}] + S_B[\bar{b}, \bar{b}]
- t \sum_{\langle \mathbf{r}\tau \rangle} \int_0^\beta d\tau \left[ \bar{a}(\mathbf{r}\tau)a(\mathbf{r}'\tau)e^{-i[\varphi(\mathbf{r}\tau) - \varphi(\mathbf{r}'\tau)]} + h.c. \right]
- i \sum_{\langle \mathbf{r}\tau \rangle} \int_0^\beta d\tau \left[ \bar{b}(\mathbf{r}\tau)b(\mathbf{r}'\tau)e^{-i[\varphi(\mathbf{r}\tau) - \varphi(\mathbf{r}'\tau)]} + h.c. \right]
+ \sum_r \int_0^\beta d\tau \left[ \bar{\mu}(\mathbf{r}\tau) + \mu e\bar{n}(\mathbf{r}\tau) \right],
\]
(27)

with the new phase action \( S_0[\varphi] \)
\[
S_0[\varphi] = \sum_r \int_0^\beta d\tau \left[ \frac{\varphi^2(\mathbf{r}\tau)}{U} - \frac{2\bar{\mu}}{iU}\varphi(\mathbf{r}\tau) \right].
\]
(28)

Then the partition function of the system in new variables is
\[
Z = \int[\mathcal{D}\bar{a}\mathcal{D}a][\mathcal{D}\bar{b}\mathcal{D}b][\mathcal{D}\varphi] e^{-S[\bar{a}, \bar{b}, \bar{a}, \bar{b}, \varphi]}.
\]
(29)

This form of the partition function will be the starting point for deriving the effective actions for the fermions and for the phase sector.

### IV. PAIRING AND COHERENCE IN EXCITON CONDENSATE

The excitonic order parameter in terms of the \( c \) and \( f \) variables is defined as
\[
\Psi = \lim_{\delta \to 0^+} \langle \bar{c}(\mathbf{r}\tau) f(\mathbf{r}\tau + \delta) \rangle.
\]
(30)

Here, an infinitesimal increment \( \delta \) is added to the Matsubara time variables for the proper definition of the equal time correlation functions. After the \( U(1) \) transformations in Eqs. (25) and (26), the order parameter takes the following form
\[
\Psi = \lim_{\delta \to 0^+} \langle \bar{a}(\mathbf{r}\tau)b(\mathbf{r}\tau + \delta) \rangle \langle z(\mathbf{r}\tau)z(\mathbf{r}\tau + \delta) \rangle = \frac{\Delta}{U} \lim_{\delta \to 0^+} G_z(\mathbf{r}\tau, \mathbf{r}\tau + \delta),
\]
(31)

where \( z(\mathbf{r}\tau) = e^{-i\varphi(\mathbf{r}\tau)} \). The averages in Eq. (31) are performed with respect to the corresponding fermionic and phase actions given in the Section VI. Furthermore, \( \Delta \) is the excitonic gap parameter
\[
\Delta = U \langle \bar{a}(\mathbf{r}\tau)b(\mathbf{r}\tau) \rangle.
\]
(32)

The non-zero value of \( \Delta \) signals the appearance of the electron-hole bound pairs, which manifests as a gap in the excitation spectrum and signals the presence of the EI state. Subsequently, \( G_z(\mathbf{r}\tau, \mathbf{r}\tau + \delta) \) is the local, equal-time phase-phase correlation function. In general,
\[
\lim_{\delta \to 0^+} G_z(\mathbf{r}\tau, \mathbf{r}\tau + \delta) = 1
\]
(33)

reflecting the unimodularity of the \( z(\mathbf{r}\tau) \)-field (\( |z(\mathbf{r}\tau)|^2 \equiv 1 \)). However, in the case of the spontaneous \( U(1) \) symmetry breaking in the phase sector, an anomalous expectation value of \( \langle e^{i\varphi(\mathbf{r}\tau)} \rangle \neq 0 \) appears signaling of the presence of the phase coherence in the system. In Section VI we will show that this is indeed the case, because the phase action contains the phase stiffnesses originating from the existence of the gap parameter \( \Delta \). As a result, the values of the function in Eq. (33) will be depleted by the amount of the condensed \( e^{i\varphi(\mathbf{r}\tau)} \) fields, so that
\[
\lim_{\delta \to 0^+} G_z(\mathbf{r}\tau, \mathbf{r}\tau + \delta) = 1 - |\psi_0|^2,
\]
(34)

where \( \psi_0 \) is the condensate transition amplitude \( \psi_0 = \langle e^{i\varphi(\mathbf{r}\tau)} \rangle \). It is important to understand what we mean by coherence in the present context. One type of coherence refers to the coherence of the wave function of the single electron and hole forming an exciton. This will be seen for example in a electrical transport properties of the system. Another type of coherence, which is crucial to the notion of a condensate is a macroscopic coherence of many excitons in the same quantum state. This is precisely what we mean by evaluating expectation value of \( z(\mathbf{r}\tau) \)-field. Therefore, from the Eqs. (31) and (32) we have for the excitonic order parameter
\[
\Psi = \frac{\Delta}{U} \left( 1 - |\psi_0|^2 \right).
\]
(35)

From the equation Eq. (35) it follows in general that the pairing and condensation are not the same. However, in the weak coupling limit \( U/t \ll 1 \), where dynamics and spatial fluctuation of the phase variables is unimportant \( z(\mathbf{r}\tau) \equiv e^{i\varphi} \) with constant (space and time independent) value of \( \varphi \) condensation and pairing occur at the same critical temperature controlled by \( \Delta \). This is what happens in the excitonic insulator in the weak coupling limit and has its analogue in a standard BCS superconductor: because the binding energy of the pair is small, the pair breaking controls the temperature. For this reason, the two different transitions the coherence and pairing are usually equated, while dealing with the exciton condensation problem. However, in a excitonic system with strong pairing, i.e., \( U/t \gg 1 \), we have the situation, in which pairs are strongly bound (thus non-zero value of \( \Delta \)), but these are incoherent pair, uncorrelated with each
other until they eventually undergo the BEC at low temperatures. Therefore, the fact that the EI state can be described by $\Delta$ is not the same as showing the coherence in the system. It must be shown that the experimental results cannot be described by an ensemble of the independent pairs. For example, the tunneling experiments in excitonic system can be explained simply by electron-hole pairing without resorting to the coherence among excitons. Exciton coherence may be evidenced by coherence of their light emission, which can be studied by interferometry measurements.

V. EXCITONIC PAIRING GAP

A. Effective fermionic action

We start the derivation of the EI gap equation with the phase averaged action obtained by the U(1) transformations given by the Eqs. (25) and (26). Within the HF approximation the many-body (interaction) part of the original Hamiltonian in Eq. (11) is decoupled according to

$$n_a(r r) n_b(r r) \approx \langle n_a(r r) \rangle \langle n_b(r r) \rangle + \langle n_b(r r) \rangle \langle n_a(r r) \rangle - \frac{1}{U} \Delta \overline{a}(r r) b(r r) - \frac{1}{U} \Delta \overline{b}(r r) a(r r).$$

Here $n_a(r r)$ and $n_b(r r)$ are the electron densities after the U(1) gauge transformation.

The Fourier transformation of the fermionic variables $a(r r)$ and $b(r r)$ is given by

$$x(r r) = \frac{1}{\beta N} \sum_{k \nu n} x_k(\nu n) e^{i(k r - \nu n \tau)}$$

with $x = a, b$ for the $a$ and $b$ type electrons. $N$ is the number of lattice sites and $\nu_n = \pi(2n + 1)/\beta$ are the Fermi-Matsubara frequencies with $n = 0, \pm 1, \pm 2, \ldots$. Using Eq. (37) the effective action of the fermionic sector takes the form

$$S_{\text{eff}}[\overline{a}, a, \overline{b}, b] = \frac{1}{\beta N} \sum_{k \nu n} \overline{a}_k(\nu n) (\mu^a_{\text{eff}} - i \nu_n - i \overline{\tau}) a_k(\nu n)
\quad + \frac{1}{\beta N} \sum_{k \nu n} \overline{b}_k(\nu n) (\mu^b_{\text{eff}} - i \nu_n - i \overline{\tau}) b_k(\nu n)
\quad - \frac{\Delta}{\beta N} \sum_{k \nu n} \overline{a}_k(\nu n) b_k(\nu n)
\quad - \frac{\Delta}{\beta N} \sum_{k \nu n} \overline{b}_k(\nu n) a_k(\nu n)$$

with the effective chemical potentials $\mu^a_{\text{eff}}$ and $\mu^b_{\text{eff}}$

$$\mu^a_{\text{eff}} = \epsilon_a - \mu + U n_b + i \langle \varphi(r r) \rangle, \quad \mu^b_{\text{eff}} = \epsilon_b - \mu + U n_a + i \langle \varphi(r r) \rangle.$$  

$n_a$ and $n_b$ in Eqs. (39) and (40) are the fermion densities $n_x = \langle n_x(r r) \rangle$. The renormalized hopping amplitudes $t_k$ and $\tilde{t}_k$ are given by the relations

$$t_k = 2g\epsilon_k(\mathbf{k}), \quad \tilde{t}_k = 2\tilde{g}\epsilon_k(\mathbf{k}),$$

where $g$ is the bandwidth renormalization factor and

$$\epsilon_k(\mathbf{k}) = \cos(d_x k_x) + \cos(d_y k_y) + \cos(d_z k_z)$$

is the three-dimensional lattice dispersion relation with $d_x (\alpha = x, y, z)$, being the components of the lattice spacing vector $d = r - r'$ with $r$ and $r'$ nearest neighbors positions. For the simple cubic geometry they are equal $d_x \equiv d$. The factor $g$ is

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

Introduction of the Nambu notations

$$\sigma_k(\nu_n) = \left[ \begin{array}{cc} a_k(\nu_n) & \overline{b}_k(\nu_n) \\
\overline{a}_k(\nu_n) & b_k(\nu_n) \end{array} \right], \quad \sigma_{\overline{k}}(\nu_n) = \left[ \begin{array}{cc} \overline{a}_k(\nu_n) & b_k(\nu_n) \\
a_k(\nu_n) & \overline{b}_k(\nu_n) \end{array} \right],$$

permits to rewrite the action in Eq. (38) in the compact form

$$S_{\text{eff}}[\overline{\sigma}, \sigma] = \frac{1}{\beta N} \sum_{k \nu n} \sigma_k(\nu_n) \hat{G}^{-1}(\nu_n) \sigma_{\overline{k}}(\nu_n),$$

where $\hat{G}^{-1}(\nu_n)$ is the inverse of the Green function matrix

$$\hat{G}^{-1}(\nu_n) = \left[ \begin{array}{cc} \mathcal{E}^a_k(\nu_n) & -\Delta \\
-\Delta & \mathcal{E}^b_k(\nu_n) \end{array} \right].$$

where $\mathcal{E}^a_k(\nu_n)$ and $\mathcal{E}^b_k(\nu_n)$ are given by

$$\mathcal{E}^a_k(\nu_n) = \mu^a_{\text{eff}} - i \nu_n - \overline{\tau}, \quad \mathcal{E}^b_k(\nu_n) = \mu^b_{\text{eff}} - i \nu_n - \overline{\tau}.$$  

The normal propagator $\mathcal{G}^{xx}(r r, r' r')$ is defined in terms of the fermionic variables $x(r r)$:

$$\mathcal{G}^{xx}(r r, r' r') = - \langle x(r r) \overline{x}(r' r') \rangle.$$  

The anomalous or the excitonic propagator is

$$\mathcal{G}^{ab}(r r, r' r') = \langle a(r r) b(r' r') \rangle.$$  

The averages in the Eqs. (50) and (51) are defined as

$$\langle \ldots \rangle = \frac{\int [D\overline{\sigma} D\sigma] \ldots e^{-S_{\text{eff}}[\overline{\sigma}, \sigma]}}{\int [D\overline{\sigma} D\sigma] e^{-S_{\text{eff}}[\overline{\sigma}, \sigma]}}.$$  

As a consequence, using Eqs. (47) and (52) we have

$$\mathcal{G}^{aa}(r r, r' r') = - \frac{1}{\beta N} \sum_{k \nu n} \mathcal{E}^a_k(\nu_n) e^{i(k r - r' - \nu_n (r' - r'))} \langle \overline{E}^a_k(\nu_n) \rangle \langle \mathcal{E}^a_k(\nu_n) \rangle - |\Delta|^2.$$  

(53)
with similar expression for $G^{aa}(\mathbf{r}, \mathbf{r}'; \tau)$ with the replacement $\xi^a_k(\nu_n) \rightarrow \xi^b_k(\nu_n)$. Furthermore, the anomalous propagators are given by

$$G^{ab}(\mathbf{r}, \mathbf{r}'; \tau) = -\frac{\Delta}{\beta N} \sum_{\mathbf{k} \nu_n} \frac{e^{-i|\mathbf{k}(\mathbf{r}-\mathbf{r}')| \nu_n(\tau-\tau')}}{\xi^a_k(\nu_n)\xi^b_k(\nu_n) - |\Delta|^2},$$

(54)

while $G^{ba}(\mathbf{r}, \mathbf{r}'; \tau)$ is obtained by the substitution $\Delta \rightarrow \Delta$. The anomalous propagators in the form given in Eq. (54) will determine furthermore the phase stiffness $\xi$.

Using the propagators in Eqs. (53) and (54), we can rewrite the Eq. (55) in an equivalent explicit form

$$\rho_{3D}(x) = \frac{1}{\pi^3} \int_{\max(-1,-2-x)}^{\min(1,2-x)} \frac{\Theta \left(1 - \frac{|x|}{\sqrt{1 - y^2}}\right)}{\sqrt{1 - y^2}} \times K \left[\sqrt{1 - \left(\frac{y}{2} + \frac{x}{2}\right)^2}\right],$$

(62)

For the three-dimensional lattice the density of states is given as

$$\rho_{3D}(x) = \frac{1}{\pi^3} \int_{\max(-1,-2-x)}^{\min(1,2-x)} \frac{\Theta \left(1 - \frac{|x|}{\sqrt{1 - y^2}}\right)}{\sqrt{1 - y^2}} \times K \left[\sqrt{1 - \left(\frac{y}{2} + \frac{x}{2}\right)^2}\right],$$

(63)

where $\Theta(x)$ is the Heaviside step function and $K(x)$ is the elliptic function of the first kind. The plot of the function $\rho_{3D}(x)$ is presented in the inset in Fig. 1. From the density difference $\tilde{n}$ between conduction and valence bands plotted as a function of the Coulomb interaction parameter $U$ in units of $t$ in the region where $\Delta \neq 0$. It is clear in Fig. 1 that in the strong coupling limit $U/t \gg 1$ the system is in the band-insulator regime, because at the upper bound of the Coulomb interaction the $f$-band is fully occupied ($n_b = 1$) and the $c$-band is totally empty ($n_a = 0$).

B. Self-consistent solution for $\Delta$, $\Delta_g$ and $\Delta_e$

From the expression of the Green functions in Eqs. (53) and (54) obtained above, we have the equations for the average electron densities $n_a$ and $n_b$ corresponding to the $a$- and $b$-orbitals respectively and also a self-consistent equation for the excitonic gap parameter $\Delta$. We have

$$n_a = G^{aa}(0,0),$$

$$n_b = G^{bb}(0,0),$$

$$\Delta = UG^{ab}(0,0).$$

(55)

Using the propagators in Eqs. (53) and (54), we can rewrite the Eq. (55) in an equivalent explicit form

$$\frac{1}{N} \sum_{\mathbf{k}} \left[ n_F(E^+_k) + n_F(E^-_k) \right] = 1,$$

(56)

$$\tilde{n} = \frac{1}{N} \sum_{\mathbf{k}} \frac{n_F(E^+_k) - n_F(E^-_k)}{\sqrt{\xi^a_k + 4\Delta^2}},$$

(57)

$$\Delta = \frac{U\Delta}{N} \sum_{\mathbf{k}} \frac{n_F(E^+_k) - n_F(E^-_k)}{\sqrt{\xi^a_k + 4\Delta^2}}.$$

(58)

Here we assumed a half-filled band case $n = n_a + n_b = 1$ and we defined the density difference $\tilde{n} = n_a - n_b$. Furthermore, $n_F(\epsilon)$ denotes the Fermi-Dirac distribution function $n_F(\epsilon) = 1/(e^{\beta\epsilon} + 1)$. Next, we have introduced the band-energy parameters $E^+_k$ and $E^-_k$

$$E^+_k = \frac{1}{2} \left( -A_k \pm \sqrt{\xi^2_k + 4\Delta^2} \right),$$

(59)

where $A_k = \tilde{t}_k - \mu^b + t_k - \mu^a$ with the quasiparticle dispersion $\xi_k$

$$\xi_k = \tilde{t}_k + \mu^a - t_k - \mu^b.$$

(60)

The energy difference

$$\Delta_e = E^+_k - E^-_k$$

(61)

defines the charge-transfer gap, which we will discuss later on in this Section. The quantities $n_a$, $n_b$, $\Delta$ and also $\mu$ can be determined by solving numerically the Eqs. (56)-(58) in a self-consistent way.

Summations over the wave vectors can be simplified by introducing the appropriate density of states (DOS) for the three-dimensional lattice $\rho_{3D}(x)$. Using Eq. (13) we write

$$\rho_{3D}(x) = \frac{1}{\pi^3} \int_{\max(-1,-2-x)}^{\min(1,2-x)} \frac{\Theta \left(1 - \frac{|x|}{\sqrt{1 - y^2}}\right)}{\sqrt{1 - y^2}} \times K \left[\sqrt{1 - \left(\frac{y}{2} + \frac{x}{2}\right)^2}\right],$$

(63)

where $\Theta(x)$ is the Heaviside step function and $K(x)$ is the elliptic function of the first kind. The plot of the function $\rho_{3D}(x)$ is presented in the inset in Fig. 1 where the electronic density difference $\tilde{n}$ between conduction and valence bands $\tilde{n}$ is plotted as a function of the Coulomb interaction parameter $U$ in units of $t$ in the region where $\Delta \neq 0$. It is clear in Fig. 1 that in the strong coupling limit $U/t \gg 1$ the system is in the band-insulator regime, because at the upper bound of the Coulomb interaction the $f$-band is fully occupied ($n_b = 1$) and the $c$-band is totally empty ($n_a = 0$). In Fig. 2 the solution for the excitonic pairing gap $\Delta$ is plotted as a function of the Coulomb interaction energy $U/t$ for different values of the hopping amplitude $\tilde{t}$. The excitonic gap is non-zero for a rather large domain of the Coulomb interaction in agreement with the result of Ref. [28] and in contrast with the results for the two-dimensional square lattice in Ref. [28]. The obtained values for the lower and upper bounds of the Coulomb interaction in Ref. [28] are about $(U_{c1}, U_{c2}) = (0.66, 6.95)$, which differ considerably from our results especially for the large hopping. The solutions of Eqs. (56)-(58) for the chemical potentials for $\Delta \neq 0$ in the intermediate and strong interaction limits, forms a well defined band for all values of the $t$ implying the formation of the single particle excitation gap $\Delta_g = \mu^{max} - \mu^{min}$, where $\mu^{max}$ and $\mu^{min}$ are the upper and lower bounds of the chemical potential (see Fig. 3). The evolution of the upper bound of the chemical potential as a function of the Coulomb interaction $U$ is presented in Fig. 3. Moving from the weak to intermediate coupling regime, single particle $\Delta_g$ and pairing $\Delta$ gaps both are increasing while in the strong coupling limit $(U/t > 8$ for $\tilde{t} = -0.3t$ for example) $\Delta$ decreases rapidly with increasing $U/t$ while $\Delta_g$ remains open. For vanishing of the pairing gap $\Delta = 0$ the single particle gap collapses $\Delta_g = 0$ and the solution for the chemical potential is single valued (see Fig. 3). For
FIG. 1: (Color online) The difference \( \dot{\bar{n}} \) between conduction and valence band average densities as a function of the interaction parameter \( U/t \) for a number of values of the hopping amplitude \( t \). In the inset the density of states (DOS) for the three-dimensional cubic lattice is presented.

the completeness the density difference between the conduction and valence bands at the EI transition boundary \( \dot{\bar{n}} \) is presented in Fig. 8.

The charge-transfer gap \( \Delta_c \) defined in Eq. (61) is calculated as a function of the Coulomb interaction \( U \). The results are presented in Figs. 7 and 8. We see in Fig. 7 that for the small values of the Coulomb interaction the charge-transfer gap is nearly zero. The small value of it is the manifestation of the semimetallic or the BCS limit. Augmenting the interaction parameter \( U \), the gap \( \Delta_c \) is gradually opening. In Fig. 8 we presented the charge-transfer gap for a smaller value of the hopping amplitude \( t = -0.1t \). With decreasing the hopping amplitude we are decreasing also the charge-transfer gap. This is consistent with the results for the excitonic gap parameter presented in Fig. 4 and with the single particle excitation gap behavior in Fig. 2. Finally, in Fig. 8 we have presented the solution of the equation \( \Delta(T, U) = 0 \), which determines the temperature \( T_\Delta \) for which the pairing gap vanishes. Our calculation regarding the pairing gap \( \Delta \) and resulting pair formation temperature \( T_\Delta \) agree very well with the analogous results in previous works (see Refs. 20–31). However, as we will show in the Section VII, the excitonic pair formation temperature \( T_\Delta \) is not coinciding in general with the excitonic condensation critical temperature, which requires the phase coherence among excitons, a feature that was not considered in the previous works.

FIG. 2: (Color online) The excitonic gap parameter \( \Delta \) as a function of the normalized Coulomb interaction energy \( U/t \) for different values of the hopping parameter \( t \).

C. The coherence length and momentum distribution functions

We can associate a characteristic decay of \( F(\mathbf{k}) \) with the coherence length \( \xi_c \) defined by the relation \( 62 \)

\[
\xi_c = \sqrt{\frac{\sum_k |\nabla_k F(\mathbf{k})|^2}{\sum_k |F(\mathbf{k})|^2}}.
\]

The quantity \( \xi_c \) provides the quantitative information about the properties of the system. To proceed we define the frequency-summed normal and anomalous momentum-dependent functions

\[
n_a(\mathbf{k}) = \frac{1}{\beta} \sum_{\nu_n} G^{aa}(\mathbf{k}\nu_n),
\]

\[
F(\mathbf{k}) = \frac{1}{\beta} \sum_{\nu_n} G^{ab}(\mathbf{k}\nu_n),
\]

where \( G^{aa}(\mathbf{k}\nu_n) \) and \( G^{ab}(\mathbf{k}\nu_n) \) are the Fourier transformations of the local normal and anomalous propagators. Using Eqs. (53) and (54) we obtain

\[
n_a(\mathbf{k}) = \frac{1}{\beta} \sum_{\nu_n} \frac{\mu_{\mathbf{k}a}^{\nu_n} - i\nu_n - \tilde{t}_n}{\mathcal{E}_{\mathbf{k}}^{\nu_n}(\nu_n)\mathcal{E}_{\mathbf{k}}^{\nu_n}(\nu_n) - |\Delta|^2},
\]

\[
F(\mathbf{k}) = -\frac{1}{\beta} \sum_{\nu_n} \frac{\Delta}{\mathcal{E}_{\mathbf{k}}^{\nu_n}(\nu_n)\mathcal{E}_{\mathbf{k}}^{\nu_n}(\nu_n) - |\Delta|^2}.
\]

Summing over the fermionic Matsubara frequencies, we get

\[
n_a(\mathbf{k}) = v_F^2 n_F(E_{\mathbf{k}}^-) - u_F^2 n_F(E_{\mathbf{k}}^+),
\]

\[
F(\mathbf{k}) = u_F v_F \left[ n_F(E_{\mathbf{k}}^+) - n_F(E_{\mathbf{k}}^-) \right],
\]
while the function \( n_b(k) \) for the \( b \)-orbital is simply \( n_b(k) = 1 - n_a(k) \). The coefficients appearing in Eq. (67) are given by

\[
\begin{align*}
    u_k^2 &= \frac{1}{2} \left( 1 + \frac{\xi_k}{\sqrt{\xi_k^2 + 4\Delta^2}} \right), \\
    v_k^2 &= \frac{1}{2} \left( 1 - \frac{\xi_k}{\sqrt{\xi_k^2 + 4\Delta^2}} \right), \\
    u_kv_k &= \frac{\Delta}{\sqrt{\xi_k^2 + 4\Delta^2}}. \\
\end{align*}
\]

In analogy with the HF approximation\(^{28}\), we will suppose that \( 2|F(k)| = 1 \) at \( k = k_F \), which is the definition of the Fermi momentum \( k_F \), i.e., \( n_a(k_F) = n_b(k_F) = 0.5 \). In Figs. 10, 11 we presented the \( k \)-dependence of the normal \( a \)-band and anomalous \( F(k) \) function. In the weak coupling regime the normal distribution function \( n_a(k) \) drops at \( k_F \) and anomalous momentum function is picked at the Fermi level. With increasing the Coulomb interaction \( n_a(k) \) spread out in the \( k \)-space and also \( k_F \) becomes broad with the Fermi level \( k_F \) displaced to the value \((0,0,0)\) in the momentum space. Across the crossover regime, the anomalous momentum function decreases for all momenta of the reciprocal space and this is consistent with the behavior of the excitonic gap parameter \( \Delta \) in the strong coupling regime presented in Fig. 12. Subsequently, in Fig. 13, we have presented the temperature dependence of the anomalous distribution function.

The \( k \) -summations in the analytical expression of \( \xi_c \) were done with the \((100 \times 100 \times 100)\) \( k \)-points in the
phase stiffness, we are interested in purely phase action and thus we will integrate out the fermions in Eq. (29) to obtain the effective phase action in the model. The partition function of the phase-only model is

$$Z = \int [\mathcal{D}\varphi] e^{-S_{\text{eff}}[\varphi]},$$  \hspace{1cm} (69)$$

where

$$S_{\text{eff}}[\varphi] = S_0[\varphi] - \frac{1}{2} \langle S^2 \rangle_{S_0[n,a,b,k]}, \hspace{1cm} (70)$$

and the action $S_0[\varphi]$ is given in Eq. (28). The detailed calculation of the average of the second order term in Eq. (70) is given in the Appendix \[B\]. As a result, we have for the phase-only action

$$S_J[\varphi] = -J \int_0^\beta d\tau \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \cos 2[\varphi(\mathbf{r},\tau) - \varphi(\mathbf{r}',\tau)],$$  \hspace{1cm} (71)$$

where $J$ is the phase stiffness parameter with the help of the lattice DOS in Eq. (63) we have (see Appendix \[B\])

$$J = \frac{4\Delta^2 t_i}{9} \int \int \rho_{3D}(x)\rho_{3D}(y)\epsilon(x)\epsilon(y) \sqrt{\xi(x) + 4\Delta^2} \left[ A_1(x,y) \tanh \left( \frac{\beta E^+(x)}{2} \right) - A_2(x,y) \tanh \left( \frac{\beta E^-(x)}{2} \right) \right],$$  \hspace{1cm} (72)$$

FIG. 7: (Color online) Momentum dependence of the charge-transfer gap $\Delta_c$ along the direction $(0,0,0) \rightarrow (\pi,\pi,\pi)$ for $t = -0.3t$ in the extended zone scheme. The wave vector $\mathbf{k}$ is measured in units of $2\pi/d$. The plots are given for different values of the Coulomb energy $U/t$. 

VI. EXCITONIC PHASE COHERENCE

A. Phase stiffness

In this section we examine the system of excitons by considering the phase stiffnesses of the conduction band electrons and valence band holes. We will show how the macroscopic phase coherence between these two solid state bands is important for the excitonic condensation at the very low temperatures. In order to consider the
The phase stiffness in units of the hopping parameter is 

\[ \frac{1}{E^+(x) - E^-(y)} \cdot \frac{1}{E^+(x) - E^-(y)} \cdot \frac{1}{E^-(x) - E^+(y)} \cdot \frac{1}{E^-(x) - E^-(y)} \]  

(73)

where \( E^+(x) \) and \( E^-(x) \) are given by Eq. (59). From the phase stiffness in Eq. (72) it follows that the non-zero value of \( J \) is linked with the pairing gap \( \Delta \) since \( J(\Delta = 0) = 0 \). Therefore, the pairing in the excitonic system is the necessary prerequisite for the phase coherence. In Fig. 10 we presented the phase stiffness parameter \( \Lambda \) as a function of the hopping amplitude \( t \). As the figures show, the values of \( J \) are strictly positive for all regions of the normalized Coulomb interaction parameter \( U/t \).

The phase stiffness in units of the hopping parameter is very small \( J/t \ll 1 \), but is persistent in the whole region with non-vanishing pairing gap \( \Delta \).

### B. Quantum rotor representation

In the discussion above, we derived the effective phase-only action \( S_{\text{eff}} \) : 

\[ S_0[\varphi] + S_{\text{coul}}[\varphi]. \]

In the following we cast the \( S_{\text{eff}}[\varphi] \) into the quantum rotor representation \( 1 \) which enables us to study a spontaneous U(1) symmetry breaking resulting in global phase coherent state among electron-hole pairs. To proceed, we replace the phase degrees of freedom by the complex unimodular field \( z(\mathbf{r}) \), which satisfy the periodic boundary conditions \( z(\mathbf{r}+\mathbf{r}_0) = z(\mathbf{r}) \), as it was implemented in the Section IV for the description of the pairing order parameter \( \Psi \):

\[ z(\mathbf{r}) = e^{i\varphi(\mathbf{r})}. \]

(74)

Now we introduce the new variables into the partition function in Eq. (60) using the following identity

\[ \int DzD\delta \left( \sum_\mathbf{r} |z(\mathbf{r})|^2 - N \right) \times \]

\[ \times e^{i\delta \left( \bar{z} - e^{-i\varphi(\mathbf{r})} \right)} = 1. \]

(75)

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

\[ \frac{1}{N} \sum_\mathbf{r} |z(\mathbf{r})|^2 = 1, \]

(76)

which forms a kind of spherical constraint on a set of unimodular variables \( z(\mathbf{r}) \). The spherical constraint in Eq. (76) can be resolved by introducing the Lagrange multiplier \( \lambda \) resulting from the Laplace transform of the functional delta representation

\[ \delta \left( \sum_\mathbf{r} |z(\mathbf{r})|^2 - N \right) = \int_{-i\infty}^{+i\infty} \left[ \frac{D\lambda}{2\pi i} \right] \times \]

\[ \times e^{-i\int_0^\beta d\tau \sum_\mathbf{r} \lambda( |z(\mathbf{r})|^2 - 1 )}. \]

(77)
This adds a quadratic term (in the z-field) to the phase action. Next, the phase stiffness action in Eq. (71) can be rewritten in more convenient form using the trigonometric half-angle transformation formula

$$
\cos 2 \left[ \phi(r\tau) - \phi(r'\tau) \right] = 2 \cos^2 \left[ \phi(r\tau) - \phi(r'\tau) \right] - 1.
$$

Then, in terms of the complex variables $z(r\tau)$, the transformation in Eq. (78) leads to a biquadratic form of the phase stiffness action in Eq. (71). We have

$$
S_J[\phi] \to S_J[\tilde{z}, z] = -J \int_0^\beta d\tau \sum_{r\tau} \left[ \tilde{z}(r\tau)z(r'\tau) + c.c. \right]^2.
$$

(79)

The four order term in Eq. (79) could be decoupled with the help of the Hubbard-Stratonovich transformation by introducing the complex variables $w(r\tau r'\tau)$ at each bond of the lattice

$$
e^{\frac{2j}{\beta} \int_0^\beta d\tau \sum_{r\tau} \left[ \tilde{z}(r\tau)z(r'\tau) + c.c. \right]^2} = \int [D\lambda] e^{-\int_0^\beta d\tau \sum_{r\tau} \frac{w(r\tau r'\tau)^2}{2j} \times e^{\int_0^\beta d\tau \sum_{r\tau} w(r\tau r'\tau) \left[ \tilde{z}(r\tau)z(r'\tau) + c.c. \right]}}.
$$

(80)

The integral in Eq. (80) over the $w(r\tau r'\tau)$ fields could be calculated using the saddle-point method, which amounts in replacing $w(r\tau r'\tau)$ variables by their saddle-point value

$$
\omega_0 = J \langle \left[ \tilde{z}(r\tau)z(r'\tau) + c.c. \right] \rangle = 2Jg,
$$

(81)

where we used the expression of the bandwidth renormalization factor $g$ given in the Eq. (44). Substituting the value of $\omega_0$ in Eq. (81) back into the Eq. (80) we obtain the part of the effective phase action pertaining to the stiffness $S_J[\tilde{z}, z]$ in a form

$$
S_J[\tilde{z}, z] = -4gJ \int_0^\beta d\tau \sum_{r\tau} \tilde{z}(r\tau)z(r'\tau).
$$

(82)

Finally, after integrating out the phase variables in Eq. (89), the partition function assumes the form

$$
\mathcal{Z} = \mathcal{Z}_0 \int [D\lambda] \int [D\tilde{z}\tilde{z}] e^{-S_\lambda[\tilde{z}, z]},
$$

(83)

where $\mathcal{Z}_0$ is the statistical sum of the non-interacting set of quantum rotators

$$
\mathcal{Z}_0 = \int [D\tilde{z}] e^{-S_0[\tilde{z}]},
$$

(84)

while the action $S_\lambda[\tilde{z}, z]$ in Eq. (83) after the Fourier transformation

$$
z(r\tau) = \frac{1}{\beta N} \sum_{k\omega_n} z(k\omega_n)e^{-i(k\tau - \omega_n\tau)}
$$

(85)
reads

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

(86)

where

$$G_z^{-1}(k\omega_n) = \lambda - 8gJ e(k) + \gamma^{-1}(\omega_n)$$

(87)

and \(\omega_n\) in Eq. (86) are the Bose-Matsubara frequencies \(\omega_n = \frac{2\pi n}{\beta}\) with \((n = 0, \pm 1, \pm 2, ...\)). Furthermore, \(\gamma^{-1}(\omega_n)\) is the inverse of the Fourier transformation of the two-point phase correlation function

$$\gamma(\mathbf{r}\tau, \mathbf{r}'\tau') = \frac{1}{Z_0} \int [\mathcal{D}\varphi] e^{-S_0[\varphi]} e^{i[\varphi(\mathbf{r}\tau) - \varphi(\mathbf{r}'\tau')]}. \quad (88)$$

The calculation of the Fourier transformation \(\gamma(\omega_n)\) of the function in Eq. (86) is straightforward

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

(89)

where

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

(90)

The summations in Eqs. (89) and (90) are over the winding numbers \(m\) of the \(U(1)\) group (see the Section III A).

C. Phase coherence line

In the thermodynamic limit \(N \to \infty\) the integration over \(\lambda\)-field in Eq. (83) and (86) can be performed exactly using the saddle-point method

$$\delta S[z, z] \bigg|_{\lambda=\lambda_0} = 0. \quad (91)$$

As a result, one can write the constraint for the saddle-point value of the Lagrange multiplier \(\lambda_0\)

$$1 = \lim_{\delta \to 0^+} \frac{\langle z(\mathbf{r}\tau)\tilde{z}(\mathbf{r}\tau + \delta) \rangle}{\langle \tilde{z}(\mathbf{r}\tau) \rangle}, \quad (92)$$

where the average in Eq. (92) is defined as

$$\langle \ldots \rangle \equiv \frac{\int [Dzdz] \ldots e^{-S_0[z, z]} \int [Dzdz] e^{-S_0[z, z]}}{\int [Dzdz]}.$$

(93)

Then with the help of the Eq. (86) we can write explicitly

$$1 = \frac{1}{(\beta N)^2} \sum_{k\omega_n} \langle z(k\omega_n)\tilde{z}(k\omega_n) \rangle \equiv \frac{1}{\beta N} \sum_{k\omega_n} G_z(k\omega_n). \quad (94)$$

Due to the presence of the phase stiffnesses \(J\) (see the Eq. (83)) we have the possibility of the spontaneous breaking of the \(U(1)\) symmetry of the phase filed leading to the non-vanishing expectation value of the \(z(\mathbf{r}\tau)\)-filed. In order to demonstrate this, we separate the single particle state \(\mathbf{k} = 0\) and the frequency mode \(\omega_n = 0\) for

FIG. 11: (Color online) The normal momentum distribution function \(n_d(k)\) and anomalous function \(2F(k)\) along the direction \((0, 0, 0) \to (\pi, \pi, \pi)\) at \(T = 0\) for different values of the normalized Coulomb interaction parameter \(U/t\) and for \(t = -0.1t\). The wave vector \(k\) is given in units of \(2\pi/d\).

FIG. 12: (Color online) The normal momentum distribution function \(n_d(k)\) and anomalous function \(2F(k)\) along the direction \((0, 0, 0) \to (\pi, \pi, \pi)\) at \(T = 0\) and for different values of the normalized Coulomb interaction parameter \(U/t\) and for \(t = -0.3t\). The wave vector \(k\) is given in units of \(2\pi/d\).
Furthermore, find \( \lambda \) which fixes the Lagrange multiplier to the value given by the equation

\[
\lambda = \frac{n_B(\varepsilon)}{\gamma^{-1}(\omega_n = 0)},
\]

where \( n_B(\varepsilon) \) is the Bose-Einstein distribution function \( n_B(\varepsilon) = 1/(e^{\beta \varepsilon} - 1) \) and the variables \( \zeta_k \) and \( \zeta_{2k} \) are given by

\[
\zeta_k = -\bar{\mu} + (-1)^a \sqrt{\bar{\mu}^2 + 4UgJ(\varepsilon(0) - \varepsilon(k))},
\]

where \( a = 1, 2 \). The simultaneous solution of the equations Eq. (101) and Eqs. (56-58) from the Section IV gives the critical temperature \( T_c(U) \) for the transition to the phase coherent excitonic condensate (see the Fig. 17 and Fig. 18). The upper curve on the same plots represents the temperature \( T_{\Delta} \) as a function of the Coulomb energy along which the excitonic gap \( \Delta \) vanishes.

We observe, that for \( U/t \ll 1 \) the temperatures \( T_{\Delta} \) and \( T_c \) coincide, signaling that in the weak coupling regime.
the formation of the excitonic condensate is dominated by pair breaking effects, in close analogy with the BCS superconducting systems. In the region of the intermediate values of the Coulomb interaction the BEC transition temperature is different from the pair formation transition temperature $T_\Delta$ (about two order of magnitude).
The reason for this is that these two critical temperatures are set by different energy scales: the pair breaking critical temperature $T_\Delta$ is controlled by the Coulomb energy $U$, while $T_c$ depends on phase stiffness $J$. Furthermore, the maximum of the condensate transition temperature $T_{c}^{\text{max}}$ coincides with the maximum of the phase stiffness parameter $J_{\text{max}}$ and this is due to the fact that both transitions are strongly interrelated. From the behavior of the excitonic gap parameter (Fig. 2) it is clear that the transition proportional to the force. This could in principle be superfluid phase-coherent state should have an acceleration proportional to the force. For excitons incoherent, then their motion under varying electric field should follow an Ohm’s law, in which their velocity is proportional to the force. The exciton in a superfluid phase-coherent state should have an acceleration proportional to the force. This could in principle be measured by optical imaging of the exciton motion. For example, the exciton phase coherence may be evidenced by the coherence of their light emission, which can be studied by interferometry. Exciton decay by emitting photons upon electron-hole recombination. Therefore, measurements of the intensity of the line-shape of this decay may be a powerful probe of the velocity spectrum in the excitonic system especially as to whether the global phase-coherent phase below the temperature $T_c$ exists.

### D. Phase coherence and spectral functions

#### 1. Excitonic correlation function

As discussed in Ref. 42, the luminescence line-shapes $I(\omega)$ in the excitonic system can be analyzed in terms of the spectral density $A_g(k\omega)$ of the interacting exciton gas, which also determines the exciton center-of-mass distribution. Quite generally, the line shape $I(\omega)$ is the sum of two distinct contributions: a narrow peak at $k = 0$, associated with the excitonic condensate and a broader distribution associated with the decay of excitons outside the condensate $k \neq 0$. Because within our theoretical approach we can access a variety of correlation functions, we concentrate now on the excitonic propagator in terms of the initial fermionic variables $c$ and $\tilde{f}$ defined as

$$G_{\text{ct}}(r_\tau, r_\tau') = \langle \tilde{c}(r_\tau) f(r_\tau') \rangle.$$  \hspace{1cm} (103)

After introducing the U(1) transformations in Eqs. (25) and (26), we have

$$G_{\text{ct}}(r_\tau, r_\tau') = G_{ab}(r_\tau, r_\tau') G_z(r_\tau, r_\tau'),$$  \hspace{1cm} (104)

where we introduced the $G_{ab}(r_\tau, r_\tau')$ fermionic and $G_z(r_\tau, r_\tau')$ phase-phase propagator, which are defined as follows

$$G_{ab}(r_\tau, r_\tau') = \langle \tilde{a}(r_\tau) b(r_\tau') \rangle,$$

$$G_z(r_\tau, r_\tau') = \langle e^{-i\varphi(r_\tau) - \varphi(r_\tau')} \rangle.$$  \hspace{1cm} (105)

Then we write the Fourier transformations

$$G_{ab}(r_\tau, r_\tau') = \frac{1}{\beta N} \sum_{k \nu_n} G_{ab}(k \nu_n) e^{i(k(r_\tau') - \nu_n(r_\tau'))},$$

$$G_z(r_\tau, r_\tau') = \frac{1}{\beta N} \sum_{k \omega_n} G_z(k \omega_n) e^{i(k(r_\tau') - \omega_n(r_\tau'))},$$  \hspace{1cm} (106)

Furthermore, the Fourier transformation of the function in Eq. (104) could be written as a convolution in the reciprocal space:

$$G_{\text{ct}}(k \nu_n) = \frac{1}{\beta N} \sum_{q \omega_n} G_z(q \omega_n) G_{ab}(k - q, \nu_n - \omega_n).$$  \hspace{1cm} (107)

On the other hand, following the Section VIII C, the phase-phase propagator $G_z(r_\tau, r_\tau')$ will be rewritten in terms of the U(1) complex variables $z(r\tau) = e^{i\varphi(r\tau)}$

$$G_z(r_\tau, r_\tau') = \langle z(r\tau) z(r_\tau') \rangle.$$  \hspace{1cm} (108)

The complex variables $z(r\tau)$ will be used for calculating the Fourier transformation of the phase-phase propagator. Putting Eq. (95) into the expression for $G_z(k \omega_n)$ in Eq. (94), we have

$$G_z(k \omega_n) = \beta N |\psi_0|^2 \delta_{k,0} \delta_{\omega_n,0} + \tilde{G}_z(k \omega_n).$$  \hspace{1cm} (109)
At the sufficiently low temperatures, the Eq. (109) defines the coherent macroscopic state, i.e., the BEC state. We can separate now the mode \( \{ q = 0, \omega_n = 0 \} \) for the condensate state of the function in Eq. (107). Using the Eq. (109) above we get

\[
G_{cf}(k\nu_n) = |\psi_0|^2 G_{ab}(k\nu_n) + \frac{1}{\beta N} \sum_{q \neq 0, \omega_n \neq 0} \tilde{G}_{z}(q\omega_n) G_{ab}(k - q, \nu_n - \omega_n) . \tag{110}
\]

As we see, the excitonic propagator composes of two parts: one responsible for the excitonic condensate and the on-condensate excitation part.

2. Spectral functions and the density of states (DOS)

Using Eq. (110) for the total excitonic propagator we can calculate the analytical form of the excitonic spectral function \( A_{cf}(k\omega) \) and, later on, the excitonic density of states (DOS) profiles for the condensate and non-condensate states in the system. We introduce here the excitonic spectral function \( A_{cf}(k\nu_n) \) that carries the same physical information as the correlation function \( G_{cf}(k\nu_n) \) itself. For this, it is sufficient to write the Cauchy formula for the correlation function by renaming it as the spectral function under the integral

\[
G_{cf}(k\nu_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{A_{cf}(k\omega)}{i\nu_n - \omega} d\omega. \tag{111}
\]

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

\[
G_{z}(k\omega_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{A_z(k\omega)}{i\omega_n - \omega} d\omega \tag{122}
\]

and

\[
G_{ab}(k\omega_n) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{A_{ab}(k\omega)}{i\nu_n - \omega} d\omega. \tag{133}
\]

Furthermore, using Eq. (110) we can write for the total spectral function \( A_{cf}(k\omega) \)

\[
A_{cf}(k\omega) = |\psi_0|^2 A_{ab}(k\omega) + \frac{1}{N} \sum_{q \neq 0} \int \frac{d\omega}{2\pi} A_z(q\omega) \times
\]

\[
\times A_{ab}(k - q, \omega - \omega') [n_B(-\omega') + n_F(\omega - \omega')]. \tag{144}
\]

From the spectral functions we can obtain the density of states (DOS) by summing over the reciprocal wave vectors \( \mathbf{k} \) with and appropriate normalization factor, hence, the total density of states is

\[
\rho_{cf}(\omega) = -\frac{1}{N} \sum_{\mathbf{k}} A_{cf}(k\omega). \tag{155}
\]

For the total excitonic DOS, we have an equation analogue to the Eqs. (109) and (113)

\[
\rho_{cf}(\omega) = |\psi_0|^2 \rho_{ab}(\omega) + \tilde{\rho}_{cf}(\omega), \tag{166}
\]

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

\[
\tilde{\rho}_{cf}(\omega) = \int_{-\infty}^{+\infty} \rho_{2}(\omega') \rho_{ab}(\omega - \omega') \times [n_B(\omega') + n_F(\omega - \omega')] d\omega'. \tag{177}
\]

A key feature of the result in Eq. (113), is that we have separated contributions from the condensate in a form of a sharp peak proportional to the amplitude \( \psi_0 \) and broader incoherent part \( \tilde{\rho}_{cf}(\omega) \). Within the thermal equilibrium the coherent part of the function \( \rho_{cf}(\omega) \) in Eq. (116) is sharp and is unaffected by the collisional broadening. This is the result of the long-range phase coherence in the excitonic system, which arises when a condensate of excitons has formed as shown in the real experiments on luminescence in the cuprous oxide excitonic system.

VII. CONCLUSION AND OUTLOOK

We have studied the excitonic phase transition in a system of conduction band electrons with transfer parameter \( t \) and valence band band holes described by the three-dimensional extended Falicov-Kimball model with tunable Coulomb interaction \( U \) between both species. To this end we implement the functional integral formulation of our model, where the Coulomb interaction term is expressed in terms of U(1) quantum phase variables \( \varphi \) conjugated to the local particle number, providing a useful representation of strongly correlated systems. At low temperatures the electron-hole system may become unstable with respect to the formation of the excitons at \( T = T_\Delta \), exhibiting a gap \( \Delta \) in the particle excitation spectrum controlled by the parameter \( U \), which gives the relevant energy scale 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 Bose-Einstein condensation at lower temperature \( T_c < T_\Delta \) controlled by the phase stiffness \( J \ll U \) between the excitonic pairs. Here, as a result the spontaneous U(1) 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 exciton 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 $U/t \gg 1$ we have the situation, where the pairs are strongly bound, but can be mutually uncorrelated with each other until they become phase coherent at $T_C$. Although, the excitonic gap can be used to explain some experimental results (like tunneling data and resistivity measurements), $\Delta$ is not signifying the macroscopic coherence in the excitonic system. For example, the exciton phase coherence may be evidenced by the coherence of their light emission, which can be studied by interferometry (see e.g., Ref. [17]) and the experiments on luminescence in the cuprous oxide excitonic system. Therefore, a possible direction for future work will be the determination of the single-particle excitation spectra, which would be instrumental for interpretation of the coherent light emission measurements in the excitonic system.

**Appendix A: Effective actions**

1. Fermionic action

We would like now to derive the effective action for fermions. Our starting point is the partition function given in the Eq. (29) derived with the help of the U(1) gauge transformation as it is introduced in the Section III which can be written as

$$Z = \int [D\bar{a}Da] [D\bar{b}Db] e^{-S_{\text{eff}}[\bar{a},a,\bar{b},b]}.$$  \hspace{1cm} (A1)

where the effective fermionic action $S_{\text{eff}}[\bar{a},a,\bar{b},b]$ in the exponential is defined as

$$S_{\text{eff}}[\bar{a},a,\bar{b},b] = -\ln \int [D\varphi] e^{-S[\bar{a},a,b]}.$$ \hspace{1cm} (A2)

Furthermore, we expand the logarithm keeping only the terms up to second order in $S$. As a result we obtain

$$S_{\text{eff}}[\bar{a},a,\bar{b},b] = S_0 + \langle S \rangle_{S_{\text{eff}}[\varphi]} - \frac{1}{2} \left[ \langle S^2 \rangle_{S_{\text{eff}}[\varphi]} - \langle S \rangle^2_{S_{\text{eff}}[\varphi]} \right].$$ \hspace{1cm} (A3)

Here, the averages with respect to the phase variables are defined as

$$\langle \ldots \rangle_{S_{\text{eff}}[\varphi]} = \frac{\int [D\varphi] \ldots e^{-S_{\text{eff}}[\varphi]} \int [D\varphi] e^{-S_{\text{eff}}[\varphi]}}. \hspace{1cm} (A4)$$

2. Phase action

In a similar way, the integration over the fermions in Eq. (29) gives the effective action for the phase sector. The partition function in this case is

$$Z = \int [D\varphi] e^{-S_{\text{eff}}[\varphi]},$$ \hspace{1cm} (A5)

where the effective phase action in the exponential is

$$S_{\text{eff}}[\varphi] = -\ln \int [D\bar{a}Da] [D\bar{b}Db] e^{-S}.$$ \hspace{1cm} (A6)

Again, expanding the logarithm in the Eq. (A6) we will have up to second order in $S$:

$$S_{\text{eff}}[\varphi] = \hat{S}_0 + \langle S \rangle_{S_{\text{eff}}[\bar{a},a,\bar{b},b]} - \frac{1}{2} \left[ \langle S^2 \rangle_{S_{\text{eff}}[\bar{a},a,\bar{b},b]} - \langle S \rangle^2_{S_{\text{eff}}[\bar{a},a,\bar{b},b]} \right].$$ \hspace{1cm} (A7)

where $\hat{S}_0$ is an unimportant constant. Here the fermionic average $\langle \ldots \rangle_{S_{\text{eff}}}$ is given by

$$\langle \ldots \rangle_{S_{\text{eff}}[\bar{a},a,\bar{b},b]} = \frac{\int [D\bar{a}Da] [D\bar{b}Db] \ldots e^{-S_{\text{eff}}[\bar{a},a,\bar{b},b]} \int [D\bar{a}Da] [D\bar{b}Db] e^{-S_{\text{eff}}[\bar{a},a,\bar{b},b]}}.$$ \hspace{1cm} (A8)

The Eq. (A3) is important for deriving the excitonic gap equation, while the relation in Eq. (A7) is crucial for deriving the phase stiffnesses.

**Appendix B: The phase stiffness**

We present here derivation of the phase stiffnesses, which are proportional to $tt'$ terms in the effective phase action in Eq. (A7). The derivation of the other term, proportional to $tt$, is very similar. Using Eq. (A7) and Eq. (27) we get for the mixed term $tt'$

$$\frac{1}{2} \sum_{(r_i,r_j)} \sum_{(r_i',r_j')} \int_0^\beta d\tau d\tau' \left( \bar{a}(r_i) a(r'_j) \bar{b}(r_j) b(r_j') \right) \times$$

$$e^{-\frac{1}{i} \left[ \varphi(r_i) - \varphi(r_j) \right]} e^{-\frac{1}{i} \left[ \varphi(r_i') - \varphi(r_j') \right]}$$

$$+ t(r_i r_i') \bar{b}(r_j r_j') \left( \bar{a}(r_i) a(r_j) \bar{b}(r_i') b(r_j') \right) \times$$

$$e^{-\frac{1}{i} \left[ \varphi(r_i) - \varphi(r_i') \right]} e^{\frac{1}{i} \left[ \varphi(r_j) - \varphi(r_j') \right]}$$

$$+ t(r_j r_j') \bar{b}(r_i r_i') \left( \bar{a}(r_j) a(r_i) \bar{b}(r_j') b(r_j') \right) \times$$

$$e^{\frac{1}{i} \left[ \varphi(r_i) - \varphi(r_i') \right]} e^{-\frac{1}{i} \left[ \varphi(r_j) - \varphi(r_j') \right]}$$

$$+ t(r_i r_j) \bar{b}(r_i r_j') \left( \bar{a}(r_i) a(r_j) \bar{b}(r_i') b(r_j') \right) \times$$

$$e^{-\frac{1}{i} \left[ \varphi(r_i) - \varphi(r_i') \right]} e^{\frac{1}{i} \left[ \varphi(r_j) - \varphi(r_j') \right]}$$

$$+ t(r_i r_j') \bar{b}(r_i r_j) \left( \bar{a}(r_i) a(r_j) \bar{b}(r_i') b(r_j') \right) \times$$

$$e^{\frac{1}{i} \left[ \varphi(r_i) - \varphi(r_i') \right]} e^{-\frac{1}{i} \left[ \varphi(r_j) - \varphi(r_j') \right]}.$$ \hspace{1cm} (B1)
As an example, we give the Wick averaging result of the first four-fermion term in the expression of Eq. (B1)

\[
\langle \bar{a}(r_1\tau)a(r_1'\tau)b(r_2'\tau')b(r_2') \rangle = \\
\langle \bar{a}(r_1\tau)a(r_1'\tau) \rangle \langle b(r_2'\tau')b(r_2') \rangle \\
- \langle \bar{a}(r_1\tau)b(r_2'\tau') \rangle \langle a(r_1'\tau)b(r_2') \rangle \\
+ \langle \bar{a}(r_1\tau)b(r_2'\tau') \rangle \langle a(r_1'\tau)b(r_2') \rangle \\
= G^{aa}(r_1' - r_1, 0)G^{bb}(r_2' - r_2, 0) \\
- G^{ab}(r_1 - r_2, \tau - \tau')G^{ba}(r_2 - r_1', \tau - \tau'). \quad (B2)
\]

We kept in Eq. (B2) only the terms proportional to excitonic gap. We neglected other terms like \(\langle \bar{a}(r\tau)b(r'\tau') \rangle\) or \(\langle a(r\tau)b(r'\tau') \rangle\), which vanish due to the symmetry of the action in Eq. (B5). Contributions, proportional to fermionic densities \(\langle \bar{a}(r\tau)a(r'\tau') \rangle\) and \(\langle b(r\tau)b(r'\tau') \rangle\) could be also omitted, since they are not contributing directly to the excitonic pair formation.

After calculating all averages in Eq. (B1) and recombining them with the similar terms coming from the component proportional to \(\dot{t}\tau\), we obtain the relevant portion of the phase action in the form

\[
S_J[\varphi] = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{rr'} \{ J(rr', r'\tau') \cos [\varphi(rr) + \varphi(rr') - \varphi(r\tau) - \varphi(r'\tau)] \\
+ G_{ab}(0, \tau - \tau')\bar{G}_{ba}(0, \tau' - \tau) \cos [\varphi(rr) - \varphi(r\tau') - \varphi(r'\tau) + \varphi(r'\tau')] \}, \quad (B3)
\]

containing phase stiffness parameter \(J\)

\[
J(rr', r'\tau') = -4\dot{t}G_{ab}(r - r', \tau - \tau')\bar{G}_{ba}(r - r', \tau' - \tau). \quad (B4)
\]

Furthermore, in order to simplify the non-local (in time variable) effective phase action in Eq. (B3) we resort to the gradient expansion of the phase field in the form

\[
\varphi(rr') = \varphi(rr) + (r' - \tau) \partial_r \varphi(rr) + O \left( (r' - \tau)^2 \right). \quad (B5)
\]

\[
G_{ab}(\tau - \tau')\bar{G}_{ba}(\tau' - \tau) = \frac{4\Delta^2 U^2}{z^2(\beta N)^2} \sum_{kk'} \sum_{\nu_n, \nu_n'} \frac{\epsilon(k) \epsilon(k')}{\sqrt{\xi_k + 4\Delta^2}} \frac{e^{-i(\nu_n - \nu_n')\delta}}{[C^a_k(\nu_n)C^b_k(\nu_n) - |\Delta|^2] [C^b_k(\nu_n')C^a_k(\nu_n') - |\Delta|^2].} \quad (B7)
\]

Here \(z = 6\) is the number of the nearest neighbor sites on the three-dimensional cubic lattice. After integrating over the imaginary time \(\tau'\) in Eq. (B6), we perform the Matsubara frequency summations in Eq. (B7) and obtain the phase stiffness parameter \(J\) in Eq. (B6) in the final form

\[
J = \frac{16\Delta^2 \dot{t}}{z^2 N^2} \sum_{kk'} \frac{\epsilon(k) \epsilon(k')}{\sqrt{\xi_k + 4\Delta^2}} \left[ \Lambda_1(kk') \tanh \left( \frac{\beta E_k^+}{2} \right) - \Lambda_2(kk') \tanh \left( \frac{\beta E_k^-}{2} \right) \right]. \quad (B8)
\]

The parameters \(\Lambda_1(kk')\) and \(\Lambda_2(kk')\) entering in Eq. (B8) are given by

\[
\Lambda_1(kk') = \frac{1}{E^+(k) - E^+(k')} \cdot \frac{1}{E^+(k) - E^-(k')}, \quad \Lambda_2(kk') = \frac{1}{E^-(k) - E^-(k')} \cdot \frac{1}{E^-(k) - E^+(k')}. \quad (B9)
\]
Following the Section VI the summations over the $k$ wave vectors in Eq. (B8) could be transformed into the integrations with the help of the density of states given in Eq. (B3). As we see, Eq. (B8) relates the phase stiffness parameter $J$ with the local pairing gap $\Delta$. The physical significance of this fact is that the excitonic pair formation is a precondition for the appearance of the phase stiffness and subsequent phase coherence of the preformed excitonic pairs. The numerical evaluations of the expression in Eq. (B8) for $T = 0$ K are presented in Fig. 16 and discussed in the Section VI of the present paper.

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