The fate of the excitonic insulator in the presence of phonons

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The fate of the excitonic insulator in the presence of phonons on the formation of the excitonic insulator has hardly been analyzed so far. Recent experiments on Ta\textsubscript{2}NiSe\textsubscript{5}, 1T-TiSe\textsubscript{2}, and TmSe\textsubscript{0.45}Te\textsubscript{0.55}, being candidates for realizing the excitonic-insulator state, suggest, however, that the underlying lattice plays an important role. Employing the Kadanoff-Baym approach we address this issue theoretically. We show that owing to the electron-phonon coupling a static lattice distortion may arise at the excitonic instability. Most importantly such a distortion will destroy the acoustic phase mode being present if the electron-hole pairing and condensation is exclusively driven by the Coulomb interaction. The absence of this mode when lattice degrees of freedom are involved challenges that the excitons in these materials form a true condensate exhibiting off-diagonal long-range order.

I. INTRODUCTION

The excitonic insulator (EI) is a longstanding problem in condensed matter physics. Although first theoretical work dates back almost a century,\textsuperscript{1–5} the experimental realization of the EI phase has proven to be quite challenging. In recent years a number of mixed-valent rare-earth chalcogenide and transition-metal dichalcogenide materials have been presented,\textsuperscript{6–8} which are promising in this respect and have renewed the interest in the EI also from the theoretical side.\textsuperscript{9–14}

An EI instability can be triggered by the Coulomb interaction between electrons and holes. Therefore, the theoretical modeling typically focuses on a purely electronic mechanism. First attempts to include a coupling to the lattice degrees of freedom have been made quite recently, motivated by several experiments indicating that the lattice is involved at the phase transition to the anticipated EI phase.\textsuperscript{15–19} For example, in the TmSe\textsubscript{0.45}Te\textsubscript{0.55} compound a drop of the specific heat and an increase of the lattice constant have been interpreted as a strong coupling between excitons and phonons.\textsuperscript{20}

Furthermore, in 1T-TiSe\textsubscript{2} there is a longstanding debate whether the charge-density-wave and the concomitant structural phase transition observed in this material are the results of an excitonic\textsuperscript{7,11} or a lattice instability.\textsuperscript{21,22} A combination of both instabilities was also proposed.\textsuperscript{23,24} Without any doubt, lattice effects are crucial in this material. Finally, at the transition to the suggested EI phase in Ta\textsubscript{2}NiSe\textsubscript{5} the lattice structure changes from orthorhombic to monoclinic, although the charge does not modulate.\textsuperscript{16,17,25} Therefore, the electron-phonon interaction seems non-negligible in this material as well.

Motivated by these findings, we analyze the EI formation in the framework of a rather generic two-band model that comprises both the Coulomb interaction and an explicit electron-phonon coupling. Besides its relevance to the materials under study, some fundamental theoretical questions are brought up in this model. So we address the electron-hole pair spectrum and the nature of condensate respectively of the ordered ground state.

The paper is organized as follows. In Sec. II we introduce our model. A mean-field treatment in terms of the electron Green functions is given in Sec. III. In Sec. IV we calculate the electronic self energies using a Kadanoff-Baym approach. From this, we argue that the considered electron-phonon interaction does not lead to a qualitative modification of the single-particle spectra. The electron-hole pair spectrum, on the other hand, indicates a strong influence of the phonons. This is shown in Sec. V. How the lattice dynamics affects the electron-hole pairing is analyzed in the framework of a Kadanoff-Baym approach. We present some numerical results in Sec. VI and show that the purely electronic model possesses an acoustic mode, whereas the collective mode becomes massive if phonons participate. Section VII finally addresses the question whether the excitonic ground state represents a true condensate. To this end, we discuss the presence of off-diagonal long range order. A short summary of our results is given in Sec. VIII.

II. MODEL

For our analysis, we start from a two-band model with interband Coulomb interaction and an explicit electron-phonon coupling,

\begin{equation}
H = H_e + H_{e-e} + H_{ph} + H_{e-ph}.
\end{equation}

The noninteracting band-electron contribution is given by

\begin{equation}
H_e = \sum_{k} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma},
\end{equation}

where \(c_{k\sigma}^{(1)}\) is the annihilation (creation) operator for an electron with momentum \(k\) in the valence band (band index \(\sigma = v\)) or in the conduction band (\(\sigma = c\)). The corresponding band dispersions are denoted as \(\varepsilon_{k\sigma}\). We
consider an electron-electron interaction of the form
\[ H_{e-e} = \sum_{k, k', q} \frac{V(q)}{N} c_{k} c_{k+q} c_{k'} c_{k'+q}, \]
where \( V(q) \) is the effective Coulomb repulsion. \( N \) is the number of unit cells. In harmonic approximation, the phonon Hamiltonian reads
\[ H_{ph} = \sum_{q} \omega_{q} b_{q}^{\dagger} b_{q}, \]
where \( \omega_{q} \) is the bare phonon frequency, and \( b_{q}^{(\dagger)} \) is the annihilation (creation) operator for a phonon with momentum \( q \). Throughout this paper we set \( \hbar = 1 \).

If the electron-phonon interaction is assumed to be
\[ H_{e-ph} = \sum_{k, q} \left( \frac{g_{q}}{\sqrt{N}} (b_{-q}^{\dagger} + b_{q}^{\dagger}) c_{k} c_{k+q} + \text{H.c.} \right), \]
the phonon directly couples to an electron-hole pair with the (real) coupling constant \( g_{q} \). Then, the annihilation of a phonon is inevitably connected with a transfer of an electron from the valence band to the conduction band and vice versa. Such a coupling of phonons to excitons may look rather specific, but for materials near the semimetal-semiconductor transition (SM-SC) it is of relevance.

In order to model the SM-SC transition, we consider the case of half-filling,
\[ n_{e} + n_{v} = 1, \]
where \( n_{\sigma} = \frac{1}{N} \sum_{k} (c_{k \sigma}^{\dagger} c_{k \sigma}) \).

III. MEAN-FIELD GREEN FUNCTIONS

The electron-phonon coupling (5) may cause a deformation of the lattice at sufficiently low temperatures. A static lattice distortion is characterized by
\[ \delta_{Q} = \frac{2}{\sqrt{N}} g_{Q} (b_{Q}^{\dagger}), \]
where the ordering vector of the dimerized phase is denoted as \( Q \). Working at half-filling, we assume that \( Q \) is either zero or half a reciprocal lattice vector. Then the parameter \( \delta_{Q} \) is a real number that measures the amplitude of the static lattice distortion. Adopting the frozen phonon approximation we replace the phonon operators by their averages. Then, the Hamiltonian (1) describes an effective electronic system.

Applying subsequently a Hartree-Fock decoupling scheme, our model reduces to
\[ H_{MF} = \sum_{k} \bar{\varepsilon}_{k} c_{k}^{\dagger} c_{k} + \sum_{k} \bar{\varepsilon}_{k+Q} c_{k+Q}^{\dagger} c_{k+Q} + \bar{x}_{Q} c_{k}^{\dagger} c_{k+Q} c_{k+Q}^{\dagger} + C_{\text{dec}} \]
with renormalized dispersions \( \bar{\varepsilon}_{k \sigma} = \varepsilon_{k \sigma} + V(0)n_{-\sigma} \). In Eq. (8),
\[ x_{Q} = \delta_{Q} - \Delta_{Q}, \]
is the gap parameter,
\[ \Delta_{Q} = \frac{1}{N} \sum_{k'} V(k' - k + Q) \langle c_{k'}^{\dagger} c_{k+Q} c_{k+Q}^{\dagger} c_{k} \rangle \]
is the Coulomb-induced hybridization between the valence band and the conduction band, and
\[ C_{\text{dec}} = \frac{1}{N} \sum_{k, k'} V(k' - k + Q) \langle c_{k+Q}^{\dagger} c_{k+Q} c_{k}^{\dagger} c_{k} \rangle \]
\[ + \frac{N}{4} \omega_{Q} \delta_{Q}^{2} - NV(0)n_{e} n_{v}, \]
For an undistorted lattice \( \Delta_{Q} \) serves as the EI order parameter, whose phase is undetermined and can be chosen arbitrarily. A finite lattice distortion removes this freedom. If \( \delta_{Q} \) is real, \( \Delta_{Q} \) is real too.

In mean-field approximation the electronic Green functions become
\[ G_{e}(k, z_{1}) = \langle c_{k}^{\dagger} c_{k} \rangle = u_{k}^{2} G_{A}(k, z_{1}) + u_{k}^{2} G_{B}(k, z_{1}), \]
\[ G_{e}(k + Q, z_{1}) = \langle c_{k+Q}^{\dagger} c_{k} \rangle = u_{k}^{2} G_{A}(k, z_{1}) + u_{k}^{2} G_{B}(k, z_{1}), \]
\[ F(k, z_{1}) = \langle c_{k+Q}^{\dagger} c_{k} \rangle = -u_{k} v_{k} [G_{B}(k, z_{1}) - G_{A}(k, z_{1})] \]
\[ = \langle c_{k+Q}^{\dagger} c_{k+Q} \rangle = F_{k}(k, z_{1}), \]
where \( z_{1} \) denotes fermionic Matsubara frequencies, and
\[ G_{A/B}(k, z_{1}) = \frac{1}{z_{1} - E_{k}/z} - \frac{1}{E_{k}/z}, \]
\[ E_{k/A/B} = \frac{1}{2} \left( \bar{\varepsilon}_{k+Q} + \bar{\varepsilon}_{k} \right) \pm \frac{1}{2} \left( \bar{\varepsilon}_{k+Q} - \bar{\varepsilon}_{k} \right)^{2} + x_{Q}^{2} \]
\[ u_{k}^{2} / v_{k}^{2} = \frac{1}{2} \pm \frac{1}{2} \left( \bar{\varepsilon}_{k+Q} - \bar{\varepsilon}_{k} \right) \pm \frac{1}{2} \left( \bar{\varepsilon}_{k+Q} - \bar{\varepsilon}_{k} \right)^{2} + x_{Q}^{2} \]

One can easily show that \( \Delta_{Q} \times \delta_{Q} \) Moreover, \( \delta_{Q} \) and \( \Delta_{Q} \) couple to the same set of operators and, therefore, enter the quasiparticle dispersion in equal manner. Hence, at the mean-field level of approximation we cannot discriminate between a Coulomb-driven or a phonon-driven phase transition.
IV. ELECTRONIC SELF ENERGY

We now analyze self-energy effects. To this end, we use the technique developed by Kadanoff and Baym and determine the self energy of the electrons.\textsuperscript{27} The imaginary-time Green functions are defined as

\begin{align}
G_v(k, t - t') &= -i \langle T [c_{kv}(t)c_{vk'}(t')] \rangle, \\
G_c(k, t - t') &= -i \langle T [c_{kv}(t)c_{kv'}(t')] \rangle, \\
F(k, t - t') &= -i \langle T [c_{kv+Q}(t)c_{kv'}(t')] \rangle, \\
F^\dagger(k, t - t') &= -i \langle T [c_{kv}(t)c_{kv+Q}(t')] \rangle,
\end{align}

with imaginary-time variables \(t\) and \(t'\).

We start from the equation of motion (EOM) for the valence-electron Green function,

\[
\left( i \frac{\partial}{\partial t} - \varepsilon_{kv} \right) G_v(k, t - t') = \delta(t - t') - i \sum_q \frac{g_q}{\sqrt{N}} G_v^\dagger(k, q, t, t') - i \sum_{k', q} V_c(q) G_v^\dagger(k, k', q, t, t'),
\]

where

\[
G_v^\dagger(k, k', q, t, t') = \left\langle T [c_{kv}(t)c_{k'v}(t)c_{k'v+q}(t)c_{kv}(t')] \right\rangle,
\]

\[
G_c^\dagger(k, q, t, t') = \left\langle T [b_{kv}^\dagger(t+b_{kv})c_{kv+q}(t)c_{k'v}(t')] \right\rangle,
\]

and proceed as follows: The auxiliary correlation functions (23) and (24) are expanded up to first order in the interactions they couple to, i.e., \(G_v^\dagger(k, k', q, t, t')\) is expanded up to linear order in \(V_c(q)\) and \(G_c^\dagger(k, q, t, t')\) is expanded up to linear order in \(g_q\). Subsequently, we decouple the correlation functions taking only electron-hole fluctuations into account.

Straight forward calculation yields

\[
\left( i \frac{\partial}{\partial t} - \varepsilon_{kv} \right) G_v(k, t - t') = \delta(t - t') + x_{kvQ} F(k, t - t') - \int_0^{-i\beta} d\tau \sigma_{vv}(k, t - \tau) G_v(k, \tau - t') - \int_0^{-i\beta} d\tau \sigma_{vF}(k, t - \tau) F(k, \tau - t'),
\]

(here \(\beta\) is the inverse temperature), with the self energies

\[
\sigma_{vv}(k, t - \tau) = \frac{1}{N^2} \sum_{q, q', Q} V_c(q) V_c(q') G_v(k + Q, t - \tau) \times G_v(Q, k + Q' - k - q, \tau - t) - \frac{i}{N} \sum_q |g_q|^2 D(q, \tau - t) G_v(k + q, t - \tau),
\]

\[
\sigma_{vF}(k, t - \tau) = \frac{1}{N^2} \sum_{q, q', Q} V_c(q) V_c(q') F(k + Q, t - \tau) \times F(Q, k + Q - q', k - q, \tau - t) - \frac{i}{N} \sum_q |g_q|^2 D(q, \tau - t) F(k + q, Q, \tau - t).
\]
with

\[
\sigma_{Fv}(k, t - \tau) = \frac{1}{N^2} \sum_{q, q', Q} V_v(q) V_v(q') F(k + Q - q, t - \tau) \\
\times H_2(Q, k + q', k + q + Q - Q, \tau - t) \\
- \frac{i}{N} \sum_q |g_q|^2 D(q, t - \tau) F^\dagger(k + Q - q, t - \tau),
\]

(36)

\[
\sigma_{FF}(k, t - \tau) = \frac{1}{N^2} \sum_{q, q', Q} V_v(q) V_v(q') G_v(k + Q - q, t - \tau) \\
\times G_2(Q, k + q + Q, k + Q - q', t - \tau) \\
- \frac{i}{N} \sum_q |g_q|^2 D(q, t - \tau) G_v(k + Q - q, t - \tau).
\]

(37)

Note that both the electron-electron interaction and
the electron-phonon interaction couple different species
(valence electrons, conduction electrons, and electrons in
the hybridized state) to each other. The structure of the
self energies shows that the one-particle spectrum cannot
be used to decide whether the ordered ground state is
the effect of the Coulomb interaction alone or if phonons
contribute, at least at this level of approximation. Let
us therefore analyze the electron-hole pair spectrum in
the following.

V. ELECTRON-HOLE PAIR SPECTRUM

In the Bethe-Salpeter equation, describing the correla-
tions of electron-hole pairs, the Coulomb interaction is
treated in ladder approximation. In the vicinity of the
SM-SC transition, the small number of free electrons and
holes makes two-particle collisions to be the dominant
process. The ladder approximation takes the sequence
of these collisions into account and is suitable to describe
both the buildup of excitons and the formation of the
EL.14

We now work out the influence of \(H_{e-ph}\) [Eq. (5)] on
the electron-hole pairs. The four-time electron-hole pair
correlation functions are defined as

\[
G_2(Q, k, k', t_1, t_2, t_3, t_4) = \\
- \langle T[c_{k}^\dagger(t_1)c_{k + Qc}^\dagger(t_2)c_{k' + Qc}^\dagger(t_4)c_{k'c}(t_3)] \rangle,
\]

(38)

\[
F_2(Q, k, k', t_1, t_2, t_3, t_4) = \\
- \langle T[c_{k - Qc}^\dagger(t_1)c_{kuc}(t_2)c_{k' + Qc}^\dagger(t_4)c_{k'c}(t_3)] \rangle.
\]

(39)

The relations to the two-time electron-hole pair correla-
tion functions, occurring in Sec. IV, are

\[
G_2(Q, k, k', t - t') = G_2(Q, k, k', t, t', t')
\]

and

\[
F_2(Q, k, k', t - t') = F_2(Q, k, k', t, t', t').
\]

In order to analyze the effects of the phonons within the Kadanoff-Baym scheme,27 we expand the correlation functions (38) and (39) to leading order in the electron-phonon coupling. Restricting
ourselves to the study of electron-hole pairs, there are no incoming or outgoing phonon branches. Hence, the phonons must be created and annihilated in one diagram, and the first non-vanishing contribution is of second
order in the electron-phonon coupling constant \(g_q\). The
many-particle correlation functions that occur in the
leading order expansion of \(G_2(Q, k, k', t_1, t_2, t_3, t_4)\) and
\(F_2(Q, k, k', t_1, t_2, t_3, t_4)\) are subsequently decoupled into
electron-hole pair correlation functions, electron Green
functions, and phonon Green functions. We identify two
effects of \(H_{e-ph}\): Excitons can be created (annihilated)
by the annihilation (creation) of a phonon, and phonons
may change the individual momenta of the electron and
the hole in the bound state without modifying the mo-
mentum of the exciton. This is illustrated by diagrams
depicted in Fig. 1.

\[FIG. 1. \text{Diagrams occurring in the equations for the electron-}\]

hole pair correlation functions. First row: Single particle
Green functions \(G_v, G_e\) (left hand side) and \(F, F^\dagger\) (right
hand side). Second row: Ladder approximation for the
Coulomb interaction. Third row: Ring diagrams including
the electron-phonon interaction. Fourth row: Ladder di-
agrams including the electron-phonon interaction. The dashed
lines with the vertex points represent the Coulomb interac-
tion, the wavy lines represent the phonon Green function, and
the vertex squares represent our electron-phonon interaction.

If both Coulomb and phonon effects are of importance,
the electron-hole pair correlation function (38) has to be
calculated according to
\[ G_2(Q, k, k', t_1, t_2, t_3, t_4) = G_2^{(0)}(Q, k, t_1, t_2, t_3, t_4) \delta_{k, k'} \]
\[- i \frac{1}{N} \int_{0}^{-i\beta} d(\tau - t_4) \sum_{q} V_{\epsilon}(q) G_2^{(0)}(Q, k, t_1, t_2, \tau, \tau) G_2(Q, k + q, k', \tau, \tau, t_3, t_4) \]
\[- i \frac{1}{N} \int_{0}^{-i\beta} d(\tau - t_4) \sum_{q} V_{\epsilon}(q) F_2^{(0)}(Q, k, t_1, t_2, \tau, \tau) F_2(Q, k + q + Q, k', \tau, \tau, t_3, t_4) \]
\[ + i \frac{1}{N} \int_{0}^{-i\beta} d(\tau - t_4) \int_{0}^{-i\beta} d(\tau' - t_4) \sum_{q} \left( |g_q|^2 D(Q, \tau - \tau') |G_2^{(0)}(Q, k, t_1, t_2, \tau, \tau) \right) \]
\[- F_2^{(0)}(Q, k, k', t_1, t_2, \tau, \tau, t_3, t_4) \]
\[ F_2^{(0)}(Q, k, t_1, t_2, t_3, t_4) = - F(k, t_3 - t_1) F(k + Q, t_2 - t_4). \]

Typical diagrams occurring in Eq. (40) are shown in Fig. 1.

If \( x_{kQ} \neq 0 \), \( G_2(Q, k, k', t_1, t_2, t_3, t_4) \) is coupled to \( F_2(Q, k, k', t_1, t_2, t_3, t_4) \), which can be calculated from

\[ F_2(Q, k, k', t_1, t_2, t_3, t_4) = F_2^{(0)}(Q, k, t_1, t_2, t_3, t_4) \delta_{k, k'} + \]
\[- i \frac{1}{N} \int_{0}^{-i\beta} d(\tau - t_4) \sum_{q} V_{\epsilon}(q) F_2^{(0)}(Q, k, t_1, t_2, \tau, \tau) G_2(Q, k + q + Q, k', \tau, \tau, t_3, t_4) \]
\[- i \frac{1}{N} \int_{0}^{-i\beta} d(\tau - t_4) \sum_{q} V_{\epsilon}(q) G_2^{(0)}(Q, k, t_1, t_2, \tau, \tau) F_2(Q, k + q + Q, k', \tau, \tau, t_3, t_4) \]
\[ + i \frac{1}{N} \int_{0}^{-i\beta} d(\tau - t_4) \int_{0}^{-i\beta} d(\tau' - t_4) \sum_{q} \left( |g_q|^2 D(Q, \tau - \tau') |G_2^{(0)}(Q, k, t_1, t_2, \tau, \tau) \right) \]
\[- F_2^{(0)}(Q, k, k', t_1, t_2, \tau, \tau, t_3, t_4) \]
\[- |g_{k-k'}|^2 D(Q + k - \tau, \tau') G_2^{(0)}(Q, k, k', \tau, \tau', t_3, t_4) \]
\[- |q_{k-k'}|^2 D(Q + k - \tau, \tau') F_2^{(0)}(Q, k, k', \tau, \tau', t_3, t_4) \]
\[ F_2^{(0)}(Q, k, k', t_1, t_2, \tau, \tau, t_3, t_4) = - F(k, t_3 - t_1) F(k + Q, t_2 - t_4). \]

where

\[ \tilde{G}_2^{(0)}(Q, k, t_1, t_2, t_3, t_4) = - G_c(k - Q, t_3 - t_1) G_c(k, t_2 - t_4), \]

\[ \tilde{F}_2^{(0)}(Q, k, k', t_1, t_2, t_3, t_4) = - F(k - Q, t_3 - t_1) F(k, t_2 - t_4). \]

For an explicit calculation of the electron-hole pair correlation functions the Matsubara technique is advantageous. Performing the transformation

\[ G_2(Q, k, k', t_1, t_2, t_3, t_4) = \int_{0}^{-i\beta} d(t_1 - t_4) e^{-i\tau_1(t_1 - t_4)} \int_{0}^{-i\beta} d(t_2 - t_4) e^{-i\tau_2(t_2 - t_4)} \int_{0}^{-i\beta} d(t_3 - t_4) e^{-i\tau_3(t_3 - t_4)} \]
\[ \times G_2(Q, k, k', t_1, t_2, t_3, t_4), \]
we obtain
\[
G_2(Q, k, k', z_1, z_2, z_3) = G_2^{(0)}(Q, k, z_1, z_2, z_3) \delta_{k, k'}
\]
\[
- i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q V_e(q) G_2^{(0)}(Q, k, z_1, z_2, z_4) G_2(Q, k + q, k', z_5, z_1 + z_2 - z_5, z_3)
\]
\[
- i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q V_e(q) F_2^{(0)}(Q, k, z_1, z_2, z_4) F_2(Q, k + q + Q, k', z_5, z_1 + z_2 - z_5, z_3)
\]
\[
+ i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q |g_Q|^2 D(Q, z_1 + z_2) \left[ G_2^{(0)}(Q, k, z_1, z_2, z_4) + F_2^{(0)}(Q, k, z_1, z_2, z_4) \right]
\]
\[
\times \left[ G_2(Q, k, k', z_5, z_1 + z_2 - z_5, z_3) + F_2(Q, q, k', z_5, z_1 + z_2 - z_5, z_3) \right]
\]
\[
- i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q \left[ |g_Q + k - q|^2 D(Q + k - q, z_4 + z_5) \right]
\]
\[
\times G_2^{(0)}(Q, k, z_1, z_2, z_4) F_2(Q, q, k', z_5, z_1 + z_2 - z_5, z_3)
\]
\[
+ |g_{k - q}|^2 D(k - q, z_4 + z_5) F_2^{(0)}(Q, k, z_1, z_2, z_4) G_2(Q, k - q, k', z_5, z_1 + z_2 - z_5, z_3) \]
\]
\[
(47)
\]
and
\[
F_2(Q, k, k', z_1, z_2, z_3) = F_2^{(0)}(Q, k, z_1, z_2, z_3) \delta_{k, k'} + Q + q + k'
\]
\[
- i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q V_e(q) G_2^{(0)}(Q, k, z_1, z_2, z_4) F_2(Q, k + q, k', z_5, z_1 + z_2 - z_5, z_3)
\]
\[
- i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q V_e(q) F_2^{(0)}(Q, k, z_1, z_2, z_4) G_2(Q, k + q + Q, k', z_5, z_1 + z_2 - z_5, z_3)
\]
\[
+ i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q |g_Q|^2 D(Q, z_1 + z_2) \left[ G_2^{(0)}(Q, k, z_1, z_2, z_4) + F_2^{(0)}(Q, k, z_1, z_2, z_4) \right]
\]
\[
\times \left[ G_2(Q, q, k', z_5, z_1 + z_2 - z_5, z_3) + F_2(Q, q, k', z_5, z_1 + z_2 - z_5, z_3) \right]
\]
\[
- i \left( \frac{1}{-i \beta} \right)^2 \sum_{z_4, z_5} \sum_q \left[ |g_Q + q - k|^2 D(Q + q - k, z_4 + z_5) \right]
\]
\[
\times \tilde{G}_2^{(0)}(Q, k, z_1, z_2, z_4) G_2(Q, q, k', z_5, z_1 + z_2 - z_5, z_3)
\]
\[
+ |g_{q - k}|^2 D(q - k, z_4 + z_5) \tilde{F}_2^{(0)}(Q, k, z_1, z_2, z_4) F_2(Q, q - k, k', z_5, z_1 + z_2 - z_5, z_3) \]
\]
\[
(48)
\]
where \( z_i, i = 1 \ldots 5 \), are fermionic Matsubara frequencies.

The collective excitations in the electron-hole pair spectrum can be assigned to phase and amplitude modes. The phase mode are determined by the poles of
\[
P(Q, z_\nu) = i \sum_{k, k'} [G_2(Q, k, k', z_\nu) - F_2(Q, k, k', z_\nu)]
\]
\[
(49)
\]
while the amplitude mode are given by the poles of
\[
A(Q, z_\nu) = i \sum_{k, k'} [G_2(Q, k, k', z_\nu) + F_2(Q, k, k', z_\nu)]
\]
\[
(50)
\]
where
\[
G_2(Q, k, k', z_\nu) = \left( \frac{1}{-i \beta} \right)^2 \sum_{z_2, z_3} G_2(Q, k, k', z_\nu - z_2, z_2, z_3)
\]
\[
(51)
\]
and \( F_2(Q, k, k', z_\nu) \) is defined accordingly.

**VI. RESULTS AND DISCUSSION**

In the numerical evaluation of the equations derived so far we work at zero temperature and assume a local Coulomb potential \([V(q) = U]\), a momentum-independent electron-phonon coupling \((g_q = g_Q)\), and dispersionless Einstein phonons \((\omega_q = \omega_Q)\). We fur-
thermore consider a direct band-gap situation, i.e., the valence-band maximum and the conduction-band minimum are located at the Brillouin-zone center. Then, the ordering vector of the low-temperature phase is \( \mathbf{Q} = 0 \). To avoid heavy numerics, we consider a two-dimensional (square) lattice. For this, the bare band dispersions 
\[ \varepsilon_{\text{ker}} = E_\sigma - 2 t_\sigma [\cos(k_x) + \cos(k_y)] \] 
(\( \sigma = v, c \)), where \( t_c \) sets the unit of energy. Typical model parameters are: \( E_v = -2.4 \), \( E_c = 0 \), \( t_v = -0.8 \), and \( \omega_Q = 0.01 \). Performing the analytic continuation \( z_\nu \to \omega + i\delta \), we use \( \delta = 2 \cdot 10^{-3} \). Moreover, we use the Hartree-Fock single-particle Green functions in the calculation.

### A. Vanishing electron-phonon coupling

We start our analysis for a system, where the phonons are neglected (\( g_Q = 0 \)). In this case, the phase and amplitude correlation functions can be calculated according to

\[
P(Q, z_\nu) = \frac{1}{2} U \left[ P^{(0)}(Q, z_\nu) + P^{(0)}(-Q, -z_\nu) \right] P(Q, z_\nu)
- \frac{1}{2} U \left[ P^{(0)}(Q, z_\nu) - P^{(0)}(-Q, -z_\nu) \right] A(Q, z_\nu)
+ P^{(0)}(Q, z_\nu)
\]

(52)

and

\[
A(Q, z_\nu) = \frac{1}{2} U \left[ P^{(0)}(Q, z_\nu) - P^{(0)}(-Q, -z_\nu) \right] P(Q, z_\nu)
- \frac{1}{2} U \left[ A^{(0)}(Q, z_\nu) - A^{(0)}(-Q, -z_\nu) \right] A(Q, z_\nu)
+ A^{(0)}(Q, z_\nu),
\]

(53)

respectively. We note that in general phase and amplitude modes are coupled to each other, i.e. the collective excitations are a mixture of both.

Figure 2 shows the phase mode for weak and strong couplings. Obviously, there exists a gapless phase mode in the EI state, i.e., \( \omega(Q) \to 0 \) for \( Q \to 0 \).\textsuperscript{29-31} The appearance of this mode can be attributed to the U(1) symmetry of the underlying electronic model \( H = H_c + H_{\text{e-e}} \).\textsuperscript{32} Because of this symmetry the phase of \( \Delta_{kQ} \) can be chosen arbitrarily, which results in such an acoustic mode.

Figure 2 furthermore reveals the different character of the phase mode for weak- and strong-coupling situations. In the weak-coupling, BCS-type pairing regime \( (U = 3.03) \) \( \omega(Q) \) exhibits a steep increase for small momenta and, as a result, quickly enters the electron-hole continuum, which it leaves again close to the Brillouin-zone corner. The lower boundary of the electron-hole continuum is given by

\[
\omega_C(Q) = \min_k (E_{kA} + Q \cdot A - E_{kB}),
\]

(54)

where \( E_{kA} \) and \( E_{kB} \) \( (E_{kA} > E_{kB}) \) are the renormalized quasiparticle energies in the ordered ground state.

In Hartree-Fock approximation the \( E_{kA,B} \) follow from Eq. (16). The momentum dependence of the excitation energy of the mode changes remarkably when the boundary to the electron-hole continuum is crossed. Contrariwise, in the strong-coupling, BEC-type pairing regime, the collective phase mode entirely lies below the electron-hole continuum and is a smooth function.\textsuperscript{31}

The existence of an acoustic phase mode can be understood as follows. Here, the static uniform limit of the noninteracting phase correlation function is well defined, i.e.,

\[
\lim_{Q \to 0} \left[ \lim_{\omega \to 0} P(Q, \pm Q, \pm \omega) \right] = \lim_{Q \to 0} \left[ \lim_{\omega \to 0} P(Q, \pm Q, \pm \omega) \right] = P(0, 0).
\]

(55)

The same does not hold for the amplitude correlation function, however,

\[
\lim_{Q \to 0} \left[ \lim_{\omega \to 0} A(Q, \omega) \right] \neq \lim_{Q \to 0} \left[ \lim_{\omega \to 0} A(Q, \omega) \right].
\]

(56)

According to Eq. (55) and since we considered interband correlations, the static, uniform limit of \( P(Q, \omega) \) exists, contrary to the case of the amplitude mode \( A(Q, z_\nu) \) to which also intraband correlations contribute.\textsuperscript{33} We find for the static, uniform phase correlation function

\[
P(0, 0) = P^{(0)}(0, 0) - U P^{(0)}(0, 0) P(0, 0)
= \frac{P^{(0)}(0, 0)}{1 + U P^{(0)}(0, 0)}.
\]

(57)

The (Hartree-Fock) gap equation (9) is

\[
1 + UP^{(0)}(0, 0) = 0.
\]

(58)

Comparing Eq. (57) with Eq. (58) unveils that \( P(0, 0) \) exhibits a pole; hence, the phase mode is acoustic.

### B. Static electron-phonon coupling

Let us now discuss the behavior of the phase mode if the lattice deforms at the EI phase transition, i.e., we
have $\delta Q \neq 0$. The lattice distortion is contained in the electron Green functions but does not explicitly appear in the Bethe-Salpeter equation. Hence, the phase and amplitude correlation functions are determined by Eqs. (52) and (53), respectively. The phase mode for this situation is displayed in Fig. 3. It shows that the phase mode is massive in this case, i.e., $\omega(Q) \propto (Q^2 + C)$ for $Q \to 0$ (the constant $C > 0$). Apart from this limit, the spectrum resembles the result for the undistorted lattice since the influence of the phonons is weak for large excitation energies.

![Figure 3](image)

**FIG. 3.** (Color online) Electron-hole excitation spectrum for a distorted lattice at zero temperature. The black, solid lines show the phase mode and the red, dashed lines show the lower boundary of the electron-hole continuum.

The absence of the acoustic phase mode can be shown analytically. The phase correlation function exhibits a pole at $z_\nu = 0$ and $Q = 0$ if the denominator of Eq. (57) vanishes. For a deformed lattice the (Hartree-Fock) gap equation takes the form

$$0 = 1 + \left( U + 4 \frac{g_0^2}{\omega_0} \right) P^{(0)}(0, 0).$$

(59)

The condition for an acoustic phase mode significantly differs from Eq. (59). We can argue that the static lattice distortion breaks explicitly the $U(1)$ symmetry of the model and removes the phase invariance of $\Delta_{kQ}$. As a consequence, any phase-mode excitation requires a finite energy. Hence, the phase mode is massive.

**C. Dynamical electron-phonon coupling**

As shown above, the softening of a phonon mode and the accompanying lattice deformation leads to a massive phase mode. Let us now analyze the effect of dynamical phonons that do not become soft but offer a way to transfer electrons from the valence band to the conduction band. Thereby, we include the phonons in the Bethe-Salpeter equations, Eqs. (40) and (43), and take the self energies resulting from the coupling to the lattice in the single-particle Green functions into account.

In particular, we ask whether the phase mode in the ordered ground state is acoustic or not. To this end, we investigate the static, uniform limit of the phase correlation function with respect to its pole structure. We note that the electron-phonon coupling leads to an effective electron-electron interaction that is nonlocal in (imaginary) time. This complicates the numerical evaluation considerably. We therefore only consider the following two limiting cases.

First, we assume the phonons to be more slower than the electrons (adiabatic regime). We then neglect the frequencies $\omega_4$ and $\omega_5$, which appear in the phonon Green function, in the electron-hole pair correlation functions since they only can attain small values. Accordingly the phase mode is determined by

$$P(Q, z_\nu) = X(Q, z_\nu) - Y(Q, z_\nu),$$

(60)

where

$$\tilde{X}^{(0)}(Q, z_\nu) = [1 - r_x(Q, z_\nu)] X(Q, z_\nu) - r_y(Q, z_\nu) Y(Q, z_\nu),$$

(61)

$$\tilde{Y}^{(0)}(Q, z_\nu) = [1 - s_y(Q, z_\nu)] Y(Q, z_\nu) - s_x(Q, z_\nu) X(Q, z_\nu),$$

(62)

(the explicit expressions for the functions are given in the Appendix A). The corresponding gap equation reads

$$1 = \frac{1}{-i\beta} \sum_{z_1} \frac{UR(z_1)}{1 - |g_0|^2 D^2(z_1)},$$

(63)

where

$$R(z_1) = \frac{1}{N} \sum_k \frac{i}{\Omega(k, z_1)},$$

(64)

$$\Omega(k, z_1) = [z_1 - \bar{\epsilon}_{kv} - \sigma_{ev}(k, z_1)] [z_1 - \bar{\epsilon}_{kc} - \sigma_{cv}(k, z_1)] - |\Delta_{kQ} + \sigma_{Fv}(k, z_1)|^2,$$

(65)

$$\bar{D} = \frac{1}{-i\beta} \sum_{z_\mu} D(0, z_\mu).$$

(66)

The $z_1$ ($z_\mu$) are fermionic (bosonic) Matsubara frequencies. However, the structure of the phase correlation function remains complicated in this case, and a comparison with Eq. (63) does not unveil the inherent physics.

Second, if the phonons are much faster than the electrons (anti-adiabatic regime), we can integrate out, in principle, the lattice degrees of freedom (instantaneous approximation). Considering this limit is technical rather than physically motivated since in most materials the phonon frequency is much smaller than the characteristic electronic energy scale. Due to the fact that the qualitative behavior of the phase mode is mainly determined by the underlying symmetry of the state, the instantaneous approximation is nevertheless instructive. In this limit, we can replace the phonon Green function according to $D(q, \tau - \tau') = D(q, 0) \delta(\tau - \tau')$ and obtain a closed system of equations for the correlation functions. Then, the phase correlation function in the static, uniform limit becomes

$$P(0, 0) = \frac{P^{(0)}(0, 0)}{1 + [U - |g_0|^2 D(0, 0)] P^{(0)}(0, 0)},$$

(67)
and the gap equation is given by
\[ 1 = [U + |g_0|^2 D(0, 0)] \frac{1}{-i\beta} \sum_{z_1} R(z_1) \]  \hspace{1cm} (68)

(again \(z_1\) are fermionic Matsubara frequencies). Obviously, the instantaneous phonons lead to a static renormalization of the Coulomb interaction. However, in the phase correlation function \(V\) the phonon contribution \(|g_0|^2 D(0, 0)\) enters with a negative sign, while \(|g_0|^2 D(0, 0)\) enters with a positive sign the gap equation \(\text{(68)}\). This discrepancy rules out that \(P(0, z_\nu)\) exhibits a pole at \(z_\nu = 0\). Consequently the phase mode is massive.

That is, if the lattice is not deformed statically the phonons affect the electrons in two ways: They enhance the effective masses of the electrons and the holes (thereby modifying the band structure) and renormalize the Coulomb interaction. The former effect is less important for the basic mechanism of exciton condensation. The latter effect, on the other hand, is crucial, since it generates an effective electron-electron interaction that explicitly breaks the \(U(1)\) symmetry. This is demonstrated by the diagrams shown in Fig. 1. Here, the incoming and outgoing branches at the vertices, i.e., at \(\tau\) and \(\tau'\) describe the effective two-particle interaction. For the Coulomb interaction, diagramed in the second row of Fig. 1, there is one incoming and outgoing branch for the valence electrons (labeled with \(\nu\) and \(\nu'\) respectively) and one incoming and outgoing branch for the conduction electrons (labeled with \(c\) and \(c'\) respectively). Hence, the interaction \(V_{\text{Coul}} \propto c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3} c_{k_4}\). In the ladder terms arising from the electron-phonon coupling (fourth row in Fig. 1) there are two incoming branches of conduction electrons and two outgoing branches of valence electrons (or vice versa), which establish an effective electron-electron interaction
\[ V_{\text{ph}} \propto c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3} c_{k_4} + c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4} \propto \cos(2\phi). \]  \hspace{1cm} (69)

Here, \(\phi\) denotes the phase of \(\Delta_{kQ}\). An electron-electron interaction of identical form might appear if exchange terms were considered.\[^{34}\] Such an interaction fixes \(\phi\) and, consequently, destroys the acoustic phase mode.

To sum up, both a static lattice distortion and the coupling of the electrons and holes to dynamical phonons lead to a massive phase mode by inducing a gap in the electron-hole pair spectrum.

D. Critical electron-hole pairing

Having analyzed the electron-hole pair spectrum, we now ask whether an additional electron-phonon coupling supports electron-hole pairing. For this, we analyze the phonon contribution in the gap equations taking the following bare phonon Green function into account:
\[ D(q, \nu) = -\frac{2\omega_q}{z_\nu - \omega_q}. \]  \hspace{1cm} (70)

In the gap equation for slow phonons, Eq. \((63)\), we find \(D = -2p(\omega_0) - 1 < 0\), where \(p(x)\) is the Bose distribution, and, since \(\frac{1}{z_\nu} \sum_{z_1} R(z_1) > 0\), we can conclude that the local Coulomb potential is effectively weakened. Self-evidently slow phonons introduce retardation effects and therefore give rise to a long-ranged electron-hole interaction potential which reduces the effect of the local potential. Instantaneous phonons act in an opposite way. In this limit, there is no retardation and, since \(D(0, 0) = 2/\omega_0 > 0\), these phonons enhance the strength of the local Coulomb interaction, see Eq. \((68)\).

VII. ACOUSTIC PHASE MODE AS INDICATOR FOR AN EXCITONIC CONDENSATE

We now turn to the question under which circumstances the excitonic ground state represents a true condensate. A widely accepted criterion in this respect is that the system exhibits off-diagonal long range order (ODLRO).\[^{31,35,36}\] ODLRO can be tested with the help of the reduced density matrix. Since we are concerned with the condensation of electron-hole pairs, ODLRO exists if the following reduced density matrix for electrons and holes is finite in case of pairs separated at arbitrarily large distances,\[^{37}\] i.e.,
\[ \rho_{2e-h}(r, r', \mathbf{R}, \mathbf{R}') = \frac{1}{N} \langle c_{\mathbf{R} + r/2}^\dagger c_{\mathbf{R} - r/2} c_{\mathbf{R}' + r'/2}^\dagger c_{\mathbf{R}' - r'/2} \rangle \]  \hspace{1cm} (71)

stays finite as \(|\mathbf{R} - \mathbf{R}'| \to \infty\). Thereby, \(\mathbf{R}\) and \(\mathbf{R}'\) denote the center-of-mass coordinates of the excitons, and \(r\) and \(r'\) are the relative coordinates of the bound electron and the bound hole in the exciton respectively. Fourier transformation of \(\rho_{2e-h}\) yields
\[ \rho_{e-h} = \frac{1}{N^2} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \langle c_{\mathbf{k} + \mathbf{q}/2}^\dagger c_{\mathbf{k} - \mathbf{q}/2} c_{\mathbf{k}' - \mathbf{q}/2}^\dagger c_{\mathbf{k}' + \mathbf{q}/2} \rangle e^{i\mathbf{k} \cdot \mathbf{r} - i\mathbf{k}' \cdot \mathbf{r}'}. \]  \hspace{1cm} (72)

The extent of the excitons, given by \(|r|\) and \(|r'|\), are of the order of the electron-hole pair coherence length, which is small compared with the system size. We therefore neglect the \(r\)- and \(r'\)-dependencies in the following and write
\[ \rho_{e-h} = -\frac{1}{N\beta} \sum_{\mathbf{q}} \sum_{\nu} X(\mathbf{q}, \nu) e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')}. \]  \hspace{1cm} (73)

with \(X(\mathbf{q}, \nu) = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} G_2(\mathbf{q}, \mathbf{k}, \mathbf{k}', \nu)\) (\(\nu\) are bosonic Matsubara frequencies). The condition for ODLRO can only be satisfied if \(\rho_{e-h}\) contains averages \(I_q\) of the order of unity.\[^{35}\] We have
\[ I_q = \frac{1}{N\beta} \sum_{\nu} X(\mathbf{q}, \nu) = \frac{1}{N} R(\omega_X). \]  \hspace{1cm} (74)
where $R(\omega_X)$ is the residuum of the pole $\omega_X$. Note that $R(\omega_X) \propto p(\omega_X)$ with the Bose distribution $p(x)$. For $R(\omega_X)$ to be of the order of $N$, $\omega_X$ must vanish. That is, an acoustic phase mode implies the presence of ODLRO. Since an acoustic mode is absent for finite electron-phonon coupling, electron-hole pair condensation only takes place in exclusively electronically driven phase transitions.

VIII. CONCLUSIONS

In this work we have revisited on what terms an excitonic insulator (EI) forms. In particular, we have analyzed the effects of an explicit electron-phonon interaction $H_{e-ph}$. The potential EI state then may possess a static lattice distortion. We have shown that $H_{e-ph}$ will not change the single-particle spectra qualitatively, even if self-energy effects are taken into account. However, $H_{e-ph}$ significantly modifies the electron-hole pair spectrum. To demonstrate this, we have calculated the contributions of the electron-phonon interaction to electron-hole pairing within the Kadanoff-Baym approach including ring and ladder diagrams. When the electron-phonon coupling is neglected the phase mode is acoustic. Phonons destroy the acoustic mode regardless if they cause a static lattice distortion or solely renormalize the effective electron-electron interaction.

We pointed out that an acoustic phase mode, or at least the vanishing of the excitation energy of a collective mode, implies the presence of off-diagonal long range order (ODLRO), and therefore characterizes a condensate. That is, the EI phase in pure electronic models, e.g., in the extended Falicov Kimball model, represents a true exciton condensate. Since in real materials, the coupling to the lattice is always present, EI materials under consideration rather resemble the phenomenon of a charge-density-wave but do not embody a true exciton condensate with super-transport properties (cf. the remark by Walter Kohn in the supplementary discussion section in Ref. 5).

To realize an exciton condensate in equilibrium experimentally, bilayer systems, such as graphene double layers and bilayers, are the most promising candidates at present. Since the interband tunneling processes that destroy the $U(1)$ symmetry can be suppressed by suitable dielectrics, an acoustic collective mode, and hence ODLRO, may emerge. In these systems electrons and holes occupy different layers and the exciton condensate is presumably accompanied by the occurrence of a dipolar supercurrent.

Let us finally emphasize that the numerical results presented in this work are obtained using rather crude approximations. That is why a more elaborated numerical treatment is highly desirable. A possible next step is to calculate the dynamical structure factor, which is accessible experimentally by electron energy-loss spectroscopy. Here collective modes show up as peaks and one might address the acoustic phase mode problem. Moreover, the behavior of the plasmon mode in the low-temperature state has not been elaborated yet. This mode is generated by intraband correlations and shows an acoustic behavior in the normal phase. Another worthwhile continuation concerns the possible formation and condensation of “polaron excitons”, i.e., the buildup of a condensate of excitons which are dressed by a phonon cloud.

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1 N. F. Mott, Philos. Mag. 6, 287 (1961).
2 R. Knox, in Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1963), p. Suppl. 5 p. 100.
3 L. V. Keldysh and H. Y. V. Kopaev, Sov. Phys. Sol. State 6, 2219 (1965).
4 D. Jérome, T. M. Rice, and W. Kohn, Physical Review 158, 462 (1967).
5 B. I. Halperin and T. M. Rice, in Solid State Physics, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1967), vol. 21, p. 115.
6 B. Bucher, P. Steiner, and P. Wachter, Phys. Rev. Lett. 67, 2717 (1991).
7 H. Cercellier, C. Monney, F. Clerc, C. Battaglia, L. Despont, M. G. Garnier, H. Beck, P. Aebi, L. Patthey, H. Berger, et al., Phys. Rev. Lett. 99, 146403 (2007).
8 Y. Wakisaka, T. Sudayama, K. Takubo, T. Mizokawa, M. Arita, H. Namatame, M. Taniguchi, N. Katayama, M. Nohara, and H. Takagi, Phys. Rev. Lett. 103, 026402 (2009).
9 F. X. Bronold and H. Fehske, Phys. Rev. B 74, 165107 (2006).
10 D. Ihle, M. Pfaffertott, E. Burovski, F. X. Bronold, and H. Fehske, Phys. Rev. B 78, 193103 (2008).
11 C. Monney, H. Cercellier, F. Clerc, C. Battaglia, E. F. Schwier, C. Didiot, M. G. Garnier, H. Beck, P. Aebi, H. Berger, et al., Phys. Rev. B 79, 045116 (2009).
12 B. Zenker, D. Ihle, F. X. Bronold, and H. Fehske, Phys. Rev. B 81, 115122 (2010).
13 V. N. Phan, K. W. Becker, and H. Fehske, Phys. Rev. B 81, 205117 (2010).
14 B. Zenker, D. Ihle, F. X. Bronold, and H. Fehske, Phys. Rev. B 85, 221102R (2012).
15 C. Monney, C. Battaglia, H. Cercellier, P. Aebi, and H. Beck, Phys. Rev. Lett. 106, 106404 (2011).
16 T. Kaneko, T. Toriyama, T. Konishi, and Y. Ohta, Phys. Rev. B 87, 035121 (2013), ibid. 87, 199902(E) (2013).
Appendix A: Functions appearing in Eqs. (61) and (62)

\[ r_x(Q, z_\nu) = \frac{1}{-i\beta} \sum_{z_2} A_x(Q, z_\nu, z_2) \left[ 1 + a(-Q, -z_\nu, z_2) \right] - b(Q, z_\nu, z_2) A_y(-Q, -z_\nu, z_2) \]

\[ r_y(Q, z_\nu) = \frac{1}{-i\beta} \sum_{z_2} A_y(Q, z_\nu, z_2) \left[ 1 + a(-Q, -z_\nu, z_2) \right] - b(Q, z_\nu, z_2) A_x(-Q, -z_\nu, z_2) \]

\[ \dot{X}^{(0)}(Q, z_\nu) = \frac{1}{-i\beta} \sum_{z_2} \dot{X}^{(0)}(Q, z_\nu, z_2) \left[ 1 + a(-Q, -z_\nu, z_2) \right] - b(Q, z_\nu, z_2) \dot{X}^{(0)}(-Q, -z_\nu, z_2) \]

\[ s_x(Q, z_\nu) = \frac{1}{-i\beta} \sum_{z_2} A_x(-Q, -z_\nu, z_2) \left[ 1 + a(Q, z_\nu, z_2) \right] - b(-Q, -z_\nu, z_2) A_x(Q, z_\nu, z_2) \]

\[ s_y(Q, z_\nu) = \frac{1}{-i\beta} \sum_{z_2} A_y(-Q, -z_\nu, z_2) \left[ 1 + a(Q, z_\nu, z_2) \right] - b(-Q, -z_\nu, z_2) A_y(Q, z_\nu, z_2) \]

\[ \dot{Y}^{(0)}(Q, z_\nu) = \frac{1}{-i\beta} \sum_{z_2} \dot{Y}^{(0)}(-Q, -z_\nu, z_2) \left[ 1 + a(Q, z_\nu, z_2) \right] - b(-Q, -z_\nu, z_2) \dot{Y}^{(0)}(Q, z_\nu, z_2) \]
\( A_x(Q, z, z_2) = -U \bar{X}_2^{(0)}(Q, z, z_2) + |g_0|^2 D(0, z) \left[ \bar{X}_2^{(0)}(Q, z, z_2) + \bar{Y}_2^{(0)}(Q, z, z_2) \right] \) (A7)

\( A_y(Q, z, z_2) = -U \bar{Y}_2^{(0)}(Q, z, z_2) + |g_0|^2 D(0, z) \left[ \bar{X}_2^{(0)}(Q, z, z_2) + \bar{Y}_2^{(0)}(Q, z, z_2) \right] \) (A8)

\( a(Q, z, z_2) = |g_0|^2 \tilde{D}(0) \bar{Y}_2^{(0)}(Q, z, z_2) \) (A9)

\( b(Q, z, z_2) = |g_0|^2 \tilde{D}(0) \bar{X}_2^{(0)}(Q, z, z_2) \) (A10)

\( \bar{X}_2^{(0)}(Q, z, z_2) = \frac{1}{-i\beta} N \sum k, k' \sum_{z_3} G_2^{(0)}(Q, k, k', z_2 - z_3, z_2, z_3) \) (A11)

\( \bar{Y}_2^{(0)}(Q, z, z_2) = \frac{1}{-i\beta} N \sum k, k' \sum_{z_3} F_2^{(0)}(Q, k, k', z_2 - z_3, z_2, z_3) \) (A12)