Exciton condensation due to electron-phonon interaction

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(Dated: May 22, 2014)

We show that the coupling to vibrational degrees of freedom can drive a semimetal excitonic-insulator quantum phase transition in an one-dimensional two-band f–c electron system at zero temperature. The insulating state typifies an excitonic condensate accompanied by a finite lattice distortion. Using the projector-based renormalization method we analyze the ground-state and spectral properties of the interacting electron-phonon model at half-filling. In particular we calculate the momentum dependence of the excitonic order parameter function and determine the finite critical interaction strength for the metal-insulator transition to appear. The electron spectral function reveals the strong hybridization of f- and c-electron states and the opening of a single-particle excitation gap. The phonon spectral function indicates that the phonon mode involved in the transition softens (hardens) in the adiabatic (non-adiabatic and extreme anti-adiabatic) phonon frequency regime.

I. INTRODUCTION

Low-dimensional electron systems are very susceptible to structural distortions driven by the electron-phonon interaction. 1 Probably the most famous one is the Peierls instability of one-dimensional metals 2 where the system spontaneously creates a periodic variation in the carrier density at any finite coupling by shifting the ions from their symmetric positions. For the half-filled band case this so-called charge density wave (CDW) is commensurate with the lattice. Since a static dimerisation of the lattice opens a gap at the Fermi surface the metal gives way to an insulator. A full understanding of such a zero-temperature quantum phase transition requires accounting for both quantum lattice fluctuations and strong electronic correlations. For example, it has been found theoretically that quantum fluctuations of the lattice ‘protect’ the metallic state at weak electron-phonon couplings below a finite critical coupling strength. 3 An intra-site Coulomb repulsion between electrons of opposite spin, on the other hand, tends to immobilize the carriers, but establishes a Mott insulating ground state with strong spin-density correlations instead of the CDW. To analyze the subtle interplay of electron-electron and electron-phonon interaction effects the one-band Holstein-Hubbard model turned out to be particularly rewarding to study. 4

If we have two electronic bands, however, forming a semimetal with only weak band overlap or a semiconductor with small band gap, the Coulomb interaction between f-band (‘hole’) and c-band (‘electron’) particles causes the formation of (electron-hole) bound states. Then, at the semimetal-semiconductor transition, the ground state of the crystal may become unstable with respect to the spontaneous formation of excitons. That is, an excitonic instability appears 5 where the number of free carriers will vary discontinuously under an applied perturbation, signalling a quantum phase transition. The new macroscopic phase-coherent quantum state can be regarded as an electron-hole pair condensate. Worth mentioning the excitonic state exhibits no ‘super’ transport properties 6 rather it typifies an ‘excitonic insulator’ (EI) which—under certain conditions—is accompanied by a CDW. 7 Such a density oscillation can, of course, trigger a lattice distortion which doubles the lattice period, just as for the Peiers state discussed above.

The challenging suggestion of electron-hole pair condensation into the EI phase at equilibrium has been intensively studied within the frameworks of purely electronic, effective-mass Mott-Wannier-type exciton 8 and extended Falicov-Kimball models. 9–13 In doing so, the coupling to the phonons was neglected. Since the nondistorted semimetal ground state of a simple two-band model with electron and hole Fermi surfaces identical in size and shape is unstable with respect to electron-hole attraction near the semimetal-semiconductor transition, just as the normal Fermi surface of a metal is unstable to the formation of Cooper pairs 1,14 one might ask whether the coupling of electrons and holes to the lattice degrees of freedom alone is sufficient to drive an EI instability. Addressing this question is the primary concern of this paper.

Whether a CDW transition arising from the coupling between valence and conduction band electrons is brought about by the electron-electron interaction or by the electron-phonon coupling has been debated for a number of materials in the recent past. For example, in spite of many experimental and theoretical studies, the origin of CDW instability in transition-metal dichalcogenide 1T-TiSe 2 remains controversial: it could be the consequence of a novel indirect Jahn-Teller effect 15 of phonon softening 16 the formation of an EI condensate 17 or the combination 18 of the latter both scenarios. 19 Also for the mixed-valent rare-earth chalcogenide TmSe 0.45 Te 0.55 20 the lattice degrees of freedom seem to play an important role forming the EI state: very recent heat capacity measurements indicate that the excitons couple to phonons in the sense of exciton-polarons. 21

In this work, we study a one-dimensional two-band
f-c electron model with a coupling to the phonon degrees of freedom only and show that this interaction mediates a ‘hybridization’ between f and c electrons. From a theoretical point of view, we employ both a standard mean-field scheme and the projector-based renormalization method (PRM). The PRM approach, described in Appendix A, thereby includes fluctuation corrections. It enables the calculation of both ground state and spectral quantities for correlated many-particle systems, and furthermore has the ability to find broken-symmetry solutions of phase transitions beyond mean-field theory. We present our numerical results in Sec. V. Our conclusions can be found in Sec. VI.

II. MODEL

Let us consider the following coupled electron-phonon system

\[ \mathcal{H} = \sum_{k} \varepsilon_{k}^{c} c^{\dagger}_{k} c_{k} + \sum_{k} \varepsilon_{k}^{e} e^{\dagger}_{k} e_{k} + \omega_{0} \sum_{q} b^{\dagger}_{q} b_{q} + \frac{g}{\sqrt{N}} \sum_{kq} \left( c^{\dagger}_{k+q} f_{k} b_{-q}^{\dagger} + b_{q} b_{q} + H.c. \right), \]  

(1)

which contains two types of spinless electrons \( (c, f) \) carrying momentum \( k \) and dispersionless phonons \( (b) \) (see Fig. 1). Here, the electronic excitation energies are given by

\[ \varepsilon_{k}^{f,c} = \varepsilon_{k}^{f,c} - t^{f,c} \gamma_{k} - \mu, \]  

(2)

where \( \omega_{0} \) is the dispersionless phonon energy. In Eq. (2), \( \varepsilon_{k}^{f,c} \) represents the local part of the respective electronic excitations, and the term \( -t^{f,c} \gamma_{k} \), with \( \gamma_{k} = 2 \cos k \), accounts for a nearest-neighbor hopping in a one-dimensional lattice. Hereafter all energies are given in units of \( t^{c} = 1 \). We furthermore note that the electronic energies are measured from the chemical potential \( \mu \); where the numerical results presented in Sec. VI contain an additional energy shift by fixing \( \varepsilon_{c} = 0 \). The last term in Eq. (1) describes a local electron-phonon interaction (with coupling constant \( g \)), written in \( k \)-space, between local f-c particle-hole excitations and lattice displacements. Apparently it represents an effective ‘exciton-phonon interaction. In Eq. (1) we have introduced Fourier transformed quantities \( f_{k}^{j} = (1/\sqrt{N}) \sum_{i}^{N} f_{i}^{j} e^{i k R_{i}}, \) \( c_{k}^{j} = (1/\sqrt{N}) \sum_{i}^{N} c_{i}^{j} e^{i k R_{i}}, \) and \( b_{q}^{j} = (1/\sqrt{N}) \sum_{i}^{N} b_{i}^{j} e^{i q R_{i}} \), where \( f_{i}^{j}, c_{i}^{j} \) and \( b_{i}^{j} \) are the local quantities. \( N \) counts the number of lattice sites \( i \).

In what follows, we consider a half-filled band, i.e.,

\[ n = \langle n_{c}^{f} \rangle + \langle n_{c}^{e} \rangle = 1, \]  

(3)

where \( n_{c}^{f} = (1/N) \sum_{k} f_{k}^{f} f_{k}^{\dagger} \), \( n_{c}^{e} = (1/N) \sum_{k} c_{k}^{e} c_{k}^{\dagger} \). The chemical potential \( \mu \) has to be adjusted in such a way that Eq. (1) is satisfied. Without loss of generality, in what follows, the \( c \) electrons will be considered as ‘light’

while the \( f \) electrons (respectively holes) are ‘heavy’, i.e. \( |t^{c}| < 1 \). For negative \( t^{f} \), and coinciding energies of \( f \) and \( e \) electrons, one is led to a picture of indirect \( c-f \) hopping (cf. Fig. 1), which suggests a possible condensation of bound \( c-f \) electron-hole pairs with finite momentum:

\[ d_{k} = \langle c_{k+Q}^{\dagger} f_{k} \rangle \neq 0, \]  

(4)

where \( Q = \pi \) in one dimension. Allowing broken symmetry solutions for non-vanishing \( d_{k} \), small infinitesimal fields must be included in model (1). We write

\[ \mathcal{H} = \sum_{k} \varepsilon_{k}^{f,c} f_{k}^{f} f_{k}^{\dagger} + \sum_{k} \varepsilon_{k}^{c} c_{k}^{e} c_{k}^{\dagger} + \omega_{0} \sum_{q} b^{\dagger}_{q} b_{q} + \Delta_{0} \sum_{k} \left( c_{k+Q}^{\dagger} f_{k} + f_{k}^{\dagger} c_{k+Q} \right) + \sqrt{N} h_{0} \left( b_{-Q}^{\dagger} + b_{Q} \right) \]  

\[ + \frac{g}{\sqrt{N}} \sum_{kq} \left( c_{k+q}^{\dagger} f_{k} b_{-q}^{\dagger} + b_{q} b_{q} + H.c. \right), \]  

(5)

where \( \Delta_{0} = 0^{+} \) and \( h_{0} = 0^{+} \). It is easily realized that the fields \( h_{0} \) and \( \Delta_{0} \) are mutually dependent. Moreover, since \( b_{Q} = b_{-Q} \) the field contribution \( \sqrt{N} h_{0} \left( b_{Q}^{\dagger} + b_{Q} \right) \) can be replaced by \( \sqrt{N} h_{0} \left( b_{-Q}^{\dagger} + b_{-Q} \right) \). Therefore a finite lattice displacement \( \propto \left( b_{Q}^{\dagger} + b_{-Q} \right) \) would give rise to the formation of a charge density wave connected to a doubling of the lattice unit cell.

FIG. 1: (Color online) Panel (a): Semimetallic f-c electron band structure used in this work. An f valence-band hole and a c conduction-band electron may form an ‘excitonic’ bound state owing to their interaction with the lattice degrees of freedom, with a Brillouin zone boundary phonon involved for momentum conservation reasons. Note that the schematic band structure shown mimics the situation in the EI material TmSeO_{1.45}TeO_{0.55}, where the quasilocalized 4f^{13} state has its maximum at the Γ point, the 5d strongly dispersive state has its minimum at the X point, and exciton formation is accompanied by a Γ-X phonon. Also in 17T-TiSe_{2} the valence-band top and the conduction-band minimum are located at different points in the Brillouin zone. Panel (b): If above a critical electron-phonon coupling strength f-c electron coherence is achieved at sufficiently low temperatures even a new symmetry-broken ground state may appear, the so-called excitonic insulator, which maybe accompanied by a finite lattice distortion and a modulation of the charge density.
III. MEAN-FIELD THEORY

To solve model (5) in mean-field approximation it is advantageous first to introduce fluctuation operators \( \Delta A = A - \langle A \rangle \) in the electron(exciton)-phonon interaction. Using

\[
\delta(c_{k+q}^\dagger f_k)\delta(b_{-q}^\dagger + b_q) = c_{k+q}^\dagger f_k(b_{-q}^\dagger + b_q)
\]

\[
+ (c_{k+q}^\dagger f_k(b_{-q}^\dagger + b_q) + [c_{k+q}^\dagger f_k(b_{-q}^\dagger + b_q)]\delta_{q,Q}
\]

the Hamiltonian \( \mathcal{H} \) is best rewritten as

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1
\]

with

\[
\mathcal{H}_0 = \sum_k \varepsilon_k^f f_k^\dagger f_k + \sum_k \varepsilon_k^c c_k^\dagger c_k + \omega_0 \sum_q b_q^\dagger b_q
\]

\[
+ \Delta \sum_k (c_{k+Q}^\dagger f_k + f_k^\dagger c_{k+Q}) + \sqrt{N} \hbar (b_{-q}^\dagger + b_{-Q}),
\]

\[
\mathcal{H}_1 = \frac{g}{\sqrt{N}} \sum_{k_q} \left[ \delta(c_{k+q}^\dagger f_k)\delta(b_{-q}^\dagger + b_q) + \text{H.c.} \right].
\]

Here the fields have acquired additional shifts, which will act as order parameters in the following:

\[
\Delta = \Delta_0 + \frac{g}{\sqrt{N}} (b_{-Q} + b_{-Q}),
\]

\[
h = h_0 + \frac{g}{\sqrt{N}} \sum_k (c_{k+Q}^\dagger f_k + f_k^\dagger c_{k+Q}),
\]

where the infinitesimal \( \Delta_0 = 0^+ \) and \( h_0 = 0^+ \) can be neglected for finite expectation values on the right hand sides.

Finally, we eliminate in Eq. (8) the term \( (b_{-Q}^\dagger + b_{-Q}) \) by defining new phonon operators

\[
B_{q}^\dagger = b_{q}^\dagger + \sqrt{N} (\hbar/\omega_0) \delta_{q,Q},
\]

where the definition is independent of the sign of \( Q \). \( \mathcal{H}_0 \) and \( \mathcal{H}_1 \) then become

\[
\mathcal{H}_0 = \sum_k \varepsilon_k^f f_k^\dagger f_k + \sum_k \varepsilon_k^c c_k^\dagger c_k + \omega_0 \sum_q B_q^\dagger B_q
\]

\[
+ \Delta \sum_k (c_{k+Q}^\dagger f_k + f_k^\dagger c_{k+Q}) + \text{const.},
\]

\[
\mathcal{H}_1 = \frac{g}{\sqrt{N}} \sum_{k_q} \left[ \delta(c_{k+q}^\dagger f_k)\delta(B_{-q}^\dagger + B_q) + \text{H.c.} \right].
\]

In \( \mathcal{H}_1 \) we have used \( \delta B_{-q}^\dagger = \delta b_{q}^\dagger \) and \( \delta B_q = \delta b_q \).

Note that the Hamiltonian \( \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \), with \( \mathcal{H}_0 \) and \( \mathcal{H}_1 \) given by Eqs. (13) and (14), is still exact. The Hamiltonian in mean-field approximation is obtained by completely neglecting the fluctuation part \( \mathcal{H}_1 \). Thus the mean-field Hamiltonian reads

\[
\mathcal{H}_{MF} = \sum_k \varepsilon_k^f f_k^\dagger f_k + \sum_k \varepsilon_k^c c_k^\dagger c_k + \omega_0 \sum_q B_q^\dagger B_q
\]

\[
+ \Delta \sum_k (c_{k+Q}^\dagger f_k + f_k^\dagger c_{k+Q}),
\]

where the constant from Eq. (13) will be suppressed. The electronic part of \( \mathcal{H}_{MF} \) is diagonalized by use of a Bogoliubov transformation. Then \( \mathcal{H}_{MF} \) is rewritten as

\[
\mathcal{H}_{MF} = \sum_k E_k^{(1)} c_{1,k}^\dagger c_{1,k} + \sum_k E_k^{(2)} c_{2,k}^\dagger c_{2,k}
\]

\[
+ \omega_0 \sum_q B_q^\dagger B_q,
\]

where the electronic quasiparticle energies and quasiparticles operators read

\[
E_k^{(1,2)} = \frac{\varepsilon_k^f + \varepsilon_k^c}{2} \pm \frac{\text{sgn}(\varepsilon_k^f - \varepsilon_k^{c+Q})}{2} W_k,
\]

and

\[
C_{1,k}^\dagger = \frac{1}{2} \left[ 1 + \text{sgn}(\varepsilon_k^f - \varepsilon_k^{c+Q}) \frac{\varepsilon_k^f - \varepsilon_k^{c+Q}}{W_k} \right],
\]

\[
C_{2,k}^\dagger = - \frac{1}{2} \left[ 1 - \text{sgn}(\varepsilon_k^f - \varepsilon_k^{c+Q}) \frac{\varepsilon_k^f - \varepsilon_k^{c+Q}}{W_k} \right],
\]

Here the prefactors are given by

\[
W_k = \sqrt{\left(\varepsilon_k^{c+Q} - \varepsilon_k^f\right)^2 + 4|\Delta|^2}.
\]

The quadratic form of Eq. (19) allows to compute all expectation values formed with \( \mathcal{H}_{MF} \). From Eqs. (10), (11), and (12) one easily obtains the following implicit equation for the order parameters \( \Delta = -(2g/\omega_0)h \),

\[
1 = \frac{4g^2}{\omega_0 N} \sum_k \text{sgn}(\varepsilon_k^f - \varepsilon_k^{c+Q}) f^F(E_k^{(1)}) - f^F(E_k^{(2)})/W_k.
\]

Here \( f^F(E_k^{(1,2)}) \) are Fermi functions, which—working at zero temperature in what follows—reduce to the corresponding \( \Theta \)-functions. Note that Eq. (23) represents a BCS-like equation for \( \Delta \). A non-zero \( \Delta \) accounts for an exciton condensation phase as was explained above. In Figs. 3 and 4 below, it will be shown that such a phase occurs for a sufficiently large coupling constant.
\( g > g_{\text{MF}}^c (\omega_0) \). We would like to point out here already, that the critical coupling constant \( g_{\text{MF}}^c \) is generally smaller than the corresponding \( g_{\text{ePRM}}^c \), obtained below by including fluctuation processes.

Let us also consider the one-particle spectral function \( A_k^{(c,f)} (\omega) \) for \( c \) and \( f \) electrons. For \( c \) electrons it is defined by

\[
A_k^c (\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle [c_{k\sigma}(t), c_{k\sigma}^\dagger]_+ \rangle e^{i\omega t} dt ,
\]

where the expectation values is formed with \( H_{\text{MF}} \). For \( A^f(k,\omega) \) and the corresponding equation for the \( f \) electrons one finds

\[
A_k^f (\omega) = \xi_k^2 \delta (\omega - E_{k-Q}^{(1)}) + \eta_k^2 \delta (\omega - E_{k-Q}^{(2)}) ,
\]

Thus both spectral functions are built up by two coherent excitations with energies \( E_{k-Q}^{(1)} \) and \( E_{k-Q}^{(2)} \). Finally, the phonon spectral function

\[
C_q (\omega) = \frac{1}{2\pi \omega} \int_{-\infty}^{\infty} \langle [b_q(t), b_q^\dagger]_+ \rangle e^{i\omega t} dt
\]

is given by

\[
C_q (\omega) = \frac{\delta (\omega - \omega_0)}{\omega_0} ,
\]

which shows a \( q \)-independent excitation at \( \omega = \omega_0 \). Note that in contrast to the electronic excitations in Eqs. (25) and (26), the phonon frequency \( \omega_0 \) in not changed in mean-field approximation.

IV. FLUCTUATION CORRECTIONS BEYOND MEAN-FIELD THEORY

In the mean-field treatment above fluctuation processes from the interaction \( H_1 \) have completely been left out. In the following, we therefore apply the PRM to evaluate the order parameters, the one-particle spectral functions \( A_k^{(c,f)} (\omega) \) and the phonon spectral function \( C_q (\omega) \) for the case that \( H_1 \) is included. To avoid technical details, the explicit application is shifted to appendix A. The general concept of the PRM is as follows: The presence of the interaction \( H_1 \) prevents a straightforward solution of the Hamiltonian \( \hat{H} = H_0 + H_1 \). For that reason the Hamiltonian is transformed into a diagonal (or at least quasi-diagonal) form by applying a sequence of small unitary transformations to \( \hat{H} \). Denoting for a moment the generator of the whole sequence by \( X = -X^\dagger \), in appendix A it is shown that one can arrive at an effective Hamiltonian \( \hat{H} = e^X \hat{H} e^{-X} \), which has the same operator structure as Hamiltonian \( H_0 \) in Eq. (13),

\[
\hat{H} = \sum_k \tilde{\epsilon}_k^c f_k^c \bar{f}_k + \sum_k \tilde{\epsilon}_k^f c_k^f \bar{c}_k + \sum_q \tilde{\omega}_q B_q^\dagger B_q 
+ \tilde{\Delta} \sum_k (c_{k+Q}^\dagger \bar{f}_k + \bar{c}_{k+Q} f_k) .
\]

Here, \( \tilde{\epsilon}_k^c, \tilde{\epsilon}_k^f, \tilde{\omega}_q, \) and \( \tilde{\Delta} \) are renormalized parameters, which have to be determined self-consistently by taking into account contributions to infinite order in the interaction \( H_1 \). Also, the phonon frequency \( \tilde{\omega}_q \) has acquired a \( q \)-dependence. Note that the PRM ensures a well-controlled disentanglement of higher order interaction terms which enter in the elimination procedure.

The PRM also allows to evaluate expectation values \( \langle A \rangle \), formed with the full Hamiltonian \( \hat{H} \). Thereby, one uses the property of unitary invariance of operator expressions under a trace. Employing the same unitary transformation to \( A \) as before for the Hamiltonian, one finds \( \langle A \rangle = \langle A \rangle \hat{H} \), where the expectation value is formed with \( \hat{H} \) and \( \hat{A} = e^{X} \hat{A} e^{-X} \). Note that Hamiltonian \( \hat{H} \) from Eq. (29) can be transformed into a diagonal form by use of a Bogoliubov transformation in analogy to the transformation from Eq. (13) to Eq. (16). Therefore, any expectation value, formed with \( \hat{H} \), can be evaluated exactly.

As an example, let us consider the spectral function \( A_k^c (\omega) \) from the former expression (24), where the expectation value should however be formed with the full Hamiltonian \( \hat{H} \) (and not with \( H_{\text{MF}} \)). Applying the unitary invariance of operator expressions under a trace, \( A_k^c (\omega) \) is rewritten as

\[
A_k^c (\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle [\tilde{c}_{k\sigma}(t), \tilde{c}_{k\sigma}^\dagger]_+ \rangle e^{i\omega t} dt ,
\]

where the expectation value is now formed with \( \hat{H} \) instead of with \( \hat{H} \). Correspondingly \( \tilde{c}_{k\sigma}^\dagger, \tilde{c}_{k\sigma} \) are the transformed electron operators, \( \tilde{c}_{k\sigma}^\dagger = e^{X} c_{k\sigma}^\dagger e^{-X} \), and the time-dependence is governed by \( \hat{H} \) as well.

V. NUMERICAL RESULTS

A. Ground-state properties

We start with a discussion of the EI order parameter \( \Delta \) and the corresponding lattice displacement \( x_Q \) in the ground state of the fully renormalized two-band model (25) in one dimension. Figure 2 at first displays the profile of the excitonic expectation value \( d_k \), in dependence on the electron-phonon coupling \( g \), for two characteristic phonon frequencies \( \omega_0 \) describing an adiabatic \( \omega_0 < 1 \) non-adiabatic \( \omega_0 > 1 \) situation. This quantity designates the range in momentum space where \( c \) electrons and \( f \) holes are perceptibly involved in the electron-hole pair formation and exciton condensation process.
Obviously $d_k$ vanishes (within numerical accuracy) for all $k$ below a critical coupling strength $|g_c| \approx 0.28 (0.6)$ at $\omega_0 = 0.5 (2.5)$. At and just above the critical coupling $d_k$ is solely finite at and near the Fermi momentum $k_F$, respectively, indicating a BCS-type electron-hole pairing instability. A further increasing electron-phonon coupling implicates more and more electron and holes states in the pairing process up to the point where Fermi surface (nesting) effects are ineffectual. Thus we expect that local, tightly bound excitons will form in the strong interaction limit and, as a consequence, Bose-Einstein condensation takes place.

The derived zero-temperature quantum-phase-transition lines, separating the semimetallic and EI phases in the $g-\omega_0$ plane, are shown in Fig. 4. In the intermediate coupling and frequency regime, we observe distinct PRM corrections to the mean-field transition points. In the anti-adiabatic limit ($\omega_0 \to \infty$), where the phononic degrees of freedom can be integrated out, the squared critical coupling $g_c^2$ scales linearly with $\omega_0$, and we find $(g_c^2/\omega_0)|_{\omega_0 \to \infty} \approx 0.14$ (see inset). Here the phase boundary basically agrees with that of mean-field theory (compare Fig. 4). An analytical proof of this finding is given in Appendix B.
FIG. 5: (Color online) Intensity plots of the $c$-electron (left-hand panels) and $f$-electron (right-hand panels) single-particle spectral functions $A_{c,f}^{k}(\omega)$ in the adiabatic regime with $\omega_0 = 0.5$. The electron-phonon coupling $g$ increases as indicated from top to bottom panels. In the lowermost two panels the corresponding mean-field results are included, without dissolving the spectral intensity however (see white dashed lines).

B. Spectral properties

We now present the PRM results for the single-particle spectral functions associated with the photoemission or inverse photoemission (injection) of a $c$ or $f$ electron with wave number $k$ and energy $\omega$, which serve as a direct measures of the occupied and unoccupied states. Figure 5 shows the variation of $A_{c,f}^{k}(\omega)$ as the electron-phonon coupling $g$ increases in the adiabatic regime. For weak couplings (see upper panels), we are in the semimetallic phase, and $A_{c,f}^{k}(\omega)$ reflect the weakly renormalized $c$- and $f$-band dispersions (note that the energy $\omega$ is measured with respect to the Fermi energy). In the EI phase, a gap opens at the Fermi energy and we observe a pronounced back-folding of the spectral signature at larger coupling. Here $c$- and $f$-electron states strongly hybridize close to the Fermi energy. The same, in principle, holds in the non-adiabatic regime. However, for the parameters used in Fig. 6 the ratio $g/\omega_0 = 0.32$ is much smaller than for the EI phase depicted in the two lowermost panels of Fig. 5 where $g/\omega_0 = 1.2$. Hence multi-phonon processes are less important in the former case and—prescinding from the gap feature—the photoemission spectrum is less affected by the lattice degrees of freedom. For comparison, we show also the outcome of mean-field theory for $A_{c}^{k}(\omega)$ and $A_{f}^{k}(\omega)$ in lower panels where $g = 0.6$. We see that the band gap is considerably overestimated, and there is, of course, no incoherent contribution at all.

More information in this respect comes from the phonon spectral function $C_{q}(\omega)$, represented in Fig. 7, below (upper panels) and above (lower panels) the semimetal-EI transition point. At weak coupling, the absorption signal is dominated by the coherent part of $C_{q}(\omega)$, which is almost dispersionless and located near the bare phonon frequency, i.e., $\tilde{\omega}_q \approx \omega_0$. This particularly holds for the case $g = 0.1$, $\omega_0 = 0.5$ shown in the top left panel. For $g = 0.5$ and a higher phonon frequency $\omega_0 = 2.5$, the overall intensity of the signal goes down, of course. Note that the phonon mode acquires a slight dispersion: It becomes larger near the Brillouin zone boundary ($\tilde{\omega}_q \gtrsim \omega_0$). Above the transition [$g > g_c(\omega_0)$], we observe two distinct features [see lower panels of Fig. 7].

Firstly, the phonon mode softens for $\omega_0 = 0.5$ while it hardens for $\omega_0 = 2.5$. That is, we find an opposite tendency for small and large phonon frequencies. This results can already be understood from perturbation the-
ory for the phonon energy as shown in Appendix A 4.

Secondly a new signal at $\omega = 0$ appears which indicates the strong coupling between electronic and phononic degrees of freedom. Note that the phonon spectral function calculated within mean-field approximation shows only a single dispersionless signal at $\omega = \omega_0$.

Besides coherent excitations all spectral functions in Figs. 5-7 also show incoherent excitations. They can be detected as (red-colored) much weaker developed contributions which deviate from the coherent ones. They possess two general features: (i) Their weight increases with increasing electron-phonon coupling $g$ since they are induced by $H_1$, and (ii) their weight is strongly suppressed in the anti-adiabatic limit. This is explained in Appendix B. To elucidate the distribution of the spectral weight in more detail, we show in Fig. 8 the coherent (left) and incoherent (right) part of the $A_c^f(\omega)$, $A_c^c(\omega)$ and $C_q(\omega)$ spectral functions separately. We choose as an example $g = 0.6$ and $\omega_0 = 0.5$, i.e., consider the system to be in the (adiabatic) EI/CDW regime (cf. Fig. 4). For these parameters the coherent signatures, given by the first terms in Eqs. (A49), (A50) and (A51) clearly dominate the spectra in each case (note that the intensity of the incoherent contributions is magnified by a factor of ten). They follow the renormalized dispersions $E_c^f$ and $E_c^c$, possessing an excitation gap and a pronounced $c$-$f$ electron hybridization. Obviously the incoherent contribution of the $c$-electron spectrum is noticeable in the range of the $f$-electron band only (and vice versa) and will be enhanced if electron-phonon coupling increases.

The phonon spectral function reveals that the signal at $\omega \simeq 0$ originates from the incoherent part of the spectrum. It acquires substantial spectral weight only if the renormalized quasiparticle bands will be ‘connected’ by phonon absorption/emission processes which are significant at large $g$.

**VI. SUMMARY**

Applying a discrete version of the projective renormalization method to a two-band $f$-$c$ electron model with coupling to the lattice degrees of freedom we show that the exciton-phonon interaction can drive a semimetal–to–excitonic insulator transition at zero temperature in one dimension. The ground-state phase diagram containing semimetallic and excitonic insulator phases is derived.
The excitonic condensate is accompanied by a charge density wave and a finite lattice dimerization, and is intimately connected with a developing f-e electron hybridization/coherence. At finite phonon frequency, this spontaneously symmetry-broken state does not appear until the interaction exceeds a finite critical coupling strength. The phase boundary determined by the projective renormalization method significantly deviates from the mean-field result in the intermediate exciton-phonon coupling and phonon frequency regime. The quantum phase transition shows up in the spectral quantities too: We notice the opening of a single-particle excitation gap in the photoemission spectrum, a substantial spectral weight transfer from the coherent to the incoherent part of the spectra, and a renormalisation of the phonon mode, which becomes softened (hardened) as the transition point is reached in the adiabatic (non-adiabatic to anti-adiabatic) regime. In this way our work points out the prominent role played by the lattice degrees of freedom establishing a charge density wave in semimetallic systems with weak (indirect) band overlap and in mixed-valent semiconductors with band gaps comparable to the exciton binding energy, such as quasi two-dimensional 1T-TiSe$_2$ and three-dimensional TmSe$_{0.45}$Te$_{0.55}$, respectively. For 1T-TiSe$_2$ it has been shown quite recently in the framework of a multiband extended Falicov-Kimball model that a purely electronic, exciton pairing and condensation mechanism is insufficient to describe the observed (long-ranged) chiral charge order. Hence the coupling to the phonons seems to be essential, and first mean-field results indicate that electron-hole Coulomb attraction and exciton-phonon coupling indeed support each other in establishing a charge-density-wave state with small but finite lattice distortion. Thereby essential electron correlation and all phonon fluctuation effects were neglected however. Here we consider a one-dimensional model, where quantum phonon fluctuations are exceedingly important and in general tend to suppress any long-range charge order or lattice dimerization, and show that an electron/hole-lattice coupling of reasonable strength can nonetheless cause an excitonic instability. A future more complete theoretical discussion of the low-temperature properties of these material classes should definitely comprise the complex interplay of electron-phonon and electron-hole interactions beyond mean field, particularly in the vicinity of the semiconductor-semimetal transition.

Acknowledgments

The authors would like to thank H. Beck, F. X. Bronold, S. Ejima, D. Ihle, S. Sykora, and B. Zanker for valuable discussions. This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.02-2012.52 and by Deutsche Forschungsgemeinschaft through SFB 652, B5.

Appendix A: Projector-based Renormalization Method

In this Appendix we demonstrate in detail how to solve Hamiltonian $H$ by means of the PRM. So far the PRM was successfully applied to the one-dimensional Holstein and extended Falicov-Kimball models and a number of other models. Its starting point is the decomposition of a many-particle Hamiltonian $H$ into an ‘unperturbed’ part $H_0$ and into a ‘perturbation’ $H_1$, where the unperturbed part $H_0$ is solvable. The perturbation is responsible for transitions between the eigenstates of $H_0$ with non-vanishing transition energies $|E^0_n - E^0_m|$. Here $E^0_n$ and $E^0_m$ denote the energies of $H_0$ between which the transitions take place. The basic idea of the PRM method is to integrate out the interaction $H_1$ by a sequence of discrete unitary transformations. Thereby, the PRM renormalization starts from the largest transition energy of the original Hamiltonian $H_0$, which will be called $\Lambda$, and proceeds in steps $\Delta \lambda$ to lower values of transition energies $\lambda$. For practical applications the unitary transformations are best done in small steps $\Delta \lambda$. Thereby, the evaluation in each step can be restricted to low orders in $H_1$. This procedure usually limits the validity of the approach to parameter values of $H_1$ which are of the same magnitude as those of $H_0$. Every renormalization step is performed by means of a small unitary transformation, where all excitations between $\lambda$ and $\lambda - \Delta \lambda$ are eliminated:

$$H_{\lambda - \Delta \lambda} = e^{X_{\lambda - \Delta \lambda}} H_{\lambda} e^{-X_{\lambda - \Delta \lambda}}.$$  \hspace{1cm} (A1)

Here, the operator $X_{\lambda, \Delta \lambda} = -X_{1, \Delta \lambda}$ is the generator of the unitary transformation for the small step. After each step both the unperturbed part of the Hamiltonian and the perturbation become renormalized and depend on the cutoff energy $\lambda$, i.e. one arrives at a renormalized Hamiltonian $H_{\lambda} = H_{0, \lambda} + H_{1, \lambda}$. Note that $H_{1, \lambda}$ now only accounts for transitions with energies smaller than $\lambda$. Proceeding the renormalization stepwise up to zero transition energies $\lambda = 0$ all transitions with energies different from zero have been integrated out. Thus, finally one arrives at a renormalized Hamiltonian $H_{\lambda = 0}$, which is diagonal or at least quasi-diagonal, since all transitions from $H_{\lambda}$ have been used up.

1. Hamiltonian $H_{\lambda}$

Assuming that all transitions with energies larger than $\lambda$ are already integrated out, an appropriate ansatz in the present case for the transformed Hamiltonian $H_{\lambda}$ reads,
The quantity $H_{1,\lambda}$ in the equation

$$H_{1,\lambda} = \frac{g}{\sqrt{N}} \sum_{kq} \left[ \Theta_{kq,\lambda}^+(\delta(c_{k+q}^+ f_k^+ \delta B_{-q}^+ + B_{q,\lambda}) + H.c.) + \Theta_{kq,\lambda}^-(\delta(c_{k+q}^+ f_k^+ \delta B_{q,\lambda}) + H.c.) \right]$$

(A5)

as long as one is only interested in renormalization equations up to linear order in the order parameters. In Eq. (A5) we have introduced two $\Theta$-functions

$$\Theta_{kq,\lambda}^{\pm} = \Theta(\lambda - |\varepsilon_{k+q,\lambda}^f - \varepsilon_{k,\lambda}^f| \pm \omega_{\pm q,\lambda}),$$

(A6)

which restrict transitions to excitation energies smaller than $\lambda$.

One can also construct the generator $X_{\lambda,\Delta\lambda}$ of the unitary transformation (A1) for the transformation from cutoff $\lambda$ to $\lambda - \Delta\lambda$. According to Ref. [19] the lowest order for $X_{\lambda,\Delta\lambda}$ is given by

$$X_{\lambda,\Delta\lambda} = \frac{1}{L_{0,\lambda}} Q_{\lambda-\Delta\lambda} H_{1,\lambda}.$$  

(A7)

Here $L_{0,\lambda}$ is the Liouville operator of the unperturbed Hamiltonian $H_{0,\lambda}$, which is defined by $L_{0,\lambda} A = [H_{0,\lambda}, A]$ for any operator quantity $A$, and $Q_{\lambda-\Delta\lambda} = 1 - P_{\lambda-\Delta\lambda}$ is the complement projector to $P_{\lambda-\Delta\lambda}$. It projects on all transition operators with excitation energies larger than $\lambda - \Delta\lambda$. With Eqs. (A5) and (A2) one finds

$$X_{\lambda,\Delta\lambda} = \frac{g}{\sqrt{N}} \sum_{kq} \left[ A_{kq}^+(\lambda, \Delta\lambda) (\delta(c_{k+q}^+ f_k^+ \delta B_{-q}^+ - H.c.) + A_{kq}^-(\lambda, \Delta\lambda) (\delta(c_{k+q}^+ f_k^+ \delta B_{q,\lambda} - H.c.) \right], \quad (A8)$$

where the prefactors are given by

$$A_{kq}^{\pm}(\lambda, \Delta\lambda) = \Theta_{kq,\lambda}^{\pm}(1 - \Theta_{kq,\lambda}^{\pm}(\lambda - \Delta\lambda)). \quad (A9)$$

Here the products of the two $\Theta$-functions in $A_{kq}^{\pm}(\lambda, \Delta\lambda)$ assure that only excitations between $\lambda$ and $\lambda - \Delta\lambda$ are eliminated by the unitary transformation (A1). Also note that the Liouville operator $L_{0,\lambda}$ in $X_{\lambda,\Delta\lambda}$ (and the projector $P_{\lambda}$ in $H_{1,\lambda}$) in principle should have been defined with respect to the full unperturbed Hamiltonian $H_{0,\lambda}$ of Eq. (A2) and not by leaving out the last term $\propto \Delta\lambda$. However, inclusion of this term would only give small higher-order corrections to $\Delta\lambda$.

2. Renormalization equations

The $\lambda$-dependence of the parameters of $H_{\lambda}$ are found from transformation (A1). For small enough width $\Delta\lambda$ of the transformation steps, the expansion of (A1) in $g$ can be limited to $O(g^2)$ terms. One obtains

$$H_{\lambda-\Delta\lambda} = H_{0,\lambda} + P_{\lambda-\Delta\lambda} H_{1,\lambda} + [X_{\lambda,\Delta\lambda}, H_{1,\lambda}]$$

$$- \frac{1}{2} \left[ X_{\lambda,\Delta\lambda}, Q_{\lambda-\Delta\lambda} H_{1,\lambda} \right] + \cdots, \quad (A10)$$

where Eq. (A7) has been used. Renormalization contributions to $H_{\lambda-\Delta\lambda}$ arise from the last two commutators which have to be evaluated explicitly. The result must be compared with the generic form (A2). (A3) of $H_{\lambda}$ (with $\lambda$ replaced by $\lambda - \Delta\lambda$) when it is written in terms of the original $\lambda$-independent variables $c_{k,\lambda}^f, f_{k,\lambda}^f$, and $b_{q,\lambda}^f$. This leads to the following renormalization equations for the parameters of $H_{0,\lambda}$:

$$\varepsilon_{k,\lambda} - \varepsilon_{k,\lambda}^{\prime} = \frac{2g^2}{N} \sum_q \left[ A_{k-q,\lambda}^+(\lambda, \Delta\lambda)(n_{-q}^B + n_{k-q}^f) + A_{k-q,\lambda}^-(\lambda, \Delta\lambda)(1 + n_{-q}^B - n_{k-q}^f) \right], \quad (A11)$$

$$\varepsilon_{k,\lambda}^{\prime} - \varepsilon_{k,\lambda} = - \frac{2g^2}{N} \sum_q \left[ A_{k-q,\lambda}^+(\lambda, \Delta\lambda)(1 - n_{k+q}^c + n_{-q}^B) + A_{k-q,\lambda}^-(\lambda, \Delta\lambda)(n_{k+q}^c + n_{-q}^B) \right]. \quad (A12)$$
and
\[ \omega_{q,\lambda-\Delta\lambda} - \omega_{q,\lambda} = -\frac{g^2}{N} \sum_k \left[ A_{k-q}^-(\lambda,\Delta\lambda)(n_{k-q}^f - n_{k-q}^c) + A_{k,\lambda}^- (\lambda,\Delta\lambda)(n_{k}^f - n_{k+q}^c) \right], \quad (A13) \]
\[ h_{\lambda-\Delta\lambda} - h_{\lambda} = -\frac{g^2}{N\sqrt{N}} \sum_k \left[ A_{k-q}^-(\lambda,\Delta\lambda)(n_{k-q}^c - n_{k}^f) + A_{k,\lambda}^- (\lambda,\Delta\lambda)(n_{k}^c - n_{k+q}^c) \right] \left( \langle b_Q \rangle + \langle b_Q^\dagger \rangle \right), \quad (A14) \]
\[ \Delta_{\lambda-\Delta\lambda} - \Delta_{\lambda} \simeq 0. \quad (A15) \]

The quantities \( n_{k}^c, n_{k}^f \) and \( n_{q}^B \) are occupation numbers for electrons and phonons,
\[ n_{k}^c = \langle c_{k}^\dagger c_k \rangle, \quad n_{k}^f = \langle f_{k}^\dagger f_k \rangle \]
\[ n_{q}^B = \langle \delta B_{q,\lambda}^\dagger \delta B_{q,\lambda} \rangle = \langle \delta b_{q}^\dagger \delta b_q \rangle, \]
and have to be evaluated separately. Note that also \( n_{q}^B \)

As in the unrenormalized case, the electronic part of \( \tilde{H} \) will be diagonalized by a Bogoliubov transformation, which gives
\[ \tilde{H} = \sum_k \tilde{E}_k^{(1)} c_{1,k}^\dagger C_{1,k} + \sum_k \tilde{E}_k^{(2)} c_{2,k}^\dagger C_{2,k} + \sum_q \tilde{\omega}_q B_{q}^\dagger B_q + \text{const.} \quad (A22) \]

In result \( A22 \), the electronic quasiparticle energies \( \tilde{E}_k^{(1,2)} \)

3. Expectation values

Next, expectation values \( \langle A \rangle \), formed with the full \( \tilde{H} \), have to be evaluated in the framework of the PRM. As already stated in Sec. \( \text{IV} \), they can be found by exploiting the unitary invariance of operator expressions below a trace. Employing the same unitary transformation to \( A \) as before for the Hamiltonian \( \tilde{H}_0 \), one finds \( \langle A \rangle = \langle A(\lambda) \rangle_{\lambda} = \langle \tilde{A} \rangle_{\tilde{H}} \). Here \( \langle A(\lambda) \rangle_{\lambda} = e^{\lambda X_{\lambda} A e^{-X_{\lambda}}} \) and \( \tilde{A} = A(\lambda = 0) \). \( X_{\lambda} \) is the generator for the unitary transformation between cutoff \( \Lambda \) and \( \lambda \). To find the expectation values of Eqs. \( A16, A17 \)

one best starts from an \textit{ansatz} for the single fermion operators \( c_{k}^\dagger (\lambda) = e^{X_{\lambda} c_{k}^\dagger / e^{-X_{\lambda}}} \), \( f_{k}^\dagger (\lambda) = e^{X_{\lambda} f_{k}^\dagger / e^{-X_{\lambda}}} \), and the phonon operator \( b_{q}^\dagger (\lambda) = e^{X_{\lambda} b_{q}^\dagger / e^{-X_{\lambda}}} \), at cutoff \( \lambda \). In second order in the electron-phonon interaction they are chosen as
\[ c_{k}^\dagger (\lambda) = x_{k,\lambda} c_{k}^\dagger + \frac{1}{\sqrt{N}} \sum_q \epsilon_{k-q,\lambda}^+ b_{k-q}^\dagger \delta(B_{q-k}^\dagger B_{q}) \]
\[ f_{k}^\dagger (\lambda) = y_{k,\lambda} f_{k}^\dagger + \frac{1}{\sqrt{N}} \sum_q \epsilon_{k-q,\lambda}^+ b_{k+q}^\dagger \delta(B_{q-k}^\dagger B_{q}) \]
\[ b_{q}^\dagger (\lambda) = z_{q,\lambda} b_{q}^\dagger + \frac{1}{\sqrt{N}} \sum_k \epsilon_{k,\lambda}^+ c_{k+q}^\dagger \delta(f_{k}^\dagger B_{q-k}) \]

In analogy to the renormalization equations for the parameters of \( \tilde{H}_\lambda \), one first derives the following set of renormalization equations for the coefficients \( \epsilon_{k-q,\lambda}^+ \), \( x_{k,\lambda}^+ \), \( y_{k,\lambda}^+ \), \( z_{q,\lambda}^+ \).
\[ u^\pm_{q,\lambda, \Delta \lambda} = u^\pm_{q,\lambda} + g x_{q,\lambda} A^\pm (\lambda, \Delta \lambda), \quad (A26) \]
\[ v^\pm_{k,\lambda, \Delta \lambda} = v^\pm_{k,\lambda} + g y_{k,\lambda} A^\pm (\lambda, \Delta \lambda), \quad (A27) \]
\[ v^\pm_{k,\lambda, \Delta \lambda} = v^\pm_{k,\lambda} + g z_{k,\lambda} A^\pm (\lambda, \Delta \lambda). \quad (A28) \]

Using the anticommutation relations for fermion operators and the commutation relations for boson operators (as for instance \( [c^\dagger_k(\lambda), c_k(\lambda)] = 1 \), valid for any \( \lambda \)) one arrives at
\[ |x_{k,\lambda}|^2 = 1 - \frac{1}{N} \sum_q \left[ |t^+_{k-q,\lambda}|^2 \right. \]
\[ + |t^{-}_{k-q,\lambda}|^2 (1 + n^B_{k-q} - n^f_{k-q}) \], \quad (A29) \]
\[ |y_{k,\lambda}|^2 = 1 - \frac{1}{N} \sum_q \left[ |u^+_{q,\lambda}|^2 \right. \]
\[ + |u^{-}_{q,\lambda}|^2 (n^B_{q,\lambda} - n^f_{k+q} + 1) \], \quad (A30) \]
\[ |z_{k,\lambda}|^2 = 1 - \frac{1}{N} \sum_k \left[ |v^+_{k-q,\lambda}|^2 \right. \]
\[ + |v^{-}_{k-q,\lambda}|^2 (n^c_{k-q} - n^f_{k}) \]. \quad (A31) \]

Note that Eqs. \( (A26)-(A28) \) together with the new set \( (A29)-(A31) \), taken at \( \lambda \rightarrow \lambda - \Delta \lambda \), represents a complete set of renormalization equations for all \( \lambda \)-dependent coefficients in Eqs. \( (A29)-(A31) \). They combine the parameter values at \( \lambda \) with those at \( \lambda - \Delta \lambda \). By integrating the full set between \( \lambda = \Lambda \), with initial parameter values
\[ \{ x_{k,\lambda}, y_{k,\lambda}, z_{k,\lambda} \} = 1, \quad \{ t^\pm_{k,\lambda}, u^\pm_{k,\lambda}, v^\pm_{k,\lambda} \} = 0, \quad (A32) \]
and \( \lambda = 0 \), one is led to the fully renormalized one-particle operators
\[ c^\dagger_k = \tilde{c}^\dagger_k + \frac{1}{\sqrt{N}} \sum_q \tilde{t}^+_{k-q,q} c^\dagger_{k-q} \delta(\tilde{B}^\dagger_{-q}), \quad (A33) \]
\[ f^\dagger_k = \tilde{f}^\dagger_k + \frac{1}{\sqrt{N}} \sum_q \tilde{u}^+_{q,k} c^\dagger_{k+q} \delta(\tilde{B}^\dagger_{q}), \quad (A34) \]
\[ \tilde{b}^\dagger_q = \tilde{b}^\dagger_{q} + \frac{1}{\sqrt{N}} \sum_k \tilde{v}^+_{k,q} d^\dagger_{k} c^\dagger_{k-q}, \quad (A35) \]

As before, the tilde symbols denote fully renormalized quantities. With Eqs. \( (A33)-(A35) \) the expectation values \( (A16), (A17) \) can be evaluated. The expectation values for fermion operators read up to order \( \mathcal{O}(q^B_k) \):
\[ \langle n^c_k \rangle = \langle \tilde{n}^c_k \rangle + \frac{1}{N} \sum_q \left[ |\tilde{t}^+_{k-q,q}|^2 \tilde{n}^f_{k-q} + 1 + \tilde{n}^B_{k-q} \right] \]
\[ + |\tilde{t}^{-}_{k-q,q}|^2 \tilde{n}^f_{k-q} \tilde{n}^B_{k-q}, \quad (A36) \]
\[ \langle n^f_k \rangle = \langle \tilde{n}^f_k \rangle + \frac{1}{N} \sum_q \left[ |\tilde{u}^+_{k+q,q}|^2 \tilde{n}^f_{k+q} \tilde{n}^B_{k-q} \right. \]
\[ + |\tilde{u}^{-}_{k+q,q}|^2 \tilde{n}^f_{k+q} \tilde{n}^B_{k-q} \]. \quad (A37) \]

Here \( d_k = \langle \tilde{c}^\dagger_{k+Q} \tilde{c}_k \rangle \) is an additional quantity, which acts as an excitonic order parameter. The expectation values on the right-hand sides of Eqs. \( (A39)-(A41) \) are formed with \( \tilde{H} \) and can be evaluated, i.e.
\[ \langle n^c_{k+Q} \rangle = \langle \tilde{n}^c_{k+Q} \rangle = c^\dagger_k f^F(\tilde{E}^\dagger_k) + n^f_k f^F(\tilde{E}^2_k), \quad (A39) \]
\[ \langle n^f_k \rangle = \langle \tilde{n}^f_k \rangle = n^c_k f^F(\tilde{E}^\dagger_k) + c^\dagger_k f^F(\tilde{E}^2_k), \quad (A40) \]
\[ \langle c^\dagger_k f^F(\tilde{E}^\dagger_k) \rangle = -[f^F(\tilde{E}^\dagger_k) - f^F(\tilde{E}^2_k)] \text{sgn}(\tilde{\varepsilon}_k^c - \tilde{\varepsilon}_k^c) \sqrt{\frac{\Lambda}{\tilde{W}_k}}, \quad (A41) \]

Here the prefactors \( \xi_k \) and \( \eta_k \) are the coefficients from the Bogoliubov transformation, used in Eq. \( (A22) \). As mentioned, they are defined by Eqs. \( (20), (21) \), when the unrenormalized one-particle energies are replaced by the renormalized ones.

The bosonic expectation value \( (A14) \) is given by
\[ \langle \tilde{n}^B_q \rangle = \langle \tilde{n}^c_q \rangle \delta(\tilde{B}^\dagger_{-q}) = \langle \tilde{n}^c_q \rangle = \langle b^\dagger_q b_q \rangle - \langle b^\dagger_q \rangle \langle b_q \rangle \delta_{q=q} = \langle \tilde{n}^c_q \rangle \quad (A42) \]
where
\[ \langle b^\dagger_q b_q \rangle = \langle \tilde{n}^c_q \rangle + \frac{1}{N} \sum_k \left[ |\tilde{t}^+_{k-q,q} \tilde{n}^f_{k-q} (1 - \tilde{n}^B_{k-q}) \right. \]
\[ + |\tilde{t}^{-}_{k-q,q} \tilde{n}^f_{k-q} \tilde{n}^B_{k-q} \]. \quad (A43) \]
\[ \langle b^\dagger_q \rangle \sim \langle \tilde{n}^c_q \rangle = \langle \tilde{n}^c_q \rangle \tilde{n}^B_{q} \tilde{n}^B_{q} - \langle \tilde{n}^c_q \rangle \]. \quad (A44) \]

We emphasize that in \( \langle b^\dagger_q \rangle \) smaller contributions from \( (A35) \) have been neglected. Using Eq. \( (A21) \) the expectation values \( \tilde{n}^b_q = \langle b^\dagger_q b_q \rangle \tilde{n}^B_q \delta_{q=q} \) and \( \langle \tilde{n}^c_q \rangle \tilde{n}^B_q \tilde{n}^B_{q} \) on the right hand sides become
\[ \tilde{n}^b_q = \langle B^\dagger_q B_q \rangle \tilde{n}^B_q \tilde{n}^B_{q} - \frac{\sqrt{Nh}}{\omega_q} \langle B^\dagger_q B_q \rangle + \frac{Nh^2}{\omega^2_q} \langle B^\dagger_q B_q \rangle \delta_{q=q} \]
\[ = f^{B}(\tilde{\omega}_q) + \frac{Nh^2}{\omega^2_q} \delta_{q=q} \quad (A45) \]
and

$$\langle b_q^\dagger \hat{n} \rangle = \left[ \langle B_q^\dagger \hat{n} \rangle - \frac{\sqrt{N} \hbar}{\omega_q} \right] \delta_{q,Q} = -\frac{\sqrt{N} \hbar}{\omega_q} \delta_{q,Q}. \quad (A46)$$

Here we have used \( \langle B_q^\dagger \hat{n} \rangle = 0 \). \( f^B(\tilde{\omega}_q) \) is the bosonic distribution function which becomes one at zero temperature. Inserting Eqs. (A35), (A46) into (A33), (A44) one finally arrives at

$$n^B_q = |\tilde{\varepsilon}_q|^2 f^B(\tilde{\omega}_q) + \frac{1}{N} \sum_k \left[ |\tilde{\nu}_{k,-q}^+|^2 n^c_k(1 - \tilde{n}_{k,-q}^c) + |\tilde{\nu}_{k,q}^-|^2 \tilde{n}_{k,q}^+(1 - \tilde{n}_k^-) \right]. \quad (A47)$$

Note that the electronic order parameter \( d_k \) and the phononic order parameter \( \Delta \) are intimately related. Due to (A38) and (A41), \( d_k \) is proportional to \( \Delta = \Delta \), so that both order parameters are mutually dependent. Finally, as a side remark, note that the lattice displacement in the EI state is given by

$$x_Q = \frac{1}{\sqrt{N}} \frac{\tilde{\varepsilon}_Q}{\sqrt{2\omega_Q}} (b^\dagger - b) \tilde{n} = -\frac{1}{N} \frac{\hbar \tilde{\varepsilon}_Q}{\omega_Q}, \quad (A48)$$

as follows from Eqs. (A44) and (A46).

4. Spectral functions

Let us first evaluate the electronic one-particle spectral functions. Here, the c-electron spectral function \( A^c_k(\omega) \) was defined before in Eq. (24)

$$A^c_k(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle [\hat{c}_{k\sigma}(t), \hat{c}_{k\sigma}^\dagger(0)] \rangle e^{i\omega t} dt, \quad (A24)$$

where the expectation value is formed with \( \mathcal{H} \). Using the unitary invariance of operator expressions under a trace one arrives at the former expression (30). By use of Eq. (A33) and Eq. (A22) the following result for \( A^c_k(\omega) \) is found

$$A^c_k(\omega) = |\tilde{\varepsilon}_k|^2 [\varepsilon_k^2 - Q^2 \delta(\omega - \tilde{E}^1_k - Q)] + n^c_k(1 - \tilde{n}_{k}^-) + \delta(\omega - \tilde{E}^2_k - Q)]$$

$$+ \frac{1}{N} \sum_q \left[ \tilde{n}_{k,-q}^+ \right]^2 (n^B_{k,-q} + \tilde{n}_{k,-q}^c) \delta(\omega - \tilde{\varepsilon}_k^- - \tilde{\omega}_q)$$

$$+ \tilde{n}_{k,q}^- \left( 1 + n^B_{k,q} - \tilde{n}_{k,q}^c \right) \delta(\omega - \tilde{\varepsilon}_k^+ - \tilde{\omega}_q) \right]. \quad (A49)$$

Similarly, for the f-electron spectral function one finds

$$A^f_k(\omega) = |\tilde{\varepsilon}_k|^2 [\varepsilon_k^2 - \delta(\omega - \tilde{E}^1_k)] + \varepsilon_k^2 \delta(\omega - \tilde{E}^2_k)]$$

$$+ \frac{1}{N} \sum_q \left[ \tilde{n}_{k,q}^+ \right]^2 (1 + n^B_{k,q} - \tilde{n}_{k,q}^c) \delta(\omega - \tilde{\varepsilon}_k^+ + \tilde{\omega}_q)$$

$$+ \tilde{n}_{k,q}^- \left( \tilde{n}_{k,q}^+ + \tilde{n}_{k,q}^c \right) \delta(\omega - \tilde{\varepsilon}_k^+ + \tilde{\omega}_q). \quad (A50)$$

The first line in both spectral functions is the coherent contribution which describes excitations at the electronic quasiparticle energies \( \tilde{E}^{1,2}_k \). The remaining lines are incoherent contributions. They are induced by the electron-phonon interaction and turn out to be small. Note that the coherent part in both cases reduce to the mean-field result, when the renormalized quantities are replaced by the unrenormalized quantities.

The phonon spectral function \( C_q(\omega) \) is found in the same way. It is defined by

$$C_q(\omega) = \frac{1}{2\pi \omega} \int_{-\infty}^{\infty} \langle [b_q(t), b_q^\dagger(0)] \rangle e^{i\omega t} dt \quad (A51)$$

$$+ \frac{1}{N} \sum_k \left[ \tilde{n}_{k,-q}^+ \right]^2 n^F_{k,-q} - n^F_{k,-q} \delta(\omega - \tilde{\varepsilon}_k^-)$$

$$+ \tilde{n}_{k,q}^- \left( \tilde{n}_{k,q}^+ - \tilde{n}_{k,q}^c \right) \delta(\omega - \tilde{\varepsilon}_k^+). \quad (A52)$$

The numerical solution of the phonon spectral function \( C_q(\omega) \) in Fig. 7 has shown that \( \tilde{\omega}_q \) hardens in the non-adiabatic case \( (\omega_0 = 0.5) \) whereas it softens in the adiabatic case \( (\omega_0 = 2.5) \). One may ask, can this opposite tendency of the phonon mode already be understood in perturbation theory? At first, note that \( \omega_0 \) is not altered by the mean-field theory, as shown in Sec. III. Therefore, the renormalization of the phonon frequency as well as the \( Q \)-dependence of \( \tilde{\omega}_q \) can only be caused by the coupling to the electronic degrees of freedom, i.e. by the influence of \( \mathcal{H}_1 \). The easiest way to derive \( \tilde{\omega}_q \) in perturbation theory is to start from the renormalization equation (A13) for \( \tilde{\omega}_q(\Lambda) \) when the renormalization from the original cutoff \( \Lambda \) to \( \lambda = 0 \) is done in one single step. Therefore, choosing
\[ \lambda = \Lambda \text{ and also } \Delta \lambda = \Lambda, \text{ one finds from Eq. (A13)} \]
\[
\tilde{\omega}_q - \omega_0 = -\frac{2g^2}{N} \sum_k \left( A^{+}_{k-q}(\Lambda, \Lambda)(n^f_k - n^f_{k-q}) + A^-_{k,q}(\Lambda, \Lambda)(n^I_k - n^I_{k+q}) \right) + \frac{2g^2}{N} \sum_k \left( \frac{n^I_{k+q} - n^I_k}{\epsilon^I_{k+q} - \epsilon^I_k + \omega_0} + \frac{n^I_{k-q} - n^I_k}{\epsilon^I_{k-q} - \epsilon^I_k - \omega_0} \right),
\]
\[ (A53) \]

which is the perturbative result up to \( O(g^2) \). Here we have used that according to Eq. (A20) the coefficients \( A^{\pm}_{kq}(\Lambda, \Lambda) \) reduce to \( A^{\pm}_{kq}(1, 1) \).

In the adiabatic limit in agreement with the numerical outcome in the adiabatic limit, which is like the result in the anti-adiabatic case \( (\omega_q \gg \epsilon^c_{k-q}, \epsilon^c_k) \). One realizes that the renormalization due to the elimination of \( \mathcal{H}_1 \) becomes rather small in this limit. This follows from expression (AS) for \( \Delta \lambda \), which has coefficients

\[
A^{\pm}_{kq}(\lambda, \Delta \lambda) = \Theta_{kq,\lambda}^{\pm}(1 - \Theta_{kq,\lambda}^{\pm} - \Delta \lambda)).
\]

(B1)

For large \( \omega_q, \lambda \sim O(\omega_0) \), expression (B1) reduces to

\[
A^{\pm}_{kq}(\lambda, \Delta \lambda) \approx \Theta_{kq,\lambda}^{\pm}(1 - \Theta_{kq,\lambda}^{\pm} - \Delta \lambda)),
\]

(B2)

where the \( \Theta \)-functions are now independent of \( k \):

\[
\Theta_{kq,\lambda}^{\pm} \approx \Theta(\lambda - |\omega_0|) = \Theta(\lambda).
\]

(B3)

Obviously, for large energy \( \omega_0 \), Eq. (B2) only allows small renormalization contributions. Moreover, the product \( \Theta_{kq}(1 - \Theta_{kq,\lambda} - \Delta \lambda) \) in the numerator prevents any \( k \)-dependent renormalization contribution between cutoff \( \lambda \) and \( \lambda - \Delta \).

(i) **Gap equation:** For the conditional equation of the order parameter \( \Delta \), obtained by the PRM, one concludes that in the anti-adiabatic limit it reduces to the mean-field expression (B3) since renormalization contributions due to \( \mathcal{H}_1 \) are suppressed. Thus, for \( \omega_0 \to \infty \) one obtains as asymptotic result

\[
1 = \frac{4g^2}{\omega_0} \frac{1}{N} \sum_k \text{sgn}(\epsilon^c_{k+Q} - \epsilon^c_k) \frac{f^F(E^{(1)}_k) - f^F(E^{(2)}_k)}{W_k},
\]

(B4)

where all quantities are unrenormalized.

At the critical electron-phonon coupling \( g_\text{c} \), the order parameter \( \Delta \) vanishes and the condition (B4) becomes

\[
1 = \frac{4g^2}{\omega_0} \frac{1}{N} \sum_k \text{sgn}(\epsilon^c_{k+Q} - \epsilon^c_k) \frac{f^F(\epsilon^c_{k+Q}) - f^F(\epsilon^c_{k+Q})}{\epsilon^c_{k+Q} - \epsilon^c_k}.
\]

(B5)

In this extreme anti-adiabatic limit, the squared critical coupling \( g_\text{c}^2 \) scales linearly with \( \omega_0 \), provided the electronic parameters in the sum over \( k \) are kept constant. This behavior is in perfect agreement with the outcome from the numerical solution of the PRM equations, as shown in the inset of Fig. 5. Even, the numerical result from (B4) \( (g^2_\text{c}/\omega_0)_{\omega_0 \to \infty} \approx 0.16 \) is in acceptable agreement with that from Sec. (V) which is \( (g^2_\text{c}/\omega_0)_{\omega_0 \to \infty} \approx 0.14 \).

(ii) **Incoherent excitations:** The above feature of \( A^{\pm}_{kq}(\lambda, \Delta \lambda) \) can also be used to explain the behavior...
of the incoherent contributions to the electronic spectral functions $A_{\omega}^{\pm}(f)(\omega)$ in Figs. 5 and 6. As long as the electron-phonon coupling $g$ is not too small, the figures show that for the non-adiabatic case ($\omega_0 = 2.5$) in Fig. 5 the incoherent contributions to the spectral functions are less pronounced than for the adiabatic case ($\omega_0 = 0.5$) in Fig. 6. This property results from the prefactors $|t_{k-q}^{\pm}|^2$ and $|u_{k-q}^{\pm}|^2$ of the incoherent contributions in Eqs. (A51) and (A52). They are found from the solution of the renormalization equations (A20) and (A27) for $t_{k-q}^{\pm}$ and $u_{k-q}^{\pm}$, and are governed by the coefficients $A_{kq}(\lambda, \Delta \lambda)$. A similar behavior is also observed for the phonon spectral function $C_{\omega}(\omega)$ in Fig. 7, where the incoherent contributions in the anti-adiabatic regime are strongly suppressed. Note that also the weight of the incoherent excitations increases when the coupling $g$ is increased.

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