Influence of Hybridization on the Properties of the Spinless Falicov-Kimball Model

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I. INTRODUCTION

The spinless Falicov-Kimball model (FKM) without hybridization is one of the simplest non-trivial interacting many-body models. It takes into account a conduction (c-) band, a lattice of localized f-electron states and an on-site Coulomb (Falicov-Kimball-) interaction between the f- and c-electrons. It was originally proposed as a model for discontinuous valence and/or metal-insulator transitions, but has also been interpreted as a model for crystallization (interpreting the f-"electrons" as ions or nuclei) and for ordering in binary alloys. The FKM can also be considered to be a simplified version of the Hubbard model in which the electrons of the one (spin) species (corresponding to the "f-electrons") have no dispersion.

Much of the older work on the FKM was based on mean-field like decouplings of the interaction, and evidence for discontinuous phase (valence) transitions was obtained. But Leder and G. Czycholl pointed out that in the presence of a finite hybridization between f- and c-electrons only continuous transitions are present in a Hartree-Fock-decoupling; this result was confirmed in higher-order decouplings. This work emphasized, in particular, the importance of a decoupling with respect to excitonic expectation values in the presence of a finite hybridization. Subsequently it was found by Brandt and Schmidt and, independently, by Kennedy and Lieb that for dimension d ≥ 2 at half filling the FKM without hybridization has an inhomogeneous ground state with a chess-board like distribution of the f-particles. Thus a phase transition from a homogeneous high temperature phase to an inhomogeneous charge-density wave (CDW) like low temperature phase has to be expected. Shortly after the discovery of the limit of high dimensions, d → ∞, Brandt and Mielsch found the exact solution of the FKM without hybridization in this limit. They could obtain exact results for the band-(c-)electron selfenergy and Green function and for the f-electron occupation and for the f-electron occupation number and confirmed the existence of the phase transition and of the inhomogeneous CDW- (chess-board-) ground state for large d. To obtain this solution the FKM has to be mapped on an effective single-site problem in an auxiliary external field, and this idea is just the foundation of the nowadays so successful "dynamical mean-field theory" (DMFT) which becomes exact for large-d correlated electron systems. But in contrast to other correlated electron models (like the Hubbard model) one does not rely on approximate or numerical (e.g. quantum Monte-Carlo) methods, but the DMFT-equations can be solved exactly for the c-electron selfenergy (the "dynamical mean-field") of the FKM. More recently the optical properties of the FKM were investigated by Portengen, Ostreich and Sham. They studied the FKM with a k-dependent hybridization (taking account of more realistic symmetries of the c- and f-states) in Hartree-Fock approximation and found, in particular, that a non-vanishing excitonic expectation value exists even in the limit of vanishing hybridization V → 0. As an applied (optical) electric field provides for excitations between c- and f-states and thus for a polarization expectation value $P_{cf} = \langle c^\dagger f \rangle$, the finding of a "spontaneous" $P_{cf}$ (without hybridization or electric field) has been interpreted as evidence for electronic ferroelectricity. Within the Brandt-Mielsch ground state, however, one has $P_{cf} = 0$. Therefore, the question arises: Is the Brandt-Mielsch ground state stable against a small, finite hybridization or is one led to a different ground state if one starts from a finite hybridization and studies the $V \to 0$ limit of the model? Does the spinless FKM with an (infinitesimal) small hybridization...
still have the inhomogeneous CDW-like ground state or does it have a ferroelectric ground state with a spontaneous, non-vanishing polarization $P_{c,\langle f \rangle}$?

These are the questions to be answered in this contribution. To my knowledge it has not yet been investigated, which influence a finite hybridization has on the Brandt-Mietsch solution; in fact, with a few exceptions most recent FKM-work neglected the hybridization. Of course, with hybridization an exact solution of the FKM is no longer possible but one has to rely on approximations. It is easy to see analytically that in the weak-coupling limit (of small interaction) the exact Brandt-Miefsch solution contains the Hartree-Fock solution in lowest order. The inhomogeneous CDW-Brandt-Miefsch ground state is even exactly reproduced within the Hartree-Fock treatment of the FKM without hybridization. Comparing the CDW-order parameter obtained in the exact Brandt-Miefsch solution and in the Hartree-Fock approximation one sees that they completely agree for zero temperature, i.e. for the ground state, but the critical temperature $T_c$ obtained in Hartree-Fock approximation is way too large compared to the Brandt-Miefsch result for $T_c$. For low temperatures, however, the Hartree-Fock result is reliable, and the Hartree-Fock treatment can, of course, also be applied to the FKM with hybridization. Then one obtains an inhomogeneous CDW-phase at low temperatures also for finite but small hybridization $V < V_c$; above the critical hybridization $V_c$, however, there is no longer an inhomogeneous CDW-phases, but only a spatially homogeneous result is obtained within mean-field theory. Thus the inhomogeneous CDW-phase exists also within Hartree-Fock theory for $V < V_c$, but it has been overlooked in previous Hartree-Fock treatments probably because a homogeneous solution was anticipated in this work. For finite $V$ there exists, of course, a finite polarization $P_{c,\langle f \rangle} = < cf^\dagger f >$, which is strongly enhanced due to the Falicov-Kimball interaction. Studying $P_{c,\langle f \rangle}$ as a function of $V$ one sees that it vanishes for $V \to 0$, if one follows the inhomogeneous CDW-solution. If one follows the (additionally existing) homogeneous Hartree-Fock solution, however, one obtains a polarization $P_{c,\langle f \rangle} \neq 0$ for $V \to 0$ in agreement with Ref. [13]. Thus a ferroelectric phase with a non-vanishing $P_{c,\langle f \rangle}$ for vanishing hybridization $V = 0$ is obtained within a Hartree-Fock treatment of the FKM, but, unfortunately, this is not the most stable (favorable) Hartree-Fock solution.

Of course, this statement concerns only the spinless FKM, which is not very realistic, because any real Fermi system has at least a spin degeneracy. In fact, I do not know of any real electronic system exhibiting the inhomogeneous ground state with a CDW (chess-board) pattern obtained for the spinless FKM (without and with hybridization $V \leq V_c$). Therefore, it has still to be investigated if more realistic models (including spin and orbital degrees of freedom for the electronic states) would not allow for different ground states, for instance the ferroelectric one. Nevertheless, the investigation of the spinless FKM with hybridization is of interest at least as a model study because it allows for a study of the influence of the Falicov-Kimball (interband-) interaction alone, because of the interpretation of the FKM as a simplified version of the Hubbard model, and because of the exactly solvable limit $V \to 0$.

The paper is organized as follows: In section 2 I describe the FKM (with and without hybridization) and the Brandt-Miefsch solution. Section 3 shows that the Hartree-Fock solution is obtained from the exact Brandt-Miefsch solution in the weak-coupling limit and that the Hartree-Fock approximation yields the exact ground state properties of the model without hybridization. Numerical Hartree-Fock results for the FKM with hybridization are presented in Section 4 indicating that also for a small finite hybridization $V \leq V_c$ the ground state is of the inhomogeneous (chess-board) type, and the final Section 5 contains a short conclusion.

II. FALICOV-KIMBALL MODEL AND BRANDT-MIELSCH SOLUTION

The spinless Falicov-Kimball model (FKM) is defined by the Hamiltonian

$$H = H_0 + H_1$$

(1)

Here

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_R E_f f_R^\dagger f_R + \sum_R U c_R^\dagger c_R f_R^\dagger f_R$$

(2)

$$= \sum_R \left( \sum_{\Delta n.n.} t c_R^\dagger c_{R+\Delta} + E_f f_R^\dagger f_R + U c_R^\dagger c_R f_R^\dagger f_R \right)$$

describes the FKM without hybridization. It consists of a conduction ($c$-)band with a tight-binding dispersion

$$\varepsilon_k = t \sum_{\Delta n.n.} \exp(i k \Delta)$$

(3)

where $t$ is the nearest neighbor hopping, $\Delta$ denotes nearest-neighbor (n.n.) lattice vectors and the band center has been chosen as the zero of the energy scale, a lattice of f-electron states localized at the lattice sites $R$ with energy $E_f$, and a short ranged Coulomb (Falicov-Kimball-) interaction $U$ between $c$- and f-electrons at the same lattice sites. The second part

$$H_1 = V \left( f_R^\dagger c_R + c_R^\dagger f_R \right)$$

(4)

describes the hybridization between the conduction and f-electron states, which for simplicity is assumed to be also on-site (local) in the present simple model study, though for realistic f- and conduction-electron ($d$- or $s$-band) states a hybridization must have a dispersion (dispersion) for symmetry (parity) reasons [13].
The large-d limit for such a correlated lattice electron model is defined as the limit \( d \to \infty, t \to 0 \) keeping \( dt^2 = \text{const} \). Then for a d-dimensional (hyper)cubic lattice with nearest neighbor hopping the unperturbed tight-binding density of states of the conduction electron band is a Gaussian function \( \rho_0(E) = \exp(-(E^2)/\sqrt{\pi} \). Instead of this a semielliptic model density of states will be considered here, i.e.

\[
\rho_0(E) = \frac{2}{\pi} \sqrt{1 - E^2}
\]

(5)

This semielliptic density of states becomes correct for a Bethe lattice in the limit of a large coordination number, and it may be considered to be advantageous compared to the Gaussian density of states, because it has a finite bandwidth and the correct 3-dimensional bandedge van-Hove singularities so that it may better model realistic 3-dimensional systems. The corresponding unperturbed band-electron one-particle Green function is given by

\[
F_0(z) = \frac{1}{N} \sum_k \frac{1}{z - \bar{\varepsilon}_k} = 2 \left( z - \sqrt{z^2 - 1} \right)
\]

(6)

Thereby half the unperturbed conduction band width has been chosen as the energy unit. The explicit form of the unperturbed conduction density of states is not important; one could also use a realistic 3-dimensional tight-binding density of states. The important issue to be adopted from the large-d limit is the fact that the self-energy (the "dynamical mean-field") of the interacting system is site-diagonal (local). Therefore the self-energy is a functional of the local Green function alone and the functional dependence is the same as that of an effective atomic or single-impurity problem. For the FKM without hybridization \( (V = 0) \), i.e. for the Hamilton \( H_0 \) alone, which case will only be discussed in the remainder of this section, Brandt and Mielisch could analytically determine this functional for the conduction electron self-energy, namely,

\[
\Sigma_R(z) = \frac{Un_{fR}}{1 - (U - \Sigma_R(z))G_{cR}(z)}
\]

(7)

Here \( G_{cR}(z) \) is the on-site matrix element of the full conduction electron Green function \( G_c(z) \), which depends itself on the selfenergy to be determined, and \( n_{fR} \) is the f-electron occupation number at site \( \mathbf{R} \). The selfenergy functional \( \Sigma_R(z) \) is just of the Hubbard-III (alloy-analog) form, or, in other words, it is just the selfenergy functional of the coherent potential approximation (CPA) for disordered alloys, if the f-electron occupation number \( n_{fR} \) is interpreted as an impurity concentration. But here the f-electron occupation of the sites does not occur at random, but it depends itself on the band-electron Green function and the occupation of the other sites. Explicitly the f-electron occupation number is given by

\[
n_{f\mathbf{R}} = \frac{1}{1 + \exp \left( (E_f - \mu)/T \right) \prod_n \left( 1 - UG_{cR0}(z_n) \right)}
\]

(8)

where, as usual, \( T \) is the temperature (measured in energy units, i.e. \( k_B = 1 \)), \( \mu \) is the chemical potential, \( z_n = \mu + i\omega_n = \mu + i(2n + 1)\pi T \) denotes the Matsubara frequencies and

\[
G_{c\mathbf{R}0}(z) = \frac{G_{c\mathbf{R}}(z)}{1 + \Sigma_{\mathbf{R}}(z)G_{c\mathbf{R}}(z)}
\]

(9)

Obviously the f-electron occupation number can also be written in the form

\[
n_{f\mathbf{R}} = f(\tilde{E}_{f\mathbf{R}})
\]

(10)

where \( f(E) = [\exp((E - \mu)/T) + 1]^{-1} \) denotes the Fermi function and the effective f-level energy \( \tilde{E}_{f\mathbf{R}} \) is given by

\[
\tilde{E}_{f\mathbf{R}} = E_f - T \sum_n \ln(1 - UG_{c\mathbf{R}0}(z_n))
\]

(11)

In the remainder of the paper only the case of half filling, i.e. one electron per lattice site \( n_{f\mathbf{R}} + n_{c\mathbf{R}} = 1 \), and the symmetric model, i.e. \( E_f = 0 \) will be considered; then the chemical potential is automatically fixed at \( \mu = U/2 \).

If one anticipates a translationally invariant form of the solution, the selfenergy \( \Sigma_R(z) \), band-electron Green function \( G_{c\mathbf{R}}(z) \) and f-electron occupation number \( n_{f\mathbf{R}} \) are translationally invariant and do not depend on the lattice site \( \mathbf{R} \). Then the Green function is simply given by

\[
G_{c\mathbf{R}}(z) = G_c(z) = \frac{1}{N} \sum_k \frac{1}{z - \Sigma(z) - \bar{\varepsilon}_k} = F_0(z - \Sigma(z))
\]

(12)

But in general an inhomogeneous solution has to be expected for the ground state, as the following simple consideration for the atomic limit (i.e. hopping \( t = 0 \)) shows: If one assumes that in the atomic limit the average occupation number for both, the f- and c-electrons is \( 1/2 \), then, of course, a spatial separation of f- and c-electrons is energetically most favorable, i.e. half of the lattice sites is filled with f- and the other half with c-electrons; then because of the short-ranged nature of the model interactions all interactions (repulsions) are avoided and all electrons have only their one-particle energies \( E_f = E_c \) (= 0 for the above choice of the energy scale). Because of the competition with the kinetic energy, the picture is no longer as simple in the case of a finite conduction band width (finite hopping \( t \)). Then also the sites occupied by f-electrons get a finite occupation probability for band-electrons. But nevertheless an inhomogeneous ground state is energetically most favorable. For a bipartite lattice with an A- and B-sublattice in the ground state the f-electron states are occupied for the sites of one sublattice, say A, and empty for \( \mathbf{R} \in B \), and therefore the band electrons see an alternating effective potential and will also inhomogeneously (alternating from A- to B-site) be occupied. Defining the A-(B-) occupation numbers as
\[ n_{aA}(T) = n_{aR} = \langle a_R^\dagger a_R \rangle \quad \text{for } R \in A \]
\[ n_{aB}(T) = n_{aR} = \langle a_R^\dagger a_R \rangle \quad \text{for } R \in B \] (13)

and \( \sigma \{ c, f \} \) one has \( n_{fA}(T = 0) = 1 \), \( n_{fB}(T = 0) = 0 \) and \( 0 \leq n_{cA}(T = 0) < n_{cB}(T = 0) \leq 1 \) and can define the CDW order parameter as
\[ m(T) = n_{cB}(T) - n_{cA}(T) \] (14)

A full polarization of the band electrons, i.e. \( m(T = 0) \to 1 \), can be expected only in the strong coupling (large \( U \)) limit. It has been shown that for half filling the ground state of the FKM without hybridization has, in fact, the chess-board symmetry, i.e. a finite CDW-order parameter \( m(T = 0) \). Furthermore, for \( d \to \infty \) correlation functions, the critical temperature \( T_c \) at which the order parameter vanishes (as a function of the correlation \( U \)), the free energy and other quantities could be calculated away from half filling indications for phase separation were obtained.

### III. BRANDT-MIELSCH AND HARTREE-FOCK SOLUTION FOR VANISHING HYBRIDIZATION

In this section I will show that for small interaction \( U < 1 \) the Hartree-Fock approximation becomes reliable and contains the most essential features of the exact Brandt-Mielsch solution (partially even quantitatively) for the FKM without hybridization. From the exact results (7) and (11) one obtains in lowest order in the correlation for the band-electron selfenergy
\[ \Sigma_R(z) = U n_R \] (15)
and for the effective f-level energy
\[ \tilde{E}_{fR} = E_f + UT \sum_n G_{cR}(z_n) = E_f + U < n_{cR} > \] (16)

Obviously this is just the standard Hartree-Fock approximation for the FKM without hybridization, which thus follows from the exact result by an expansion with respect to \( U \) in lowest (linear) order in \( U \). This result is certainly not surprising but rather as it should be expected.

For the inhomogeneous CDW-phase the agreement between Hartree-Fock and exact solution is even stronger and – at least for \( T = 0 \), i.e. for the ground state—rigorously fulfilled (i.e. without \( U \)-expansion). Because of the full polarization of the f-electrons at \( T = 0 \), i.e. \( n_{fA}(T = 0) = 1 \) and \( n_{fB}(T = 0) = 0 \), one gets from (11)
\[ \Sigma_A(z) = U \quad \Sigma_B(z) = 0 \] (17)

which obviously corresponds to the Hartree-Fock result in this case. Therefore, if the f-electron system is fully polarized, the band-electron spectral function obtained in Hartree-Fock approximation (shown in Fig. 1 for \( U=0.4 \)) is identical to the exact spectral function. But even for

![FIG. 1. A- and B-sublattice band electron spectral function for \( U = 0.4, T = 0 \) in the inhomogeneous CDW phase](image)

![FIG. 2. Band electron spectral function for the homogeneous phase within the exact Brandt-Mielsch solution and in Hartree-Fock approximation for \( U = 0.4 \)](image)

![FIG. 3. Temperature dependence of the CDW order parameter \( m(T) \) for the FKM without hybridization (\( V = 0 \)) within the exact Brandt-Mielsch solution and within the Hartree-Fock approximation for \( U = 0.4 \) and \( U = 0.6 \)](image)
the homogeneous phase \((n_{fA} = n_{fB} = 0.5)\), which may be artificially enforced for low \(T\) or becomes the only solution for high \(T\), the difference between the Hartree-Fock and the exact solution for the spectral function may be small, as shown in Fig. 3; this holds true if the correlation \(U\) is sufficiently small so that the (around \(\mu = U/2\) symmetric) exact conduction electron density of states does not show indications of the splitting into the upper and lower Hubbard band. In Fig. 3 I present results for the temperature dependence of the CDW order-parameter obtained in Hartree-Fock approximation and exactly for \(U = 0.4\) and \(U = 0.6\). Obviously there is full agreement between the exact and Hartree-Fock result for \(m(T)\) for low temperatures \(T \to 0\) in agreement with the above argumentation. But with increasing temperature (when the \(f\)-electrons are no longer fully polarized) \(m(T)\) in Hartree-Fock becomes different from the exact result and, in particular, the critical temperature \(T_c\) above which the CDW order parameter vanishes is way too large in Hartree-Fock approximation compared to the exact (Brandt-Mielsch-) result. But at least for the low temperature (ground state) properties and small to intermediate values of the \(cf\)-correlation \(U\) \((U \leq 1)\), which is realistic for the Falicov-Kimball interaction, the Hartree-Fock approximation yields already good results for the FKM without hybridization in agreement with the exact Brandt-Mielsch result.

\section*{IV. HARTREE-FOCK TREATMENT FOR FINITE HYBRIDIZATION}

The FKM with hybridization is no longer exactly solvable, but, of course, approximations like the Hartree-Fock-treatment can be applied. As these Hartree-Fock results become correct for the groundstate properties of the model without hybridization, it can be expected that this simple approximation also reproduces the essential ground state properties of the FKM with hybridization, at least qualitatively and for \(U \leq 1\). Within Hartree-Fock theory the FKM Hamiltonian \((\ref{eq:22})\) is replaced by the following effective one-particle Hamiltonian:

\begin{equation}
H_{\text{eff}} = \sum_{\mathbf{R}} \left( \tilde{E}_{\mathbf{R}} c_{\mathbf{R}}^\dagger c_{\mathbf{R}} + t \sum_{\Delta n.n.} c_{\mathbf{R}+\Delta}^\dagger c_{\mathbf{R}} + \tilde{E}_{\mathbf{fR}} f_{\mathbf{fR}}^\dagger f_{\mathbf{fR}} + \tilde{V}_{\mathbf{R}} (f_{\mathbf{fR}}^\dagger c_{\mathbf{R}} + c_{\mathbf{R}}^\dagger f_{\mathbf{fR}}) \right)
\end{equation}

where the effective parameters are given by

\begin{align*}
\tilde{E}_{\mathbf{R}} &= U n_{f\mathbf{R}} \\
\tilde{E}_{\mathbf{fR}} &= E_f + U n_{c\mathbf{R}} \\
\tilde{V}_{\mathbf{R}} &= V - U P_c_{f\mathbf{R}} = V - U < c_{\mathbf{R}}^\dagger f_{\mathbf{fR}} >
\end{align*}

and have to be determined selfconsistently. Of course, as the exact solution for \(V = 0\) is of the spatially inhomogeneous CDW type, one has to allow for an inhomogeneous Hartree-Fock solution in the case of finite hybridization \(V\), too, i.e. one should not only look for a translationally invariant solution of \((\ref{eq:22})\), for which the expectation values \(n_f, n_c, P_c\) are independent on the lattice site \(\mathbf{R}\), as it has been done in previous Hartree-Fock studies of the FKM with hybridization \((\ref{eq:22})\). Again different expectation values and thus effective one-particle parameters will be admitted for lattice sites from the A- or B-sublattice. The expectation values are given by

\begin{align*}
n_{f\mathbf{R}} &= \langle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle = -\frac{1}{\pi} \int dE f(E) \operatorname{Im} G_{c\mathbf{R}}(E + i0) \\
n_{f\mathbf{fR}} &= \langle f_{\mathbf{fR}}^\dagger f_{\mathbf{fR}} \rangle = -\frac{1}{\pi} \int dE f(E) \operatorname{Im} G_{f\mathbf{fR}}(E + i0) \\
P_{c\mathbf{fR}} &= \langle c_{\mathbf{R}}^\dagger f_{\mathbf{fR}} \rangle = -\frac{1}{\pi} \int dE f(E) \operatorname{Im} G_{c\mathbf{R}f\mathbf{fR}}(E + i0)
\end{align*}

In the case of a finite hybridization and a possible AB-sublattice structure the on-site matrix elements of the Green function are explicitely given by

\begin{align*}
G_{f\mathbf{R}}(z) &= \frac{1}{z - \tilde{E}_{f\mathbf{R}}} \left( 1 + \tilde{V}_{\mathbf{R}} G_{f\mathbf{R}}(z) \right) \\
G_{f\mathbf{fR}}(z) &= \frac{\tilde{V}_{\mathbf{R}}}{z - \tilde{E}_{f\mathbf{R}}} G_{c\mathbf{R}}(z) \\
G_{c\mathbf{A(B)}\mathbf{R}}(z) &= \sqrt{Z_{\mathbf{B(A)}} Z_{\mathbf{A(B)}}} F_0(\sqrt{Z_{\mathbf{A}} Z_{\mathbf{B}}})
\end{align*}

with

\begin{equation}
Z_{\mathbf{A(B)}} = Z_{\mathbf{R}} = z - \tilde{E}_{c\mathbf{R}} - \frac{\tilde{V}_{\mathbf{R}}^2}{z - \tilde{E}_{f\mathbf{R}}} \quad \text{for} \quad \mathbf{R} \in \mathbf{A(B)}
\end{equation}

The above selfconsistency equations can easily be solved numerically by iteration, and some of the results are shown in the following figures. Fig. 4 shows the temperature dependence of the CDW order parameter \(m(T) = n_{cB}(T) - n_{cA}(T)\) for different values of the hybridization \(V\). According to the discussion in the previous section the \(T \to 0\) value of \(m(T)\) can be expected to correspond to the exact value, whereas the critical temperature \(T_c\) is probably too large, as in most Hartree-Fock-studies. Obviously the order parameter strongly decreases with increasing hybridization. This results from the fact that for any non-vanishing hybridization the \(f\)-electron occupation is no longer a good quantum number for the FKM; consequently the \(f\)-electron occupation number of one lattice site is no longer exactly 0 or 1 in the ground state, and therefore the band-electron polarization is also smaller than without hybridization and is the smaller the larger the hybridization is. Fig. 5 shows the low temperature order parameter \(m(T,V)\) \((T = 0.008)\) as a function of the hybridization, which confirms the decrease of the CDW-phase with increasing \(V\). Obviously there is a critical value \(V_c\) of the hybridization at which the CDW-order-parameter vanishes. For
larger $V$ only a homogeneous, translationally invariant solution exists. Finally the hybridization dependence of the off-diagonal expectation value $P_{c\bar{f}R} = \langle c^\dagger_{\bar{R}} f_R \rangle$ is shown in Fig. 5. Obviously, for the most stable, inhomogeneous CDW-solution $P_{c\bar{f}R}$ vanishes linearly with the hybridization:

$$P_{c\bar{f}R} = \langle c^\dagger_{\bar{R}} f_R \rangle \to 0 \text{ for } V \to 0$$  \hspace{1cm} (23)

But the above Hartree-Fock selfconsistency equations have also a homogeneous, translationally invariant solution, for which the CDW order parameter $m(T)$ vanishes and for which $P_{c\bar{f}}(V)$ is given by the dashed line in Fig. 5, if one starts from the high-$V$ homogeneous solution and follows it to small values of $V$. Obviously, for the homogeneous Hartree-Fock solution one has $P_{c\bar{f}}(V) \neq 0$ for $V \to 0$. Then one would have a built-in polarization, a nonvanishing excitonic expectation value $\langle c^\dagger_{\bar{R}} f_R \rangle$ for vanishing hybridization, a different kind of symmetry breaking formally resembling superconductivity (also concerning the type of selfconsistency equation and of the temperature dependence of the order parameter $P_{c\bar{f}}(V = 0, T)$). But this homogeneous Hartree-Fock solution is not the most stable one, the inhomogeneous CDW solution has the lower energy as becomes clear immediately from the densities of states of Fig. 1.2.

**V. SUMMARY AND CONCLUSION**

To summarize, I have studied the simple spinless Falicov-Kimball model for half filling (i.e. one electron per lattice site) and in the symmetric case and found that without hybridization the simple Hartree-Fock approximation reproduces the exact CDW ground state first obtained by Brandt and coworkers. Furthermore I found that also for finite but small hybridization, for which no exact result is available, an inhomogeneous CDW ground state is obtained, i.e. this ground state remains stable when turning on a hybridization (or applying a field providing for c-f-transitions and thus for an effective hybridization). But the CDW-order parameter decreases with increasing hybridization, and a critical value of the hybridization $V_c$ exists above which only a homogeneous solution and no CDW phase is obtained. For the inhomogeneous phase the "polarization" (or the c-f-transition rate $\langle c^\dagger_{\bar{R}} f_R \rangle$) vanishes in the limit $V \to 0$; so there is no built-in polarization, which the for $V \to 0$ nonvanishing $P_{c\bar{f}}$ of the (unstable) homogeneous Hartree-Fock solution might suggest.
Nevertheless, the principal idea of Ref. 13 remains valid, namely that the Falicov-Kimball interaction may be of importance in particular for a description of the optical properties of correlated electron systems. When there is a (small) finite hybridization (or field providing for c-f-transitions) the effective hybridization $\tilde{V}$ (cf. Eq. 14) is strongly enhanced due to the Falicov correlation. Furthermore, if the one-particle hybridization has a dispersion (e.g. the for parity reasons more realistic p-wave symmetry), the Falicov-Kimball interaction provides for an effective hybridization, which has also an on-site (s-wave) component, and this may be of importance for an understanding of the gap formation in heavy-fermion (Kondo-) insulators. Finally, it is certainly not excluded that models with more realistic (spin and orbital) degeneracy still have the built-in polarization, which has been interpreted as electronic ferroelectricity.

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