Hartree-Fock study of electronic ferroelectricity in the Falicov-Kimball model with $f$-$f$ hopping

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Abstract

The Hartree-Fock (HF) approximation with the charge-density-wave (CDW) instability is used to study the ground-state phase diagram of the spinless Falicov-Kimball model (FKM) extended by $f$-$f$ hopping in two and three dimensions. It is shown that the HF solutions with the CDW instability reproduce perfectly the two-dimensional intermediate coupling phase diagram of the FKM model with $f$-$f$ hopping calculated recently by constrained path Monte Carlo (CPMC) method. Using this fact we have extended our HF study on cases that have been not described by CPMC, and namely, (i) the case of small values of $f$-electron hopping integrals, (ii) the case of weak Coulomb interactions and (iii) the three-dimensional case. We have found that ferroelectricity remains robust with respect to the reducing strength of coupling ($f$-electron hopping) as well as with respect to the increasing dimension of the system.

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The Falicov-Kimball model (FKM) is a paradigmatic example of simple model to study correlation effects in interacting fermion systems on a lattice [1]. The model was originally proposed to describe metal-insulator transitions and has since been investigated in connection with a variety of problems such as binary alloys [2], the formation of ionic crystals [3], and ordering in mixed-valence systems [4]. In the last few years the FKM was extensively studied in connection with the exciting idea of electronic ferroelectricity [5, 6, 7, 8, 9, 10]. The motivation for these studies comes from the pioneering work of Portengen at al. [11, 12] who studied the FKM with a k-dependent hybridization in the Hartree-Fock (HF) approximation and found that the Coulomb interaction $U$ between the itinerant $d$-electrons and the localized $f$-electrons gives rise a non-vanishing excitonic $\langle f^+d \rangle$-expectation value even in the limit of vanishing hybridization $V \to 0$. As an applied (optical) electrical field provides for excitations between d- and f-states and thus for a polarization expectation value $P_{fd} = \langle f^+d \rangle$, the finding of a spontaneous $P_{fd}$ (without hybridization or electric field) has been interpreted as evidence for electronic ferroelectricity. This result stimulated further theoretical studies of the model. Analytical calculations within well controlled approximation (for $U$ small) performed by Czycholl [5] in infinite dimensions did not confirm the existence of electronic ferroelectricity. In contrast to results obtained by Portengen et al. [11, 12] he found that the FKM in the symmetric case ($n_f = n_d = 0.5$) does not allow for a ferroelectric ground state with a spontaneous polarization, i.e., there is no nonvanishing $\langle f^+d \rangle$-expectation value in the limit of vanishing hybridization. The same conclusion has been also obtained independently by extrapolation of small-cluster exact-diagonalization and density matrix renormalization group (DMRG) calculations in the one dimension for both intermediate and strong interactions [6]. In these regions the finite-size effects are negligible and thus the results can be satisfactory extrapolated to the thermodynamic limit.

Hybridization between the itinerant $d$ and localized $f$ states, however, is not the
only way to develop $d$-$f$ coherence. Recent theoretical works of Batista et al. [8, 9] showed that the ground state with a spontaneous electric polarization can also be induced by $f$-$f$ hopping for dimensions $D > 1$. In the strong coupling limit this result has been proven by mapping the extended FKM into the $xxz$ spin 1/2 model with a magnetic field along the $z$-direction, while in the intermediate coupling regime the ferroelectric state has been identified numerically by constrained path Monte Carlo (CPMC) technique. On the base of these results the authors postulated the following conditions that favor the formation of the electronically driven ferroelectric state: (a) The system must be in a mixed-valence regime and the two bands involved must have different parity. (b) It is best, though not necessary, if both bands have similar bandwidths. (c) A local Coulomb repulsion ($U$) between the different orbitals is required.

In the present paper we study the extended FKM (the spinless FKM with $f$-$f$ hopping) in the HF approximation with the charge-density-wave (CDW) instability. For reasons mentioned above we restrict our studies on dimensions $D > 1$. First we show that the HF solutions with the CDW instability reproduce perfectly the ground-state phase diagram obtained by the CPMC method ($D = 2$) for intermediate Coulomb interactions [9]. This “calibration” allows us to extend calculations to the case of small values of the $f$-electron hopping integral $|t_f| < 0.1$, that has been omitted in the CPMC phase diagram for numerical problems. Just in this region we have found a new phase that corresponds to the inhomogeneous solution for $\langle f^+d \rangle$-expectation value. This result completes the ground-state phase diagram of the two-dimensional FKM extended by $f$-$f$ hopping for intermediate couplings. The same calculations we have performed also in the weak coupling limit (for $D = 2$) as well as in three dimensions. We have found that the ferroelectricity remains robust with respect to the reducing strength of the coupling as well as with respect to the increasing dimension of the system.
1 The model

The extended FKM for the spinless fermions on a $D$-dimensional hypercubic lattice is

$$H = -t_d \sum_{\langle ij \rangle} d_i^+ d_j - t_f \sum_{\langle ij \rangle} f_i^+ f_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i,$$

where $f_i^+ (f_i)$ and $d_i^+ (d_i)$ is the creation (annihilation) operator of heavy ($f$) and light ($d$) electron at lattice site $i$.

The first two terms of (1) are the kinetic energies corresponding to quantum-mechanical hopping of $d$ and $f$ electrons between the nearest neighbor sites $i$ and $j$ with hopping probabilities $t_d$ and $t_f$, respectively. The third term represents the on-site Coulomb interaction between the $d$ electrons with density $n_d = \frac{1}{L} \sum_i d_i^+ d_i$ and the $f$ electrons with density $n_f = \frac{1}{L} \sum_i f_i^+ f_i$, where $L$ is the number of lattice sites. Usually, the hopping integral of the $d$ electrons is taken to be the unit of energy ($t_d = 1$) and the $f$-electron hopping integral is considered in the limit $|t_f| < 1$. This is a reason why the $d$ electrons are called light and the $f$ electrons heavy.

In our HF study of the extended FKM we go beyond the usual HF approach [13] in which only homogeneous solutions are postulated. In accordance with [14] we consider here also inhomogeneous solutions modeled by a periodic modulation of the order parameters:

$$\langle n_i^f \rangle = n^f + \delta_f \cos(Q \cdot r_i),$$

$$\langle n_i^d \rangle = n^d + \delta_d \cos(Q \cdot r_i),$$

$$\langle f_i^+ d_i \rangle = \Delta + \Delta_P \cos(Q \cdot r_i).$$

where $\delta_d$ and $\delta_f$ is the order parameter of the CDW state for the $d$- and $f$-electrons and $\Delta$ is the exciton average. The nesting vector $Q = (\pi, \pi)$ for $D = 2$ and $Q = (\pi, \pi, \pi)$ for $D = 3$.

Using expressions for $\langle n_i^f \rangle, \langle n_i^d \rangle$ and $\langle f_i^+ d_i \rangle$ the HF Hamiltonian of the extended
FKM can be written as

\[ \mathcal{H} = \sum_{\langle i,j \rangle} d^+_i d_j - t_f \sum_{\langle i,j \rangle} f^+_i f_j + E_f \sum_i n^f_i + U \sum_i \left( \delta_f \cos(\mathbf{Q} \cdot \mathbf{r}_i) \right) n^d_i \]

\[ + U \sum_i \left( \delta_d \cos(\mathbf{Q} \cdot \mathbf{r}_i) \right) n^f_i - U \sum_i \left( \Delta + \Delta_P \cos(\mathbf{Q} \cdot \mathbf{r}_i) \right) d^+_i f_i + h.c. \quad (5) \]

Following the work of Brydon et al. [14] the effective HF Hamiltonian is diagonalized by canonical transformation

\[ \gamma^m_k = u^m_k d_k + v^m_k d_{k+\mathbf{Q}} + a^m_k f_k + b^m_k f_{k+\mathbf{Q}} , \quad m = 1, 2, 3, 4 \quad (6) \]

where \( a^m_k, b^m_k, u^m_k, v^m_k \) are solutions of the associated Bogoliubov-de Gennes (BdG) eigenequations:

\[ H_k \Psi^m_k = E^m_k \Psi^m_k , \quad (7) \]

with

\[ H_k = \begin{pmatrix} \epsilon^d_k + Un^f & U\delta_f & -U \Delta & -U \Delta_P \\ U\delta_f & \epsilon^d_{k+\mathbf{Q}} + Un^f & -U \Delta_P & -U \Delta \\ -U \Delta & -U \Delta_P & \epsilon^f_k + Un^d + E_f & U \delta_d \\ -U \Delta_P & -U \Delta & U \delta_d & \epsilon^f_{k+\mathbf{Q}} + Un^d + E_f \end{pmatrix} \quad (8) \]

and

\[ \Psi^m_k = \begin{pmatrix} u^m_k \\ v^m_k \\ a^m_k \\ b^m_k \end{pmatrix} \quad (9) \]

The corresponding energy dispersions \( \epsilon^d_k \) and \( \epsilon^f_k \) can be obtained directly by the Fourier transform of the \( d- \) and \( f- \) electron hopping amplitudes and for the case of hypercubic lattice they are given by \( (\alpha = d, f) \):

\[ \epsilon^\alpha_k = -2t_{\alpha} (\cos(k_x) + \cos(k_y)), \quad \text{for } D=2, \quad (10) \]

\[ \epsilon^\alpha_k = -2t_{\alpha} (\cos(k_x) + \cos(k_y) + \cos(k_z)), \quad \text{for } D=3. \quad (11) \]
The HF parameters $n_d, \delta_d, n_f, \delta_f, \Delta, \Delta_P$ can be written directly in terms of the Bogoliubov-de Gennes eigenvectors:

$$n_d = \frac{1}{N} \sum_k' \sum_m \{u_m^ku_m^k + v_m^kv_m^k\} f(E_k^m).$$  \hspace{1cm} (12)

$$\delta_d = \frac{1}{N} \sum_k' \sum_m \{v_m^ku_m^k + u_m^kv_m^k\} f(E_k^m).$$  \hspace{1cm} (13)

$$n_f = \frac{1}{N} \sum_k' \sum_m \{a_m^ma_m^k + b_m^mb_m^k\} f(E_k^m).$$  \hspace{1cm} (14)

$$\delta_f = \frac{1}{N} \sum_k' \sum_m \{b_m^ka_m^k + a_m^mb_m^k\} f(E_k^m).$$  \hspace{1cm} (15)

$$\Delta = \frac{1}{N} \sum_k' \sum_m \{a_m^ku_m^k + b_m^kv_m^k\} f(E_k^m).$$  \hspace{1cm} (16)

$$\Delta_P = \frac{1}{N} \sum_k' \sum_m \{b_m^ku_m^k + a_m^kv_m^k\} f(E_k^m).$$  \hspace{1cm} (17)

where the prime denotes summation over half the Brillouin zone and $f(E) = 1/[1 + \exp[\beta(E - \mu)]]$ is the Fermi distribution function.

The same approach has been used recently by Brydon et al. [14] to study the interplay between excitonic effects and the CDW instability in the FKM with on-site as well as non-local hybridization. Here we use the zero temperature variant of this procedure to describe ground-state phase diagram of the spinless FKM with $f-f$ hopping.

2 Results and Discussion

To determine the ground-state phase diagram of the extended FKM in the $E_f-t_f$ plane (corresponding to selected $U$) the HF equations are solved self-consistently for each pair of $(E_f, t_f)$ values. We use an exact diagonalization method to solve the Bogoliubov-de Gennes equation. We start with an initial set of order parameters. By solving Eq. (7), the new order parameters are computed via Eqs. (12) to (17) and are substituted back into Eq. (7). The iteration is repeated until a desired accuracy is achieved.
First we have examined the two-dimensional extended FKM model in the intermediate coupling regime and $t_f$ negative. For this case there exists the comprehensive phase diagram of the model obtained by a CPMC technique [9] for $f$-electron hopping integrals $|t_f| \geq 0.1$. According these Monte-Carlo studies the phase diagram of the extended FKM consists of only three main phases, and namely, (i) the integral-valent state ($n_f = 0, 1, n_d = 1, 0$), (ii) the mixed-valent CDW state ($n_f = n_d = 0.5$), and (iii) the mixed-valent ferroelectric state that is stable for remaining values of $n_f (n_d)$.

In Fig. 1 we have displayed typical examples of our HF solutions obtained for $n_d, \delta_d, n_f, \delta_f, \Delta, \Delta_F$ in the intermediate coupling regime $U = 2$. It is seen that the extended FKM in the HF approximation with the CDW instability exhibits non-vanishing excitonic $\langle f^+d \rangle$-expectation value for all $f$-electron densities except the case when $n_f = 0, 1/2$ and 1. Thus in accordance with the Quantum Monte-Carlo studies [9] we have found that the ferroelectric ground state with the spontaneous polarization is stabilized when the system is in the mixed valence regime and the sign of the $f$-electron hopping integral is opposite to the sign of the $d$-electron one. The fact that HF solutions can describe the existence of ferroelectric ground-state with spontaneous polarization is not surprising, since this state has been found already in the homogeneous HF solution of the conventional FKM ($t_f = 0$) in the limit of vanishing hybridization $V \rightarrow 0$ [11, 12], even for all $f$-electron concentrations (for all values of $E_f$ from the $d$-electron band). What is however surprising is that the HF solutions with the CDW instability reproduce perfectly the ground-state phase diagram obtained by CPMC method for all examined values of $f$-electron hopping ($|t_f| \geq 0.1$). This is clearly demonstrated in Fig. 2, where both phase diagrams are compared.

The fact that the HF approximation with the CDW instability can describe qualitatively as well as quantitatively ground-state properties of the FKM with $f$-electron
hopping motivated us to extend our HF study on cases that have been not described by Quantum Monte-Carlo simulations. At first this is the case of small $f$-electron hopping integrals ($|t_f| < 0.1$) that has been not considered in the original work of Batista et al. [9] because numerical difficulties which appear in the Quantum Monte-Carlo simulations for small $t_f$ (the limitations in the numerical accuracy).

The second interesting case that we would like to study here within the HF theory is the three-dimensional case for which the numerical results are very rare due to numerical limitations on the size of clusters.

Let us first discuss our two-dimensional results obtained in the limit of small values of $f$-electron hopping integrals. In Fig. 3 we present results of detailed HF analysis performed in this limit for $\Delta, \Delta_P$ and $\delta_d$. It is seen that the non-vanishing excitonic $\langle f^+d \rangle$ expectation value persists also for small values of $|t_f|$ but now the inhomogeneous solution $\Delta_P \neq 0$ (with AB-sublattice oscillations in the excitonic and charge order parameters) is stabilized against the homogeneous one ($\Delta_P = 0$).

The effect is especially strong when we approach the $t_f = 0$ limit. This is clearly demonstrated in Fig. 4, where the complete intermediate-coupling phase diagram of the FKM with $f$-$f$-hopping is displayed. Five different phases depicted in Fig. 4 as $\alpha$ (the full $f$ band), $\beta, \beta'$ (the excitonic phases), $\gamma$ (the CDW phase) and $\epsilon$ (the full $d$ band) correspond to following HF solutions:

\[
\begin{align*}
\alpha & \text{ phase: } \Delta = 0, \quad \Delta_P = 0, \quad \delta_f = 0, \quad \delta_d = 0, \quad n_f = 1 \\
\beta & \text{ phase: } \Delta > 0, \quad \Delta_P = 0, \quad \delta_f = 0, \quad \delta_d = 0, \quad 0 < n_f < n_f^c, \quad 1 - n_f^c < n_f < 1 \\
\beta' & \text{ phase: } \Delta > 0, \quad \Delta_P < 0, \quad \delta_f < 0, \quad \delta_d > 0, \quad n_f^c < n_f < 1/2, \quad 1/2 < n_f < 1 - n_f^c \\
\gamma & \text{ phase: } \Delta = 0, \quad \Delta_P = 0, \quad \delta_f < 0, \quad \delta_d > 0, \quad n_f = 1/2 \\
\epsilon & \text{ phase: } \Delta = 0, \quad \Delta_P = 0, \quad \delta_f = 0, \quad \delta_d = 0, \quad n_f = 0
\end{align*}
\]

The stability of different HF solutions was also checked numerically by calculating the total energy and it was found that all phases presented in the ground-state phase diagram represent the most stable HF solutions. To determine the type of transitions
between different phases we have performed an exhaustive numerical study of the \( E_f \) dependence of the HF order parameters (the typical examples are shown in Fig. 1 and Fig. 3). At a first glance it seems that there are both first-order \((t_f \text{ large})\) and second-order \((t_f \text{ small})\) phase transitions in the extended FKM with \( f-f \) hopping. However, a more detailed analysis of numerical data (with much higher resolution than used in Fig. 1 and Fig. 3) showed that the \( \beta' \) phase persists also for large \( t_f \), although its stability region is now considerably reduced (see insets in Fig. 1). Thus there is no difference between the case of small and large values of \( t_f \). In both cases the HF order parameters change continuously indicating that the phase transitions between different phases presented in the \((E_f-t_f)\) ground-state phase diagram are of the second order.

The same calculations we have performed also in the weak coupling limit \((U \leq 1)\). We have found that the phase diagrams obtained in the weak and intermediate coupling regime have qualitatively the same form and only one difference between them is that the ferroelectric domain \((\beta)\) is stabilized against remaining phases with decreasing Coulomb interaction (see Fig. 4). Of course, this fact does not imply automatically that the excitonic \( \langle f^+d \rangle \) expectation value persists also for vanishing \( U \) and that the Coulomb interaction \( U \) is not necessary for a stabilization of the ferroelectric state, what should be in a contradiction with conclusions based on the CPMC simulations. Indeed, calculations that we have performed for different values of \( t_f \) at the selected \( f \)-electron density \( n_f = 1/4 \) showed (see Fig. 5) that the excitonic \( \langle f^+d \rangle \) expectation value is zero for \( U = 0 \), rapidly increases with increasing \( U \) and tends to the saturated state for \( U \) sufficiently large. This confirms independently the third postulate of Batista et al. [9] and namely, that the local Coulomb interaction between the different orbitals is required in order to stabilize the ferroelectric state with the spontaneous polarization.

Before discussing the case of positive \( t_f \) let us show explicitly the HF solution
for the limit of the conventional FKM ($t_f = 0$). For this case we have found that
$\Delta = \Delta_P = 0$ in the $\alpha, \gamma$ and $\varepsilon$ phase, while $\Delta = -\Delta_P$ in the $\beta'$ phase. The last solution implies that the excitonic $\langle f_i^+d_i \rangle$-expectation value is equal to $2\Delta$ on the $A$ sublattice of the hypercubic lattice, while $\langle f_i^+d_i \rangle = 0$ on the $B$ sublattice. For the symmetric case $E_f = 0$ our solutions are fully consistent with the Czycholl’s ones obtained in the limit of infinite dimensions [5]. On the other hand both these inhomogeneous solutions fully differ from the homogeneous one [11, 12] that predicts a non-zero excitonic $\langle f_i^+d_i \rangle$-expectation value for all $E_f$ from the mixed valence regime with maximum of $\langle f_i^+d_i \rangle$ at $E_f = 0$.

Similar calculations as for $t_f < 0$ we have performed also for $t_f > 0$. We have found that the ground-state phase diagram for $t_f > 0$ has exactly the same form as for $t_f < 0$, however five different phases $\alpha, \beta, \beta', \gamma$ and $\varepsilon$ are now characterized by:

- **$\alpha$ phase:** $\Delta = 0$, $\Delta_P = 0$, $\delta_f = 0$, $\delta_d = 0$, $n_f = 1$
- **$\beta$ phase:** $\Delta = 0$, $\Delta_P < 0$, $\delta_f = 0$, $\delta_d = 0$, $0 < n_f < n_f^c$ for $E_f > 0$ and $1 - n_f^c < n_f < 1$ for $E_f < 0$
- **$\beta'$ phase:** $\Delta > 0$, $\Delta_P < 0$, $\delta_f < 0$, $\delta_d > 0$, $n_f^c < n_f < 1/2$ for $E_f > 0$ and $1/2 < n_f < 1 - n_f^c$ for $E_f < 0$
- **$\gamma$ phase:** $\Delta = 0$, $\Delta_P = 0$, $\delta_f < 0$, $\delta_d > 0$, $n_f = 1/2$
- **$\varepsilon$ phase:** $\Delta = 0$, $\Delta_P = 0$, $\delta_f = 0$, $\delta_d = 0$, $n_f = 0$

Thus the main difference between the phase diagrams obtained for negative and positive $t_f$ is that the ferroelectric domain $\beta$ at $t_f < 0$ is replaced by the antiferroelectric one at $t_f > 0$. These two large domains are separated by a relatively narrow $\beta'$ domain within which the sublattice excitonic averages ($P_{fd}^A, P_{fd}^B$) change continuously (see Fig. 6) from the ferroelectric case ($P_{fd}^A = P_{fd}^B$) to the antiferroelectric case ($P_{fd}^A = -P_{fd}^B$).

Qualitatively the same picture we have observed also for the three-dimensional case. This is illustrated in Fig. 7, where the ground-state phase diagrams of the extended FKM are plotted for two different values of Coulomb interaction ($U = 2$ and $U = 4$). These results indicate that ferroelectricity remains robust with respect to
the increasing dimension of the system, what should be important for an application of HF solutions on a description of real three dimensional systems.

In conclusion, we have calculated the ground-state phase diagram of the spinless FKM with $f$-$f$ hopping in the HF approximation with the CDW instability. We have found that the HF solutions with the CDW instability reproduce perfectly the two-dimensional intermediate coupling phase diagram of the extended FKM calculated by CPMC method. Using this fact we have extended our HF study on cases that have been not described by CPMC and namely, the case of small values of $f$-electron hopping integrals, the case of weak Coulomb interactions and the three-dimensional case. We have found that the ferroelectric ground state with the spontaneous polarization remains stable in all examined cases.

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*Note added.*- After submitting this work we came to know about the work of Schneider and Czycholl [15] who studied the extended FKM in the limit of infinite dimensions and obtained results similar to ours.
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Figure Caption

Fig. 1. Dependence of the HF parameters $n_f, \delta_f, n_d, \delta_d, \Delta$ and $\Delta_P$ on the $f$-level energy $E_f$ calculated (with step $\Delta E_f = 0.005$) for three different values of $t_f$ ($t_f = -0.2, -0.5, -0.8$) and $U = 2$. Insets show the $t_f = -0.5$ case at much higher resolution (the numerical data have been obtained with step $\Delta E_f = 0.00005$). The case of $t_f = -0.8$ is analogous to $t_f = -0.5$.

Fig. 2. The HF (●) and CPMC [9] (□) phase diagram of the two dimensional FKM with $f$-$f$ hopping obtained for $U = 2$.

Fig. 3. Dependence of the HF parameters $\Delta, \Delta_P$ and $\delta_d$ on the $f$-level energy $E_f$ calculated for different values of $t_f$ ($t_f = 0, -0.01, -0.02, -0.05$) and $U = 2$.

Fig. 4. The complete HF phase diagram of the two-dimensional extended FKM in the intermediate ($U = 2$) and weak coupling ($U = 1$) regime.

Fig. 5. Dependence of the HF parameter $\Delta$ on the Coulomb interaction $U$ calculated for different values of $t_f$ and $n_f = 1/4$.

Fig. 6. Dependence of the excitonic expectation value $P_{fd} = \langle f^+_i d_i \rangle$ on $t_f$ calculated for $E_f = 0.7$ and $U = 2$.

Fig. 7. The complete HF phase diagram of the three-dimensional extended FKM calculated for $U = 2$ and $U = 4$. 
$U=2, D=2, n_f+n_d=1$

Excitonic phase $\langle f_i^+d_i \rangle > 0$

Excitonic phase $\langle f_i^+d_i \rangle > 0$

Full f band

Full d band

CDW

- CPMC
- HF
$D=2$, $n_f=1/4$

$\Delta$ vs $U$ for different values of $t_f$:
- $t_f=-0.1$
- $t_f=-0.3$
- $t_f=-0.5$
- $t_f=-0.7$
$P_{td} = \langle t_d^* d_1 \rangle$

$U=2, D=2, E_t=0.7$

- $\beta$ phase
- $\beta'$ phase
- A sublattice
- B sublattice
