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

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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 perfectly reproduce the two-dimensional intermediate-coupling phase diagram of the FKM model with *f-f* hopping, which was recently calculated using the constrained path Monte Carlo (CPMC) method. Using this fact, we have extended our HF study on cases that have been not described by CPMC, 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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I. INTRODUCTION

The Falicov-Kimball model (FKM) is a paradigmatic example of a simple model to study correlation effects of 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 past few years, the FKM was extensively studied in connection with the exciting idea of electronic ferroelectricity.[5–10] The motivation for these studies comes from the pioneering work of Portengen *et 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 to a nonvanishing excitonic $\langle f^{+}d\rangle$-expectation value even in the limit of a vanishing hybridization $V\rightarrow 0$. As an applied (optical) electrical field provides for excitations between d and f states and, thus, for a polarization expectation value $P_{fd}=\langle f_i^{+}d_i\rangle$, the finding of a spontaneous P_{fd} (without hybridization or electric field) has been interpreted as evidence of 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 a vanishing hybridization. The same conclusion has also been obtained independently by an extrapolation of small-cluster exact-diagonalization and density matrix renormalization group 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 satisfactorily 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 numerically identified by a constrained path Monte Carlo (CPMC) technique. On the basis 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 parities. (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 perfectly reproduce 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 $|t_f|<0.1$, which has been omitted in the CPMC phase diagram for numerical problems. Just in this region we have found a phase that corresponds to the inhomogeneous solution for the $\langle f^{+}d\rangle$-expectation value. This result completes the ground-state phase diagram of the two-dimensional FKM extended by *f-f* hopping for intermediate couplings. We have also performed the same calculations 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.

II. MODEL

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

$$H = -t_d \sum_{\langle ij \rangle} d_i^+ d_j - t_f \sum_{\langle ij \rangle} f_i^+ f_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i, \tag{1}$$

where f_i^+ (f_i) and d_i^+ (d_i) are the creation (annihilation) operators of heavy (f) and light (d) electrons at lattice site i.

The first two terms of Eq. (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 $n_d = \frac{1}{L}\Sigma_i d_i^+ d_i$ and the f electrons with density $n_f = \frac{1}{L}\Sigma_i f_i^+ f_i$, 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 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 Ref. 14, here, we also consider inhomogeneous solutions modeled by a periodic modulation of the order parameters:

$$\langle n_i^f \rangle = n^f + \delta_f \cos(\mathbf{Q} \cdot \mathbf{r}_i), \tag{2}$$

$$\langle n_i^d \rangle = n^d + \delta_d \cos(\mathbf{Q} \cdot \mathbf{r}_i), \tag{3}$$

$$\langle f_i^+ d_i \rangle = \Delta + \Delta_P \cos(\mathbf{Q} \cdot \mathbf{r}_i), \tag{4}$$

where δ_d and δ_f are the order parameters of the CDW state for the d and f electrons and Δ is the excitonic average. The nesting vectors are $\mathbf{Q} = (\pi, \pi)$ for $D = 2$ and $\mathbf{Q} = (\pi, \pi, \pi)$ for $D = 3$.

Using the 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

$$\begin{aligned} \mathcal{H} = & -t_d \sum_{\langle i,j \rangle} d_i^+ d_j - t_f \sum_{\langle i,j \rangle} f_i^+ f_j + E_f \sum_i n_i^f + U \sum_i [n^f \\ & + \delta_f \cos(\mathbf{Q} \cdot \mathbf{r}_i)] n_i^d + U \sum_i [n^d + \delta_d \cos(\mathbf{Q} \cdot \mathbf{r}_i)] n_i^f \\ & - U \sum_i [\Delta + \Delta_P \cos(\mathbf{Q} \cdot \mathbf{r}_i)] d_i^+ f_i + \text{H.c.} \end{aligned} \tag{5}$$

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

$$\gamma_k^m = u_k^m d_k + v_k^m d_{k+\mathbf{Q}} + a_k^m f_k + b_k^m f_{k+\mathbf{Q}}, \quad m = 1,2,3,4, \tag{6}$$

where $a_k^m, b_k^m, u_k^m, v_k^m$ are solutions of the associated Bogoliubov–de Gennes eigenequations,

$$H_k \Psi_k^m = E_k^m \Psi_k^m, \tag{7}$$

with

$$H_k = \begin{pmatrix} \epsilon_k^d + Un^f & U\delta_f & -U\Delta & -U\Delta_P \\ U\delta_f & \epsilon_{k+Q}^d + Un^f & -U\Delta_P & -U\Delta \\ -U\Delta & -U\Delta_P & \epsilon_k^f + Un^d + E_f & U\delta_d \\ -U\Delta_P & -U\Delta & U\delta_d & \epsilon_{k+Q}^f + Un^d + E_f \end{pmatrix} \tag{8}$$

and

$$\Psi_k^m = \begin{pmatrix} u_k^m \\ v_k^m \\ a_k^m \\ b_k^m \end{pmatrix}. \tag{9}$$

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

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

$$\epsilon_k^\alpha = -2t_\alpha[\cos(k_x) + \cos(k_y) + \cos(k_z)] \quad \text{for} \quad D = 3. \tag{11}$$

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,

$$n^d = \frac{1}{N} \sum_k{}' \sum_m \{u_k^m u_k^m + v_k^m v_k^m\} f(E_k^m), \tag{12}$$

$$\delta_d = \frac{1}{N} \sum_k{}' \sum_m \{v_k^m u_k^m + u_k^m v_k^m\} f(E_k^m), \tag{13}$$

$$n^f = \frac{1}{N} \sum_k{}' \sum_m \{a_k^m a_k^m + b_k^m b_k^m\} f(E_k^m), \tag{14}$$

$$\delta_f = \frac{1}{N} \sum_k{}' \sum_m \{b_k^m a_k^m + a_k^m b_k^m\} f(E_k^m), \tag{15}$$

$$\Delta = \frac{1}{N} \sum_k{}' \sum_m \{a_k^m u_k^m + b_k^m v_k^m\} f(E_k^m), \tag{16}$$

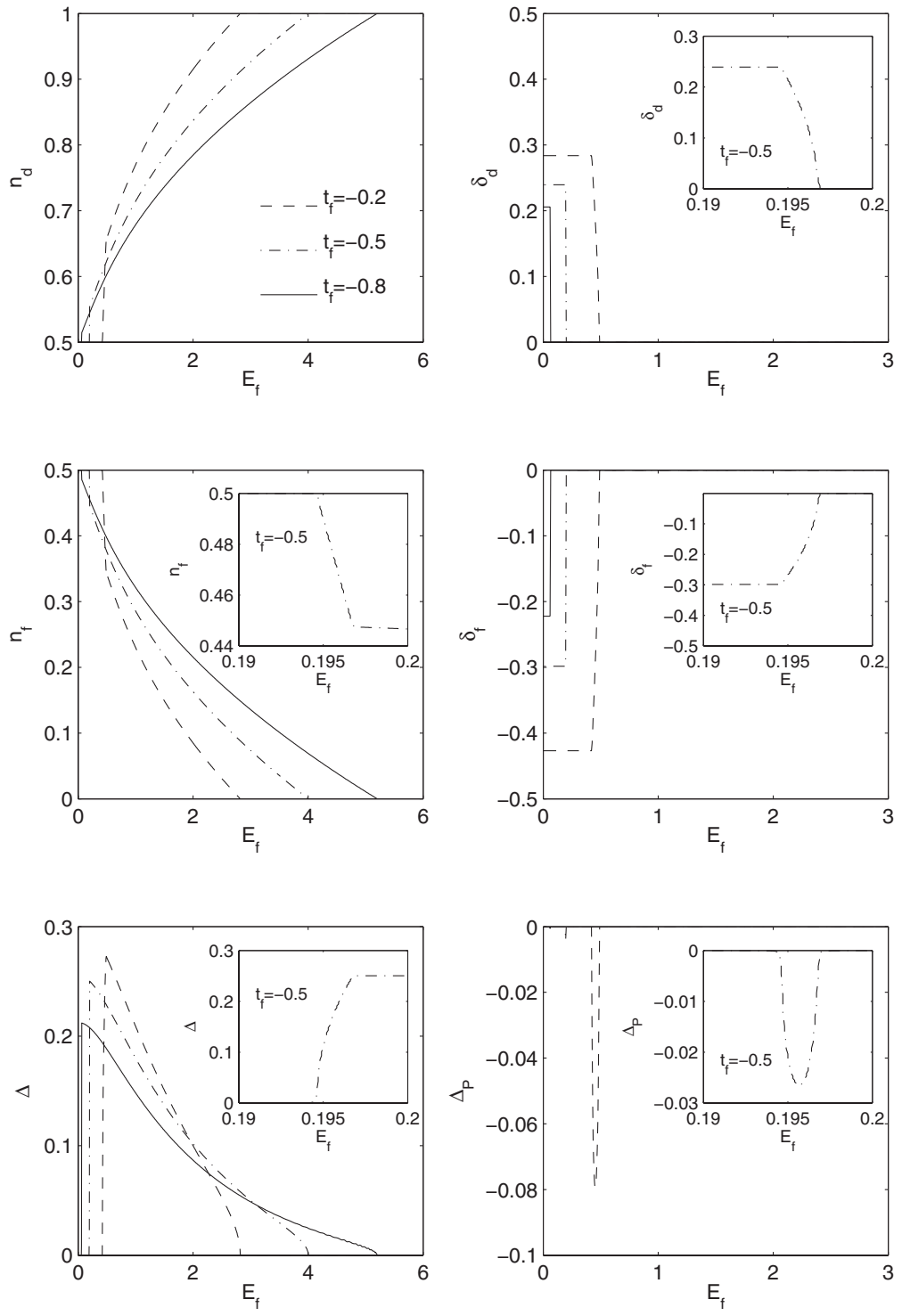

FIG. 1. Dependence of the HF parameters n_f, δ_f, n_d, δ_d, Δ, and Δ_P on the f-level energy E_f calculated (with step $\Delta E_f=0.005$) for three different values of t_f ($t_f=-0.2,-0.5,-0.8$) and $U=2$. Insets show the $t_f=-0.5$ case at much higher resolution (the numerical data have been obtained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

$$\Delta_P = \frac{1}{N}\sum_k{}' \sum_m \{b_k^m u_k^m + a_k^m v_k^m\} f(E_k^m), \tag{17}$$

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 was recently used 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 nonlocal 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.

III. RESULTS AND DISCUSSION

To determine the ground-state phase diagram of the extended FKM in the E_f-t_f plane (which corresponds 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)–(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 to these Monte Carlo studies, the phase diagram of the extended FKM consists of only three main phases, namely, (i) the integer-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, which is stable for the remaining values of n_f (n_d).

In Fig. 1, we have displayed typical examples of our HF solutions obtained for $n_d, \delta_d, n_f, \delta_f, \Delta, \Delta_P$ in the intermediate-coupling regime $U=2$. It is seen that the extended FKM in the HF approximation with the CDW instability exhibits nonvanishing excitonic $\langle f^+ d\rangle$-expectation value for all f-electron densities except for 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 the sign of the d-electron one. The fact that HF solutions can describe the existence of a ferroelectric ground state with spontaneous polarization is not surprising, since this state has already been found in the homogeneous HF solution of the conventional FKM ($t_f=0$) in the limit of vanishing hybridization $V \to 0$,[11,12] even for all f-electron concentrations (for all values of E_f from the d-electron band). However, what is surprising is that the HF solutions with the CDW instability perfectly reproduce the ground-state phase diagram obtained by the 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, there is the case of small f-electron hopping integrals ($|t_f| < 0.1$), which were not considered in the original work of Batista *et al.*[9] because of 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 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

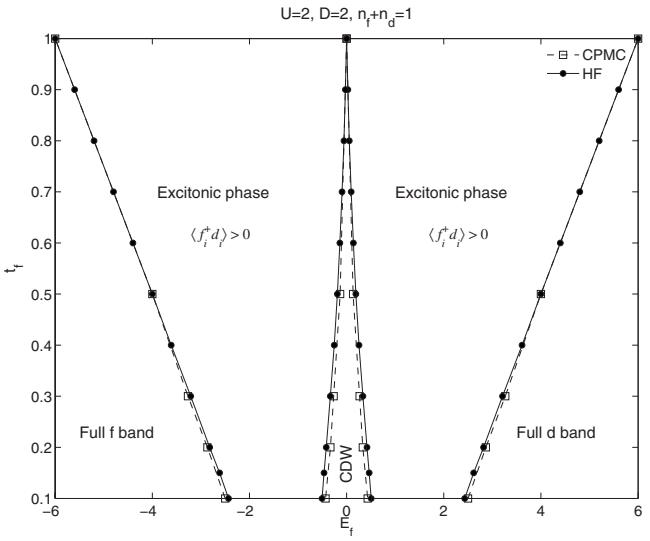

FIG. 2. The HF (●) and CPMC (Ref. 9) (□) phase diagram of the two-dimensional FKM with f-f hopping obtained for $U=2$.

Fig. 3, we present results of a detailed HF analysis performed in this limit for Δ, Δ_P, and δ_d. It is seen that the nonvanishing excitonic $\langle f^+ d\rangle$-expectation value also persists 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 α (the full f band), β, β' (the excitonic phases), γ (the CDW phase), and ϵ (the full d band) correspond to following HF solutions:

$$\alpha \text{ phase}, \quad \Delta = 0, \quad \Delta_P = 0, \quad \delta_f = 0, \quad \delta_d = 0, \quad n_f = 1,$$

$$\beta \text{ phase}, \quad \Delta > 0, \quad \Delta_P < 0, \quad \delta_f = 0, \quad \delta_d = 0, \quad 0 < n_f < n_f^c \quad \text{for} \quad E_f > 0,$$

$$1 - n_f^c < n_f < 1 \quad \text{for} \quad E_f < 0,$$

$$\beta' \text{ phase}, \quad \Delta > 0, \quad \Delta_P < 0, \quad \delta_f < 0, \quad \delta_d > 0, \quad n_f^c < n_f < 1/2 \quad \text{for} \quad E_f > 0,$$

$$1/2 < n_f < 1 - n_f^c \quad \text{for} \quad E_f < 0,$$

$$\gamma \text{ phase}, \quad \Delta = 0, \quad \Delta_p = 0, \quad \delta_d > 0, \quad n_f = 1/2,$$

$$\varepsilon \text{ phase}, \quad \Delta_P = 0, \quad \delta_f = 0, \quad \delta_d > 0, \quad n_f = 0. \quad (18)$$

The stability of different HF solutions was also numerically checked 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 Figs. 1

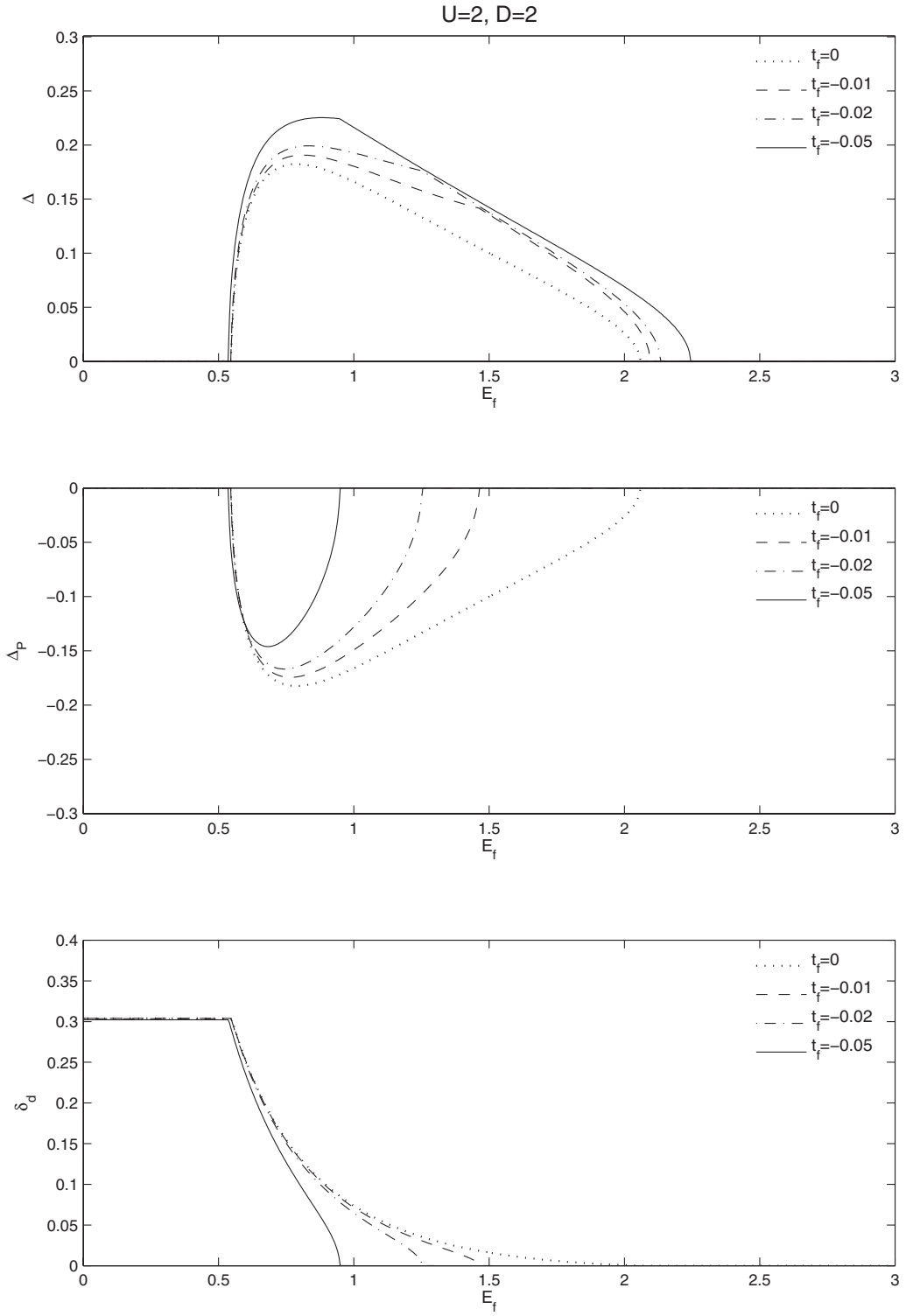

FIG. 3. Dependence of the HF parameters Δ, Δ_P, and δ_d on the f-level energy E_f calculated for different values of t_f (t_f=0,−0.01, −0.02,−0.05) and U=2.

and 3). At first glance, it seems that there are both first-order (t_f large) and second-order (t_f small) phase transitions in the extended FKM with f-f hopping. However, a more detailed analysis of numerical data (with much higher resolution than those used in Figs. 1 and 3) showed that the β' 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.

We have also performed the same calculations in the weak-coupling limit ($U \leq 1$). We have found that the phase

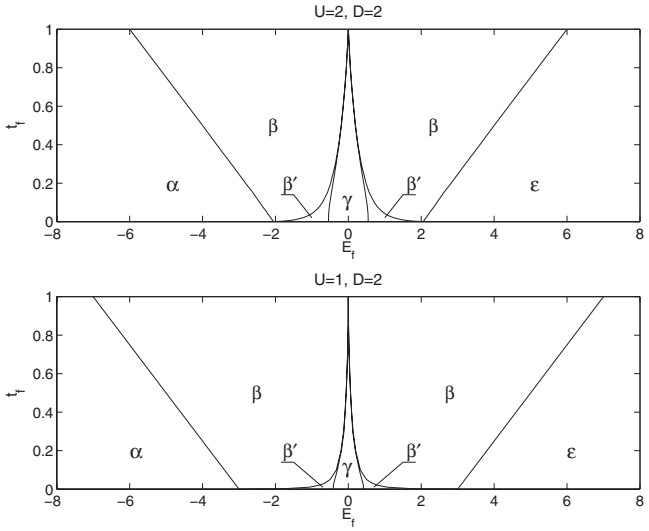

FIG. 4. The complete HF phase diagram of the two-dimensional extended FKM in the intermediate-coupling ($U=2$) and weak-coupling ($U=1$) regimes.

diagrams obtained in the weak- and intermediate-coupling regimes have qualitatively the same form and the only difference between them is that the ferroelectric domain (β) is stabilized against remaining phases with decreasing Coulomb interaction (see Fig. 4). Of course, this fact does not automatically imply that the excitonic $\langle f^{+}d\rangle$ expectation value also persists for vanishing U and that the Coulomb interaction U is not necessary for a stabilization of the ferroelectric state, a fact that should be in 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 $U=0$; it rapidly increases with increasing U and tends to the saturated state for sufficiently large U. This independently confirms the third postulate of Batista *et al.*,[9] namely, that the local

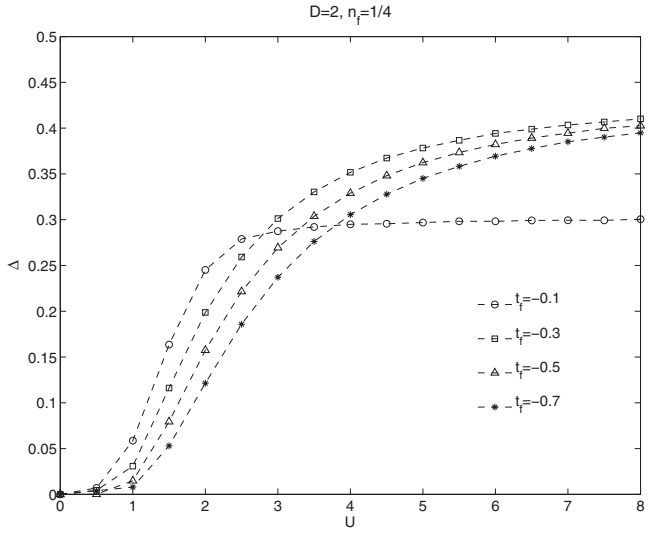

FIG. 5. Dependence of the HF parameter Δ on the Coulomb interaction U calculated for different values of t_f and $n_f=1/4$.

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 explicitly show 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 α, γ, and ε phases, while $\Delta=-\Delta_P$ in the β' phase. The last solution implies that the excitonic $\langle f_i^{+}d_i\rangle$-expectation value is equal to 2Δ on the A sublattice of the hypercubic lattice, while $\langle f_i^{+}d_i\rangle=0$ on the B sublattice. For the symmetric case of $E_f=0$, our solutions are fully consistent with the ones obtained by Czycholl[5] in the limit of infinite dimensions. On the other hand, both these inhomogeneous solutions fully differ from the homogeneous one,[11,12] which predicts a nonzero 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 for $t_f<0$ have also been performed $t_f>0$. We have found that the ground-state phase diagram for $t_f>0$ has exactly the same form as that for $t_f<0$. However, five different phases, α, β, β', γ, and ε, are now characterized by

$$\alpha \text{ phase}, \quad \Delta=0, \quad \Delta_P=0, \quad \delta_f=0, \quad \delta_d=0, \quad n_f=1,$$

$$\beta \text{ phase}, \quad \Delta=0, \quad \Delta_P<0, \quad \delta_f=0, \quad \delta_d=0, \quad 0<n_f<n_f^c \quad \text{for} \quad E_f>0,$$

$$1-n_f^c<n_f<1 \quad \text{for} \quad E_f<0,$$

$$\beta' \text{ phase}, \quad \Delta=0, \quad \Delta_P<0, \quad \delta_f=0, \quad \delta_d=0, \quad n_f^c<n_f<1/2 \quad \text{for} \quad E_f>0,$$

$$1/2<n_f<1-n_f^c \quad \text{for} \quad E_f<0,$$

$$\gamma \text{ phase}, \quad \Delta=0, \quad \Delta_P=0, \quad \delta_f<0, \quad \delta_d=0 \quad n_f=1/2,$$

$$\varepsilon \text{ phase}, \quad \Delta_P=0, \quad \delta_f=0, \quad \delta_d>0, \quad n_f=0. \quad (19)$$

Thus, the main difference between the phase diagrams obtained for negative and positive t_f is that the ferroelectric domain β at $t_f<0$ is replaced by the antiferroelectric one at $t_f>0$. These two large domains are separated by a relatively narrow β' 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 $(P_{fd}^A=-P_{fd}^B)$.

We have also observed qualitatively the same picture 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, which should be important for an application of HF solutions on a description of real three-dimensional systems.

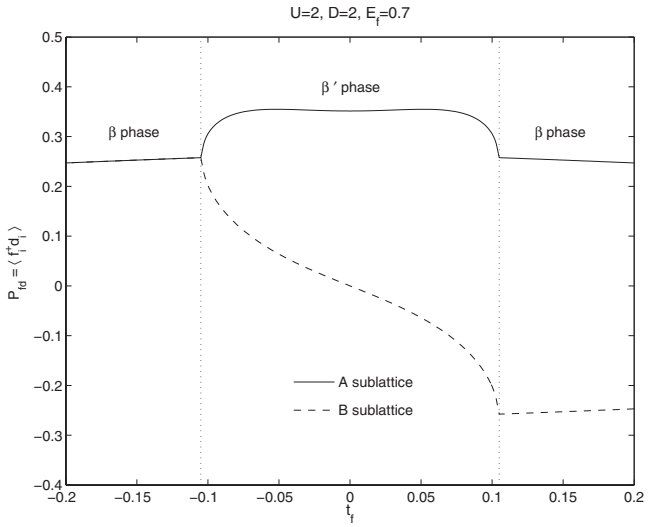

FIG. 6. Dependence of the excitonic expectation value $P_{fd}=\langle f_i^+ d_i\rangle$ on t_f calculated for $E_f=0.7$ and $U=2$.

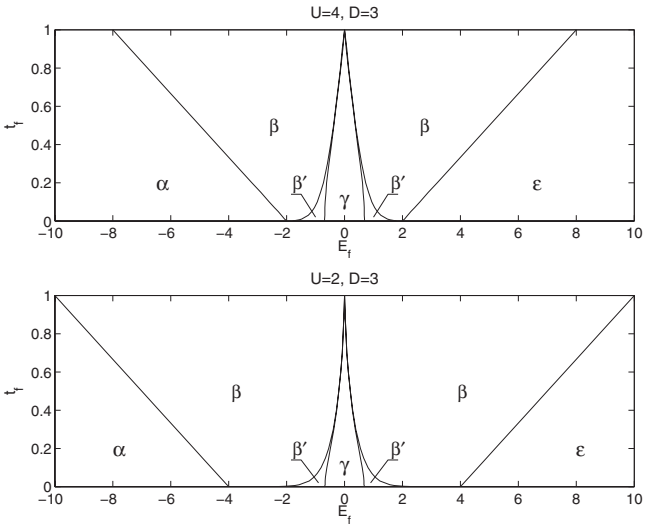

FIG. 7. The complete HF phase diagram of the three-dimensional extended FKM calculated for $U=2$ and $U=4$.

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 perfectly reproduce the two-dimensional intermediate-coupling phase diagram of the extended FKM as calculated by the CPMC method. Using this fact, we have extended our HF study on cases that have been not described by CPMC, 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.

Note added. Recently, 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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