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Competing orderings in an extended Falicov-Kimball model

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We present a Hartree-Fock study of the Falicov-Kimball model extended by both on-site and nonlocal hybridization. We examine the interplay between excitonic effects and the charge-density wave (CDW) instability known to exist at zero hybridization. It is found that the CDW state remains stable in the presence of finite hybridization; for on-site hybridization the Coulomb interaction nevertheless strongly enhances the excitonic average above its value in the noninteracting system. In contrast, for nonlocal hybridization, we observe no such enhancement of the excitonic average or a spontaneous on-site hybridization potential. Instead, we find only a significant suppression of the excitonic correlations in the CDW state. A phenomenological Ginzburg-Landau analysis is also provided to understand the interplay.

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The Falicov-Kimball model (FKM) describes a tight-binding system of itinerant d electrons interacting via on-site Coulomb repulsion U with localized f electrons of energy ϵ_f. The FKM was originally introduced as a minimal model of valence transitions in systems such as SmB_6 and Ce: by varying the interorbital Coulomb repulsion U or the f-level ϵ_f, both discontinuous and continuous changes in the distribution of the electrons across the localized and itinerant states were found.[1] It was soon realized, however, that some overlap between the d and f wave functions was an essential feature of most systems displaying valence instabilities.[2] This "mixing" of the electron wave functions may be explicitly introduced by the inclusion of a hybridization potential V. A variety of methods, including Hartree-Fock,[3] real-space renormalization group,[4] and alloy-analog approximation,[5] revealed that the hybridization removed the previously observed discontinuous valence transitions. Work on the FKM ceased in the mid-1980s as it became apparent that the periodic Anderson model offered a more realistic description of valence transition physics.[6]

As interest in the FKM as a model of valence transitions waned, it was adopted as a model of a simple binary alloy.[7] In the limit of vanishing hybridization the f-electron occupation at each site is a good quantum number: fixing the f and d populations, the ground state is identified as the configuration adopted by the f electrons that minimizes the energy of the conduction electrons. In particular, for a bipartite lattice at half filling and equal concentration of d and f electrons, the f electrons occupy the sites of one sublattice only, the so-called checkerboard phase. For dimension $d \geqslant 2$, this checkerboard charge-density wave (CDW) state obtains for temperatures below a critical temperature T_{CDW}; above this temperature a disordered phase is realized. For $d=1$ the critical temperature is zero. We note that the FKM as a binary alloy has been extensively studied in the case of infinite dimension $d \to \infty$: the dynamical mean-field theory (DMFT) gives an exact solution in this limit.[8]

The FKM with hybridization has lately attracted renewed attention due to the investigation of optical properties in this model by Portengen *et al.*[9] Following closely Leder's Hartree-Fock (HF) work,[3] they found that the Coulomb repulsion induced an effective on-site hybridization; this effect was sufficiently strong that it persists in the limit of negligible hybridization. In fact, their calculations were performed exclusively in this limit: their solution with nonzero polarization or excitonic average $\langle d^{\dagger} f \rangle$ is indistinguishable from the well-known excitonic insulator (EI) state.[10] The "spontaneous" excitonic average was interpreted as evidence of electronic ferroelectricity. Their HF solution, however, assumed a homogeneous ground state for the system; the possibility of a CDW ground state was not considered.

The problem of reconciling the results of Portengen *et al.* with the known CDW instability has only been partially addressed. Since the DMFT equations are no longer exactly solvable for nonzero hybridization potential, Czycholl[11] performed a HF analysis for the $d \to \infty$ model. It was found that for $V=0$ there was no spontaneous excitonic average and that the CDW phase was stable against sufficiently small on-site hybridization. For a given U there was a critical hybridization $V_c(U)$ under which the CDW phase prevails. Czycholl nevertheless concluded that the interorbital U could strongly renormalize the hybridization, and so could be important in the description of the optical properties of strongly correlated electron systems. Also working in the limit of large spatial dimensions, Zlatić *et al.* noted that for $V=0$ the hybridization susceptibility diverges as $T \to 0$, although they concluded that a generalization of the FKM would be required for $\langle d^{\dagger} f \rangle \neq 0$ at finite temperatures.[12]

Comparatively little work has been done on this problem in finite dimensions. Farkašovský has used exact-diagonalization and the density matrix renormalization group methods on small one-dimensional systems to rule out the possibility of a spontaneous excitonic average at zero temperature.[13] By the same methods, Farkašovský has also analyzed the effect of local[14] and nonlocal[15] hybridization; these works are more concerned with the effect of the hybridization on valence transitions, ignoring the possibility of an excitonic renormalization of the hybridization potentials. Batista and co-workers have claimed that a nonlocal hybridization stabilizes ferroelectricity in a FKM extended by f hopping;[16] Sarasua and Continentino have investigated a similar system.[17]

The FKM extended by hybridization cannot be solved exactly and so it is necessary to use approximate methods to understand the properties of the model. In this paper, we present a HF study of the effect of the hybridization upon the CDW state on a two-dimensional square lattice. The HF approximation is reliable for small temperatures. It tends, however, to overestimate the stability of ordered phases: in particular, the HF result for the critical temperature T_{CDW} is very likely to be larger than the exact value. Nevertheless, we can reasonably expect that the HF approximation will give at least a qualitatively correct account of the relative stability of ordered phases, even in two dimensions. The HF is therefore an appropriate tool to study the competition between the EI and CDW phases in the FKM. We consider only $\epsilon_f=0$ and half filling (the particle-hole symmetry point) as the CDW state here adopts the simple checkerboard form; for these parameters also the excitonic average takes its maximum as shown in the analysis of Portengen *et al.*[9]

The FKM Hamiltonian for spinless fermions is written

$$\mathcal{H} = -t\sum_{\langle i,j\rangle} d_i^\dagger d_j + \epsilon_f \sum_j n_j^f + \sum_{i,j} (V_{ij} d_i^\dagger f_j + \text{H.c.}) + U\sum_j n_j^d n_j^f. \tag{1}$$

Some overlap between the d- and f-electron wave functions is assumed, hence the hybridization term V_{ij}. The concentration of electrons is fixed at $1=(1/N)\Sigma_j(\langle n_j^f\rangle+\langle n_j^d\rangle)$ where N is the number of sites. We measure all energies in terms of the d-electron hopping integral t.

In our HF decoupling of the Coulomb interaction, we include the possibility of the CDW state by allowing for a periodic modulation of the order parameters:

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

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

$$\langle f_j^\dagger d_j\rangle = \Delta + \Delta_Q \cos(\mathbf{Q}\cdot\mathbf{r}_j). \tag{4}$$

The nesting vector $\mathbf{Q}=(\pi/a,\pi/a)$ where a is the lattice constant. The order parameter of the CDW state is δ_d and δ_f for the d and f electrons, respectively. Note that we require $\text{sgn}(\delta_f)=-\text{sgn}(\delta_d)$. Δ is the excitonic average; in the absence of an on-site hybridization potential V, $\Delta\neq 0$ indicates the EI phase. When $V\neq 0$, the EI-normal phase transition is lifted from criticality, in analogy to the ferromagnet-paramagnet transition in an external magnetic field. In this case, we cannot speak of an EI phase, but rather an excitonic enhancement of the hybridization. This will be apparent if Δ exceeds its value in the $U=0$ system. The modulation factor Δ_Q is included in Eq. (4) for completeness. In the usual HF treatment[3,9] a homogeneous solution is assumed and so $\delta_d=\delta_f=\Delta_Q=0$ for all values of the Coulomb interaction.

We thus obtain for the HF Hamiltonian

$$\begin{aligned}\mathcal{H}_{\text{HF}} = & -t\sum_{\langle i,j\rangle} d_i^\dagger d_j + U\sum_j [n^f + \delta_f\cos(\mathbf{Q}\cdot\mathbf{r}_j)]n_j^d \\ & + U\sum_j [n^d + \delta_d\cos(\mathbf{Q}\cdot\mathbf{r}_j)]n_j^f \\ & + \sum_{ij} (\{V_{ij} - U[\Delta + \Delta_Q\cos(\mathbf{Q}\cdot\mathbf{r}_j)]\delta_{ij}\}d_i^\dagger f_j + \text{H.c.}).\end{aligned} \tag{5}$$

An important feature of this Hamiltonian is the mean-field renormalization of the d-f hybridization potential by the interorbital Coulomb interaction, $V_{ij}\to V_{ij}-U[\Delta+\Delta_Q\cos(\mathbf{Q}\cdot\mathbf{r}_j)]\delta_{ij}$. The effective on-site hybridization potential introduced by the decoupling of the interaction is responsible for the spontaneous polarization in Portengen *et al.*'s work. $\mathcal{H}_{\text{HF}}$ is diagonalized by the canonical transform

$$\gamma_{\mathbf{k}}^m = u_{\mathbf{k}}^m d_{\mathbf{k}} + v_{\mathbf{k}}^m d_{\mathbf{k}+\mathbf{Q}} + \xi_{\mathbf{k}}^m f_{\mathbf{k}} + \zeta_{\mathbf{k}}^m f_{\mathbf{k}+\mathbf{Q}}, \tag{6}$$

where $m=1,2,3,4$. The coefficients in Eq. (6) are obtained by solving the associated Bogoliubov–de Gennes (BdG) eigenequations:

$$H_{\mathbf{k}}\Psi_{\mathbf{k}}^m = E_{\mathbf{k}}^m\Psi_{\mathbf{k}}^m, \tag{7}$$

where

$$H_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}} + Un^f & U\delta_f & V_{\mathbf{k}} - U\Delta & -U\Delta_Q \\ U\delta_f & \epsilon_{\mathbf{k}+\mathbf{Q}} + Un^f & -U\Delta_Q & V_{\mathbf{k}+\mathbf{Q}} - U\Delta \\ V_{\mathbf{k}}^* - U\Delta^* & -U\Delta_Q^* & Un^d & U\delta_d \\ -U\Delta_Q^* & V_{\mathbf{k}+\mathbf{Q}}^* - U\Delta^* & U\delta_d & Un^d \end{pmatrix} \tag{8}$$

and

$$\Psi_{\mathbf{k}}^m = (u_{\mathbf{k}}^m, v_{\mathbf{k}}^m, \xi_{\mathbf{k}}^m, \zeta_{\mathbf{k}}^m)^{transpose}. \tag{9}$$

Here $\epsilon_{\mathbf{k}}=-2t[\cos(k_x a)+\cos(k_y a)]$ is the d-electron energy dispersion. The self-consistency equations for the HF parameters may be written in terms of the BdG eigenvectors:

$$\begin{aligned} n^d &= \frac{1}{N}\sum_{\mathbf{k}}{}'(\langle d_{\mathbf{k}}^\dagger d_{\mathbf{k}}\rangle + \langle d_{\mathbf{k}+\mathbf{Q}}^\dagger d_{\mathbf{k}+\mathbf{Q}}\rangle) \\ &= \frac{1}{N}\sum_{\mathbf{k}}{}'\sum_m (u_{\mathbf{k}}^{m*}u_{\mathbf{k}}^m + v_{\mathbf{k}}^{m*}v_{\mathbf{k}}^m)f(E_{\mathbf{k}}^m), \end{aligned} \tag{10}$$

$$\begin{aligned} \delta_d &= \frac{1}{N}\sum_{\mathbf{k}}{}'(\langle d_{\mathbf{k}+\mathbf{Q}}^\dagger d_{\mathbf{k}}\rangle + \langle d_{\mathbf{k}}^\dagger d_{\mathbf{k}+\mathbf{Q}}\rangle) \\ &= \frac{1}{N}\sum_{\mathbf{k}}{}'\sum_m (v_{\mathbf{k}}^{m*}u_{\mathbf{k}}^m + u_{\mathbf{k}}^{m*}v_{\mathbf{k}}^m)f(E_{\mathbf{k}}^m), \end{aligned} \tag{11}$$

$$\begin{aligned} n^f &= \frac{1}{N}\sum_{\mathbf{k}}{}'(\langle f_{\mathbf{k}}^\dagger f_{\mathbf{k}}\rangle + \langle f_{\mathbf{k}+\mathbf{Q}}^\dagger f_{\mathbf{k}+\mathbf{Q}}\rangle) \\ &= \frac{1}{N}\sum_{\mathbf{k}}{}'\sum_m (\xi_{\mathbf{k}}^{m*}\xi_{\mathbf{k}}^m + \zeta_{\mathbf{k}}^{m*}\zeta_{\mathbf{k}}^m)f(E_{\mathbf{k}}^m), \end{aligned} \tag{12}$$

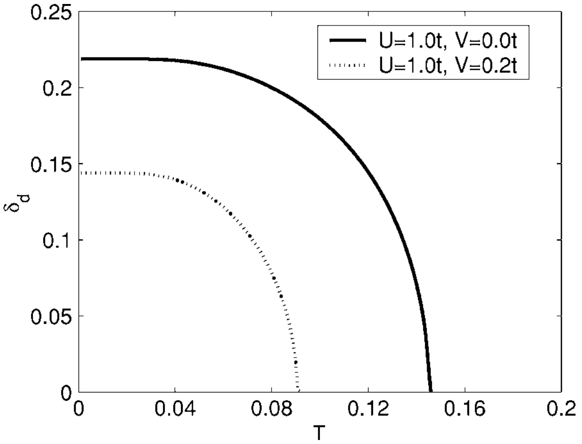

FIG. 1. Variation of the CDW order parameter δ_d with temperature in the absence (solid line) and presence (dotted line) of an on-site hybridization potential.

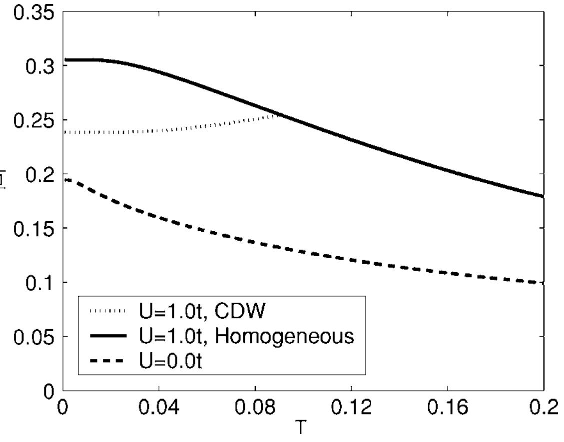

FIG. 2. Comparison of the excitonic average $|\Delta|$ in the absence (solid line) and presence (dotted line) of the CDW instability for $U=1.0t$ with the value in the noninteracting system (dashed line) for $V=0.2t$.

$$\delta_f = \frac{1}{N}\sum_{\mathbf{k}}{}'(\langle f^\dagger_{\mathbf{k+Q}} f_{\mathbf{k}}\rangle + \langle f^\dagger_{\mathbf{k}} f_{\mathbf{k+Q}}\rangle) = \frac{1}{N}\sum_{\mathbf{k}}{}'\sum_m (\zeta^{m*}_{\mathbf{k}}\xi^m_{\mathbf{k}} + \xi^{m*}_{\mathbf{k}}\zeta^m_{\mathbf{k}})f(E^m_{\mathbf{k}}), \tag{13}$$

$$\Delta = \frac{1}{N}\sum_{\mathbf{k}}{}'(\langle f^\dagger_{\mathbf{k}} d_{\mathbf{k}}\rangle + \langle f^\dagger_{\mathbf{k+Q}} d_{\mathbf{k+Q}}\rangle) = \frac{1}{N}\sum_{\mathbf{k}}{}'\sum_m (\xi^{m*}_{\mathbf{k}} u^m_{\mathbf{k}} + \zeta^{m*}_{\mathbf{k}} v^m_{\mathbf{k}})f(E^m_{\mathbf{k}}), \tag{14}$$

$$\Delta_Q = \frac{1}{N}\sum_{\mathbf{k}}{}'(\langle f^\dagger_{\mathbf{k+Q}} d_{\mathbf{k}}\rangle + \langle f^\dagger_{\mathbf{k}} d_{\mathbf{k+Q}}\rangle) = \frac{1}{N}\sum_{\mathbf{k}}{}'\sum_m (\zeta^{m*}_{\mathbf{k}} u^m_{\mathbf{k}} + \xi^{m*}_{\mathbf{k}} v^m_{\mathbf{k}})f(E^m_{\mathbf{k}}). \tag{15}$$

The prime denotes summation over half the Brillouin zone; $f(E)=1/\{1+\exp[\beta(E-\mu)]\}$ is the Fermi distribution function. The chemical potential μ is determined by the condition $1=(1/N)\Sigma_{\mathbf{k}}'\Sigma_m f(E^m_{\mathbf{k}})$. We use an exact diagonalization method to solve the BdG equation (7) self-consistently. We start with an initial set of order parameters. By solving Eq. (7), the new order parameters are computed via Eqs. (10)–(15) and are substituted back into Eq. (7). The iteration is repeated until a desired accuracy is achieved.

We first consider the case of an on-site hybridization, $V_{ij}=V\delta_{ij}$. In agreement with previous work[11–13] we find that for vanishing hybridization the CDW phase is *always* stable against the EI phase and there is no spontaneous excitonic average. The CDW order displayed by the $V=0$ ground state will persist in the presence of sufficiently small hybridization potentials, although the transition temperature T_{CDW} will be considerably suppressed (see Fig. 1). We find, however, that for finite hybridization the Coulomb interaction will strongly enhance the magnitude of Δ. We plot the variation of $|\Delta|$ with temperature in Fig. 2. Note that since $\Delta=-|\Delta|$ there is a large renormalization of the hybridization potential due to the mean-field decoupling of the Coulomb interaction Eq. (5). Comparing the homogeneous solution without the CDW ordering (the solid line) with the solution with a coexisting CDW ordering (the dotted line), we find a significant suppression of $|\Delta|$ at the onset of the CDW order at $T\sim 0.1t$. Even within the CDW phase, however, the excitonic enhancement of the on-site hybridization is still apparent as $|\Delta|$ exceeds its value within the noninteracting system (the dashed line in Fig. 2). We do not find any evidence of nonzero Δ_Q.

This competition can be understood from a phenomenological Ginzburg-Landau (GL) theory. The GL free energy density, in terms of both the CDW (δ_d) and EI (Δ) order parameters, can be constructed from a symmetry analysis:

$$f = \alpha_{EI}|\Delta|^2 + \alpha_{CDW}|\delta_d|^2 + \beta_1|\Delta|^4 + \beta_2|\delta_d|^2 + \beta_3|\Delta|^2|\delta_d|^2 - \beta_4(\Delta^{*2}\delta_d^2 + \Delta^2\delta_d^{*2}), \tag{16}$$

where we assume $\alpha_{EI}=\alpha'_{EI}(T-T^0_{EI})$ and $\alpha_{CDW}=\alpha'_{CDW}(T-T^0_{CDW})$. We assume β_i $(i=1,2,3,4)$ are all positive. In the region where $T^0_{EI}>T^0_{CDW}$,[18] the second phase transition temperature for the CDW ordering is renormalized by the preexisting EI order parameter:

$$T_{CDW} = T^0_{CDW} - \frac{(\beta_3-2\beta_4)(T^0_{EI}-T^0_{CDW})}{2\beta_1\alpha'_{CDW}/\alpha'_{EI} - (\beta_3-2\beta_4)}. \tag{17}$$

It means that when the EI order parameter preexists, the second phase transition temperature for the appearance of the CDW order parameter can be strongly suppressed by the dominant EI order parameter. This explains why the transition temperature T_{CDW} decreases with increased hybridization potential V, as shown in Fig. 1. Below the second phase transition temperature T_{CDW}, a little algebra yields

$$\Delta = \left(\frac{-2\beta_2\alpha_{EI} + \alpha_{CDW}(\beta_3-2\beta_4)}{4\beta_1\beta_2 - (\beta_3-2\beta_4)^2}\right)^{1/2}, \tag{18}$$

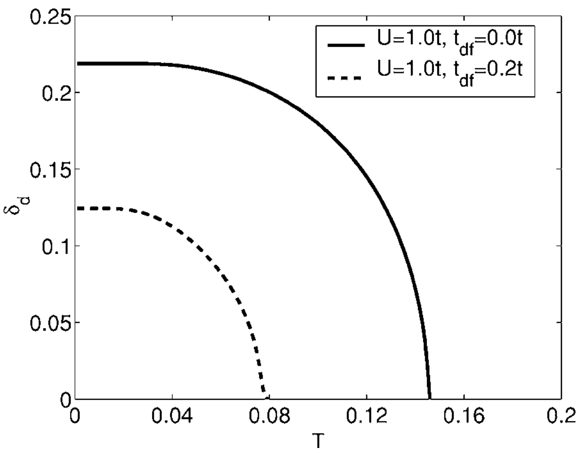

FIG. 3. Variation of the CDW order parameter δ_d in the absence (solid line) and presence (dotted line) of a nonlocal hybridization potential.

$$\delta_d = \left(\frac{-2\beta_1 \alpha_{CDW} + \alpha_{EI}(\beta_3 - 2\beta_4)}{4\beta_1\beta_2 - (\beta_3 - 2\beta_4)^2} \right)^{1/2}. \tag{19}$$

Under the condition that the temperature derivative α'_{CDW} is larger than α'_{EI}, which is indeed confirmed by our numerical results near T_{CDW} (see Figs. 1 and 2), α_{CDW} changes more rapidly than α_{EI} when the temperature is lowered. Consequently, the CDW order δ_d increases while the EI order Δ decreases with the lowered temperature.

Despite the popularity of the on-site hybridization potential, this is actually forbidden in real *d*-*f* systems by parity considerations.[6] We are instead required to consider a nonlocal hybridization with inversion symmetry: the simplest such potential is

$$V_{ij} = t_{df}[\delta_{i_x j_x}(\delta_{i_y j_y+1} - \delta_{i_y j_y-1}) + \delta_{i_y j_y}(\delta_{i_x j_x+1} - \delta_{i_x j_x-1})], \tag{20}$$

where any site on the lattice is given by $\mathbf{r}_i = i_x a\hat{\mathbf{x}} + i_y a\hat{\mathbf{y}}$. This is a particularly interesting case as the Coulomb-induced hybridization has a different (*s*-wave) symmetry. In the noninteracting system, the (on-site) excitonic average Δ vanishes; the nonlocal hybridization potential instead gives rise to an anisotropic excitonic average

$$\Xi = \mathrm{Im}\left(\frac{1}{N} \sum_{\mathbf{k}} [\sin(k_x a) + \sin(k_y a)] \langle f^{\dagger}_{\mathbf{k}} d_{\mathbf{k}} \rangle \right). \tag{21}$$

The study of this quantity allows us to assess the effect of the interorbital Coulomb repulsion upon the *d*-*f* hybridization.

As with the on-site hybridization, we find that for given U the CDW phase is suppressed by the presence of the nonlocal hybridization (see Fig. 3). We do not, however, find any evidence for a Coulomb-induced on-site hybridization when the CDW instability is allowed: for all nonzero t_{df} we have $\Delta = \Delta_Q = 0$. Czycholl considered the appearance of an on-site average Δ to be likely due to the substantial excitonic enhancement of the on-site hybridization potential by the Coulomb interaction.[11] Our results clearly demonstrate that this EI-like scenario, and the consequent formation of an electronic ferroelectric state, is severely compromised by the presence of nonlocal hybridization.

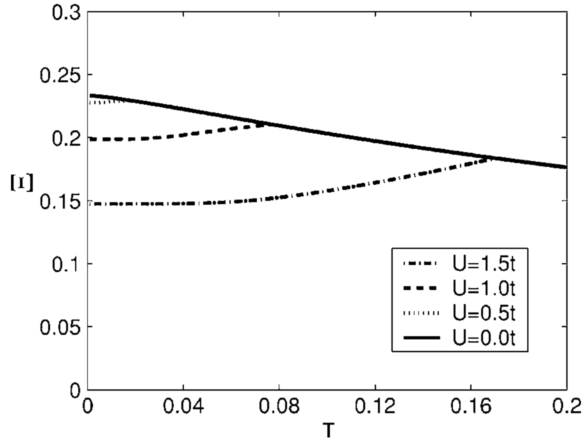

FIG. 4. Comparison of the anisotropic exciton average Ξ in the noninteracting and interacting systems. We have $t_{df} = 0.2t$.

In Fig. 4 we plot Ξ as function of temperature in both the interacting and noninteracting systems. The onset of CDW order for the given Coulomb values occurs at the point of intersection of the broken lines with the noninteracting (solid) line. Remarkably, for the standard homogeneous solution there is no effect on Ξ due to the Coulomb interaction: the variation of Ξ with temperature exactly follows the curve for the noninteracting system. Within the CDW phase, however, Ξ is suppressed below its value in the noninteracting system. We offer the following explanation for this anomaly: the hybridization potential Eq. (20) connects the *A*-sublattice *d* orbitals with *B*-sublattice *f* orbitals, and vice versa. Assume that in the CDW state the *A*-sublattice *d* orbitals has $n^d > 0.5$ and so the *B*-sublattice *f* orbitals have $n^f > 0.5$; clearly *A*-*B* sublattice *d*-*f* hopping will be suppressed, hence also the reduction in Ξ.

In conclusion, we have examined the competition between excitonic and CDW instabilities in the FKM extended by both on-site and nonlocal hybridization. In both cases, we find that the CDW phase remains stable at low temperatures even in the presence of a finite hybridization. For the local hybridization we find that the Coulomb interaction nevertheless strongly renormalizes the hybridization potential in agreement with previous work.[11] The situation is qualitatively different for the more realistic nonlocal hybridization: there is no enhancement of the nonlocal hybridization and the Coulomb interaction does not induce a spontaneous on-site hybridization. Within the CDW phase, the nonlocal hybridization is suppressed in line with the increasing localization of the *d* and *f* electrons. The failure of the Coulomb interaction to induce an effective on-site hybridization except when such a term is already present casts significant doubt on the usefulness of Eq. (1) as a minimal model for electronic ferroelectricity. Interorbital Coulomb repulsion may nevertheless still be important for understanding optical properties of strongly correlated electron systems: for example, a recent extension of the FKM by f-electron hopping offers a plausible scenario where the formation of an exciton Bose-Einstein condensate gives a spontaneous excitonic average.[16]

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[18] Note that for a finite hybridization potential the expectation value of the particle-hole pair operator, $\langle f^{\dagger}d\rangle$ is a quantity characterizing the charge polarization, not the spontaneous EI order. As such, the characteristic temperature T_{EI}^{0} is not a real EI phase transition temperature.