Electronic Ferroelectricity in the Falicov-Kimball Model

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I show that a spontaneous electric polarization exists in the solution of the Falicov-Kimball model by mapping the strong coupling limit of this Hamiltonian into an xxz spin 1/2 model with a magnetic field. In this way, I determine the phase diagram of the strongly interacting model and show the existence of a transition to a mixed-valence regime containing two phases: an orbitally ordered state and a Bose-Einstein condensation of excitons with a built-in electric polarization.

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The Falicov-Kimball [1] model (FKM) was introduced to explain semiconductor-metal transitions and has been extensively used to describe valence transitions in heavy fermion compounds. Its original version contains a dispersive band of itinerant d electrons interacting with localized f orbitals via an on-site Coulomb interaction. If hybridization between both bands is included, the f charge occupation is no longer a good quantum number, and it is possible to build coherence between the d electrons and the f holes. Based on a mean field solution of the FKM with a hybridization term, Portengen *et al.* [2] proposed that this coherence gives rise to a spontaneous electric polarization associated with a Bose-Einstein condensate (BEC) of $d-f$ excitons.

Ferroelectrics are of considerable theoretical and technological interest because of their highly unusual properties [3]. The ferroelectric (FE) transitions have traditionally been considered as a subgroup of the structural phase transitions. As in the case of superconductivity, the existence of ferroelectrics based on a purely electronic mechanism would provide a new set of physical properties [2] and technological applications; for instance, it would open the possibility of controlling optical properties with magnetic fields.

The proposal of electronic ferroelectricity in the FKM was recently tested theoretically using different techniques. An analytical calculation in infinite dimension for the weak coupling limit [4] did not confirm its existence. By using numerical methods to solve finite-size chains, Farkašovský [5] arrived at the same conclusion for the intermediate and the strong coupling regimes. Recently, Zlatić *et al.* [6] calculated the spontaneous polarization in the FKM from its exact solution in infinite dimensions. They found that the spontaneous hybridization susceptibility diverges at zero temperature, indicating a possible nonzero polarization of the ground state.

Hybridization between the bands, however, is not the only way to develop $d-f$ coherence. An $f-f$ hopping also induces it. Furthermore, I will show that in the mixed-valence regime, the ground state of the FKM with $f-f$ hopping is either an orbitally ordered (chessboard) state or a BEC of electron-hole pairs (excitons). In particular, the condensate has a built-in spontaneous FE or antiferroelectric (AFE) polarization induced by a pure electronic mechanism.

I obtain the complete phase diagram of the extended FKM by mapping the original Hamiltonian into an effective spin model. The mapping is exact in the strong coupling limit and the resulting Hamiltonian is a spin 1/2 xxz model with an applied magnetic field along the $\hat{\mathbf{z}}$ axis. This model is exactly solvable in one dimension, and its phase diagram has been determined very accurately for two dimensional ($D=2$) systems (the exact solution has been numerically obtained for a 96×96 square lattice [7]). In this way, the results obtained in this paper prove that the phase diagram of the extended FKM contains FE and AFE phases induced by an electronic mechanism.

Recently, high dielectric constants were observed in oxides of the type $ACu_3Ti_4O_{12}$. In particular, the largest dielectric constant ever observed is exhibited by $CaCu_3Ti_4O_{12}$ ($\epsilon_0 \simeq 80\,000$ for single-crystal samples at room temperature) [8–10]. In addition, high resolution x-ray and neutron powder diffraction measurements of $CaCu_3Ti_4O_{12}$ rule out a conventional FE structural phase transition. The electronic ferroelectricity proposed by Portengen *et al.* [2] was also ruled out due to the large value of the optical gap ($\Delta \sim 1.5$ eV) [11]. The strong coupling theory introduced in this paper shows that the excitons condense in the presence of a large gap.

I will consider an extended FKM for spinless fermions on a D-dimensional hypercubic lattice:

$$H = \epsilon_d \sum_{\mathbf{i}} n_{\mathbf{i}}^d + \epsilon_f \sum_{\mathbf{i}} n_{\mathbf{i}}^f + t_d \sum_{\langle \mathbf{i},\mathbf{j}\rangle} d_{\mathbf{i}}^\dagger d_{\mathbf{j}} + U^{fd} \sum_{\mathbf{i}} n_{\mathbf{i}}^d n_{\mathbf{i}}^f + t_f \sum_{\langle \mathbf{i},\mathbf{j}\rangle} f_{\mathbf{i}}^\dagger f_{\mathbf{j}}, \quad (1)$$

where $n_{\mathbf{i}}^d = d_{\mathbf{i}}^\dagger d_{\mathbf{i}}$, and $n_{\mathbf{i}}^f = f_{\mathbf{i}}^\dagger f_{\mathbf{i}}$ are the occupation numbers of each orbital. For historical reasons, I denote the orbitals by f and d, but in general they can represent any pair of atomic orbitals with different parity. For instance, in $CaCu_3Ti_4O_{12}$ there are d states which are hybridized with p bands [11].

The Hamiltonian H can be rewritten as an asymmetric Hubbard model if the orbital flavor is represented by a pseudospin variable. A spin 1/2 is required to describe the two orbitals (flavors) on each site:

$$c^\dagger_{\mathbf{i}\uparrow} = d^\dagger_{\mathbf{i}}, \qquad c_{\mathbf{i}\uparrow} = d_{\mathbf{i}}, \qquad c^\dagger_{\mathbf{i}\downarrow} = f^\dagger_{\mathbf{i}}, \qquad c_{\mathbf{i}\downarrow} = f_{\mathbf{i}}, \quad (2)$$

where the pseudospin generators are

$$\tau^x_{\mathbf{i}} = \frac{1}{2}(d^\dagger_{\mathbf{i}} f_{\mathbf{i}} + f^\dagger_{\mathbf{i}} d_{\mathbf{i}}), \qquad \tau^y_{\mathbf{i}} = \frac{i}{2}(f^\dagger_{\mathbf{i}} d_{\mathbf{i}} - d^\dagger_{\mathbf{i}} f_{\mathbf{i}}),$$
$$\tau^z_{\mathbf{i}} = \frac{1}{2}(n^d_{\mathbf{i}} - n^f_{\mathbf{i}}). \quad (3)$$

The expression for H in the new language is

$$H = e_d \sum_{\mathbf{i},\sigma} n_{i\sigma} + \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\boldsymbol{\sigma}} t_\sigma (c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) + U^{fd} \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + B_z \sum_{\mathbf{i}} \tau^z_i, \quad (4)$$

where $e_d = \frac{1}{2}(\epsilon_d + \epsilon_f)$ and $B_z = \epsilon_d - \epsilon_f$. The new version of H is a Hubbard model with different hoppings for each spin flavor, $t_\uparrow = t_d$ and $t_\downarrow = t_f$, plus a Zeeman coupling with a magnetic field B_z. Both terms break the SU(2) symmetry of the original Hubbard model ($t_\uparrow = t_\downarrow$ and $B_z = 0$). The remaining symmetries are the U(1) groups associated with the conservation of the total charge and the total τ^z. In the original language, these U(1) symmetries correspond to the conservation of the total number of particles in each band ($[H, \sum_{\mathbf{i}} n^f_{\mathbf{i}}] = [H, \sum_{\mathbf{i}} n^d_{\mathbf{i}}] = 0$).

I will consider from now on the half-filled case, i.e., one particle per site. For this concentration, it is well known that the Hubbard model in the strong coupling limit can be reduced to an effective Heisenberg model. In a similar fashion, I can reduce H to an effective spin model when $t_\sigma \ll U^{fd}$. The lowest energy subspace for infinite U^{fd} is the one generated by states having one particle at each site, i.e., the charge degrees of freedom are frozen (the system is a Mott insulator) and an effective spin is localized at each site. In this limit there is a complete spin degeneracy because the energy does not depend on the orientation of each spin. To lift this degeneracy it is necessary to consider the lowest order processes in t_σ/U^{fd}. This can be done by a canonical transformation which eliminates the linear terms in the hopping t_σ and keeps the terms of quadratic order. Up to an irrelevant constant $C = -N\mathcal{Z}J_z/8$, where $\mathcal{Z}$ is the coordination number and N is the number of sites, the resulting effective spin Hamiltonian is [12]

$$H_{\text{eff}} = \sum_{\langle \mathbf{i},\mathbf{j}\rangle} J_z \tau^z_{\mathbf{i}} \tau^z_{\mathbf{j}} + J_\perp (\tau^x_{\mathbf{i}} \tau^x_{\mathbf{j}} + \tau^y_{\mathbf{i}} \tau^y_{\mathbf{j}}) + B_z \sum_{\mathbf{i}} \tau^z_{\mathbf{i}}, \quad (5)$$

with $J_z = \frac{2(t^2_\uparrow + t^2_\downarrow)}{U^{fd}}$ and $J_\perp = \frac{4t_\uparrow t_\downarrow}{U^{fd}}$. H_{eff} is a spin 1/2 xxz model with an applied magnetic field along the $\hat{\mathbf{z}}$ direction. The model is Ising-like ($J_z > J_\perp$). However, it is important to consider the whole phase diagram because the ratio $J_z/J_\perp$ can take any value if nonzero nearest-neighbor repulsions are added to H.

H_{eff} has been exactly solved in one dimension by means of the Bethe ansatz technique [13]. The one dimensional (1D) quantum phase diagram is similar to the 2D one that I describe below. The only important difference is that, as required by the Mermin-Wagner theorem [14], the excitonic condensate is critical at zero temperature (power law correlations) for the 1D case. The phase diagram of H_{eff} has been determined recently for 2D systems by solving up to 96×96 lattices with quantum Monte Carlo loop algorithm [7]. The zero temperature phase diagram is shown in Fig. 1 and the corresponding name of each phase translated back to the original language of the FKM. Since H_{eff} is symmetric under a reflection in the xy plane, the phase diagram must be symmetric under a change of sign of the magnetic field. The fully polarized solutions, obtained for large values of $|B_z|$, correspond to a full f band for positive B_z ($\epsilon_f \ll \epsilon_d$) and a full d band for negative B_z ($\epsilon_f \gg \epsilon_d$). The spectrum of both phases has a finite charge transfer (pseudospin gap) $\Delta_{\text{CT}} = |B_z - \mathcal{Z}(|J_\perp| + J_z)/2|$. This gap vanishes at the quantum critical points $|B^c_z| = \frac{\mathcal{Z}}{2}(|J_\perp| + J_z)$, which are the boundaries for the mixed-valence phase that emerges when the f and d bands are sufficiently close: $|\epsilon_f - \epsilon_d| < \frac{\mathcal{Z}}{2}(|J_\perp| + J_z)$. If $J_z > J_\perp$, two phases are possible within the mixed-valence regime. For small values of $|B_z|$, the J_z term dominates and induces a longitudinal antiferromagnetic (AFM) phase (chessboard state in the original language). When $|B_z|$ is larger than a critical value, the magnetic field suppresses the Ising-like ordering and the $J_\perp$ term induces a magnetic ordered state in the xy plane (BEC of electron-hole pairs). The line separating the orbitally ordered state and the BEC

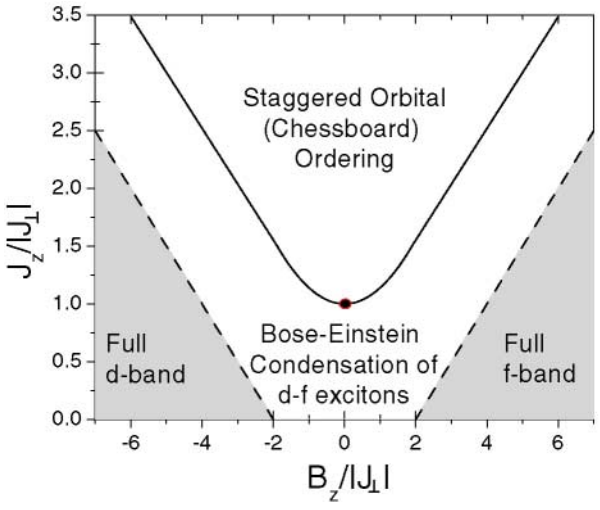

FIG. 1 (color online). Two dimensional quantum phase diagram of H_{eff} obtained from Ref. [7]. The small circle indicates the position of the Heisenberg point. The dashed line denotes the quantum phase transition between the mixed valence (non-shadowed) and the non-mixed valence regimes.

corresponds to a first order transition. This line ends at the Heisenberg point ($J_z = J_\perp$) where both phases coexist. For $J_z < J_\perp$, the only phase in the mixed-valence regime is the BEC. In a real material, changing $B_z = \epsilon_d - \epsilon_f$ can be achieved by applying pressure or alloying.

The $d - f$ exciton condensate has a built-in electric polarization [2]. This can easily be seen by realizing that the spin version of the order parameter for the BEC is the uniform xy magnetization for negative $J_\perp$ (condensation at $\mathbf{k} = \mathbf{0}$) and the staggered xy magnetization for positive $J_\perp$ (condensation at the AFM wave vector $\mathbf{k} = \mathbf{Q}$):

$$\begin{aligned} \mathbf{M}^\perp &= \sum_{\mathbf{i}} (\tau_{\mathbf{i}}^x \hat{\mathbf{x}} + \tau_{\mathbf{i}}^y \hat{\mathbf{y}}) \quad \text{for } J_\perp < 0, \\ \mathbf{M}_{ST}^\perp &= \sum_{\mathbf{i}} e^{i\mathbf{Q}\cdot\mathbf{r}_\mathbf{i}} (\tau_{\mathbf{i}}^x \hat{\mathbf{x}} + \tau_{\mathbf{i}}^y \hat{\mathbf{y}}) \quad \text{for } J_\perp > 0. \end{aligned} \tag{6}$$

Since $\mathbf{M}^\perp$ is a two dimensional vector, it can also be represented by a complex number $|\mathbf{M}^\perp| e^{i\phi}$ ($\tan\phi = M^x/M^y$) which is the usual expression for the order parameter of the BEC. The sign of $J_\perp$ is determined by the relative sign of t_d and t_f. On the other hand, the uniform polarization operator is [2]

$$\mathbf{P} = \frac{\boldsymbol{\mu}}{\Omega} \sum_{\mathbf{i}} (d_{\mathbf{i}}^\dagger f_{\mathbf{i}} + d_{\mathbf{i}} f_{\mathbf{i}}^\dagger) = \frac{2\boldsymbol{\mu}}{\Omega} M^x, \tag{7}$$

where $\boldsymbol{\mu}$ is the interband dipole matrix element and Ω is the volume of the system. Therefore, the condensate has a built-in electric polarization which is proportional to the $\hat{\mathbf{x}}$ (real) component of its order parameter. For positive $J_\perp$, the condensate becomes AFE because the staggered electric polarization is proportional to M_{ST}^x:

$$\mathbf{P}_{ST} = \frac{\boldsymbol{\mu}}{\Omega} \sum_{\mathbf{i}} e^{i\mathbf{Q}\cdot\mathbf{r}_\mathbf{i}} (d_{\mathbf{i}}^\dagger f_{\mathbf{i}} + d_{\mathbf{i}} f_{\mathbf{i}}^\dagger) = \frac{2\boldsymbol{\mu}}{\Omega} M_{ST}^x. \tag{8}$$

The three dimensional (3D) quantum phase diagram of H_{eff} [15] is similar to the two dimensional (2D) one shown in Fig. 1. The same is not true for the finite temperature phase diagrams due to the Mermin-Wagner theorem [14]. The transition temperature associated with the BEC is finite only for the 3D case. From the finite temperature phase diagram obtained in Ref. [7], the BEC of electron-hole pairs undergoes a Kosterlitz-Thouless phase transition in a 2D system.

I will now analyze the effect that a time dependent electric field $\mathbf{E}e^{i\omega t}$ induces in our FE or AFE condensate of excitons. The coupling term between the electric field and the uniform polarization,

$$H_I = \mathbf{E}\cdot\boldsymbol{\mu}\, \frac{e^{i\omega t}}{\Omega} \sum_{\mathbf{i}} (d_{\mathbf{i}}^\dagger f_{\mathbf{i}} + d_{\mathbf{i}} f_{\mathbf{i}}^\dagger), \tag{9}$$

corresponds, in the spin language, to the application of a uniform time dependent magnetic field $\mathbf{B}_1(t) = 2\mathbf{E}\cdot\boldsymbol{\mu} e^{i\omega t}\hat{\mathbf{x}}/\Omega$. From the point of view of the spin variables this is like a magnetic resonance experiment since H_{eff} already includes a uniform static field $B_z\hat{\mathbf{z}}$. Therefore, the equivalent magnetic system will have a resonant absorption at the frequency which tends to $\omega_0 = B_z/\hbar$ when $\mathbf{B}_1$ tends to zero. Back to the original language, this means that for small electric fields the optical absorption will be resonant at $\hbar\omega_0 = \epsilon_d - \epsilon_f$. This is an experimental fingerprint of the excitonic condensate.

Since the above theory is valid only in the strong coupling limit, it is natural to ask whether the chessboard ordering and the excitonic condensate survive in the intermediate and weak coupling regimes. To answer this question it is more convenient to use the Hubbard-like representation of H [see Eq. (4)]. The dispersion relation for the noninteracting part of H ($U^{fd} = 0$) is $\epsilon(\mathbf{k}, \sigma) = e_d + B_z\sigma + 2t_\sigma \sum_\nu \cos(k_\nu)$. At half-filling and for $B_z = 0$ the Fermi surface of the noninteracting problem nests at $\mathbf{k}=\mathbf{Q}$. This indicates that an infinitesimal value of U^{fd} is sufficient to induce an AFM (chessboard ordering in the original language) instability. Again the presence of a nonzero magnetic field will induce a transition from the orbitally ordered state to the BEC of excitons. For the 3D case, if $U^{fd} < U_c^{fd} \sim 2.85(|t_a| + |t_b|)$ the magnetic field B_z induces an insulator-metal transition before the saturation of the magnetization (nonmixed valence regime) is reached [16]. This means that for weak coupling a new metallic phase appears between the BEC of excitons and the nonmixed valence regime (see Fig. 1). For these reasons, I expect the phase diagram of H to contain an electric polarized BEC in the weak and intermediate coupling regimes as well.

What happens if we consider electrons instead of spinless fermions? In this case each orbital can be occupied by two electrons, and therefore it is natural to include local Coulomb repulsions U^{ff} and U^{dd}. By doing so the FKM is replaced by a two orbital Hubbard model and the large $U^{\alpha,\beta}$ expansion gives rise to a Kugel-Khomskii–like model [17] containing spin $\mathbf{s}$ (magnetic) and pseudospin $\boldsymbol{\tau}$ (orbital) degrees of freedom. If $t_a = -t_b = t$ and $U^{ff} = U^{dd} = U$ (the most general case will be analyzed in Ref. [19]), the effective spin Hamiltonian is

$$\begin{aligned} H_{\text{eff}}^{s,\tau} = {} & \frac{J_0}{2} \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \mathbf{S}_\mathbf{i}\cdot\mathbf{S}_\mathbf{j} + (J_z - J_0) \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \tau_\mathbf{i}^z \tau_\mathbf{j}^z + B_z \sum_\mathbf{i} \tau_\mathbf{i}^z \\ & + 2 \sum_{\langle \mathbf{i},\mathbf{j}\rangle} [J_0 \boldsymbol{\tau}_\mathbf{i}^\mathbf{z} \boldsymbol{\tau}_\mathbf{j}^\mathbf{z} - J_\perp (\tau_\mathbf{i}^x \tau_\mathbf{j}^x + \tau_\mathbf{i}^y \tau_\mathbf{j}^y)] \left(\mathbf{S}_\mathbf{i}\cdot\mathbf{S}_\mathbf{j} + \frac{1}{4} \right), \end{aligned}$$

where $J_0 = 4t^2/U$. The ground state of $H_{\text{eff}}^{s,\tau}$ is ferromagnetic (FM) if $J_0 < J_0^c$. For the FM solution, $H_{\text{eff}}^{s,\tau}$ reduces to H_{eff} because all the electrons have the same spin orientation and hence can be considered as spinless fermions. Therefore the charge degrees of freedom ($\boldsymbol{\tau}$) of the FM solution are exactly described by H_{eff}, and the phase diagram is the one of Fig. 1; i.e., ferromagnetism coexists with chessboard ordering or a FE BEC of excitons. If $J_0 > J_0^c$, the system becomes AFM. In this case the effective transverse coupling for the pseudospin variables, $J_\perp^{\text{eff}} = -2J_\perp \langle (\mathbf{S}_\mathbf{i}\cdot\mathbf{S}_\mathbf{j} + \frac{1}{4}) \rangle$, changes its sign because $\langle (\mathbf{S}_\mathbf{i}\cdot\mathbf{S}_\mathbf{j} + \frac{1}{4}) \rangle$ turns to be negative. For this reason the AFM

solution coexists with an AFE condensate. This means that when a magnetic field induces a transition from an AFM phase to a FM one, it simultaneously changes the electric polarization from AFE to FE.

From now on I will continue with the spinless case just to isolate the basic mechanism for FE and AFE which is associated with the charge degrees of freedom. An important aspect of this analysis is the inclusion of a nonzero hybridization term,

$$H_V = V \sum_{\mathbf{i},\nu} (d^\dagger_{\mathbf{i}} f_{\mathbf{i}+\hat{\mathbf{e}}_\nu} + f^\dagger_{\mathbf{i}+\hat{\mathbf{e}}_\nu} d_{\mathbf{i}} - f^\dagger_{\mathbf{i}} d_{\mathbf{i}+\hat{\mathbf{e}}_\nu} - d^\dagger_{\mathbf{i}+\hat{\mathbf{e}}_\nu} f_{\mathbf{i}}), \tag{10}$$

where ν runs over the different spatial directions (x, y, and z in three dimensions). The different signs in the hybridization terms are due to the different parities of the two orbitals. (The crystal has inversion symmetry.) By adding H_V to H, we get the following additional terms for H_{eff} (large U expansion):

$$H'_{\text{eff}} = J' \sum_{\mathbf{i},\nu} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_{\mathbf{i}+\hat{\mathbf{e}}_\nu} + J'_{xz} \sum_{\mathbf{i},\nu} (\tau^z_{\mathbf{i}} \tau^x_{\mathbf{i}+\hat{\mathbf{e}}_\nu} - \tau^z_{\mathbf{i}+\hat{\mathbf{e}}_\nu} \tau^x_{\mathbf{i}}) - iJ'_{yz} \sum_{\mathbf{i},\nu} (\tau^z_{\mathbf{i}} \tau^y_{\mathbf{i}+\hat{\mathbf{e}}_\nu} - \tau^z_{\mathbf{i}+\hat{\mathbf{e}}_\nu} \tau^y_{\mathbf{i}}) - 2J' \sum_{\mathbf{i},\nu} \tau^x_{\mathbf{i}} \tau^x_{\mathbf{i}+\hat{\mathbf{e}}_\nu},$$

where $J' = 4V^2/U^{fd}$ and $J'_{xz} = 4V(t_a + t_b)/(U^{fd} - B_z\alpha)$, $J'_{yz} = 4V(t_a + t_b)\alpha/(U^{fd} - B_z\alpha)$ and $\alpha = B_z/U^{fd}$. Let me now consider the perturbative effects of the hybridization ($J', J'_{xz} \ll J_z, J_\perp$) on the phase diagram of Fig. 1 for the FE case ($J_\perp < 0$). The first term is a Heisenberg interaction which just produces a renormalization of J_z and $J_\perp$. The mean value of the second and the third terms are zero in the FE phase (BEC of excitons), and therefore they do not make any contribution. The last term introduces an easy axis anisotropy along the $\hat{\mathbf{x}}$ direction and lifts the U(1) degeneracy. The BEC then is replaced by an Ising-like FE state characterized by the breaking of the remaining Z_2 symmetry. Therefore, the spontaneous ferroelectricity remains when the hybridization is included perturbatively; however, the resonant response to a time dependent electric field [see Eq. (9)] disappears due to the absence of Goldstone modes. In other words, the hybridization makes the electronically induced FE phase similar to the ones induced by structural phase transitions.

In summary, I derived the phase diagram of the FKM with a t_f hopping term in the strong coupling limit. The insulating phase obtained at half-filling has a transition from a nonmixed valence to a mixed-valence regime as a function of the energy difference between the centers of both bands. Two different phases are present in the mixed-valence regime: a BEC of excitons with a built-in electrical polarization which starts just at the valence transition and an orbitally ordered (chessboard) state which appears when the centers of the bands are sufficiently close. These results were extended to the intermediate and weak coupling regimes due to the nesting property of the Fermi surface of hypercubic lattices. I also mentioned the effect of including spin degrees of freedom in H: the interplay between magnetic and charge degrees of freedom gives rise to the coexistence of FE and FM phases which are coupled to each other. This opens the possibility of controlling optical (magnetic) properties by applying magnetic (electric) fields.

The effect of a nonzero hybridization was also considered. The main conclusion is that the U(1) degeneracy associated with the BEC of excitons is lifted by the hybridization and replaced by an Ising-like FE state (broken Z_2 symmetry). Then, the resonant response to a time dependent electric field disappears because the Goldstone modes acquire a finite mass (gap).

These results indicate that the following characteristics are favorable to the formation of an electronically driven FE 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^{fd}) between the different orbitals is required. (d) The hybridization between the bands must be small compared to their bandwidths.

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