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Effects of nonlocal hybridization on valence and metal-insulator transitions in the Falicov-Kimball model

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The density matrix renormalization group and small cluster exact diagonalization calculations are used to examine effects of nonlocal hybridization on ground-state properties of the Falicov-Kimball model in one dimension. Special attention is devoted to the problem of hybridization induced insulator-metal transitions. It is shown that the picture of insulator-metal transitions found for the Falicov-Kimball model with nonlocal hybridization strongly differs from one found for the Falicov-Kimball model without hybridization (as well as with local hybridization). The effect of nonlocal hybridization is so strong that it can induce the insulator-metal transition, even in the half-filled band case where the ground states of the Falicov-Kimball model without hybridization are insulating for all finite Coulomb interactions. Outside the half-filled band case the metal-insulator transition driven by pressure is found for finite values of nonlocal hybridization.

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I. INTRODUCTION

The Falicov-Kimball model (FKM) has become, since its introduction in 1969, one of the most popular examples of a system of interacting electrons with short-range interactions. The model was originally proposed to describe metal-insulator transitions[1] 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.[4–6] It is the latter language we shall use here, considering a system of localized f electrons and itinerant d electrons coupled via the local interaction U. A d-f hybridization term may or may not be added to the model. Thus the Hamiltonian of the FKM can be written as the sum of four terms

$$H=\sum_{ij} t_{ij} d_i^+ d_j + U\sum_i f_i^+ f_i d_i^+ d_i + \sum_{ij} V_{ij}(d_i^+ f_j + f_j^+ d_i) + E_f \sum_i f_i^+ f_i, \qquad (1)$$

where f_i^+, f_i are the creation and annihilation operators for an electron in the localized state at lattice site i with binding energy E_f and d_i^+, d_i are the creation and annihilation operators of the itinerant spinless electrons in the d-band Wannier state at site i.

The first term of Eq. (1) is the kinetic energy corresponding to quantum-mechanical hopping of the itinerant d electrons between sites i and j. These intersite hopping transitions are described by the matrix elements t_{ij}, which are $-t$ if i and j are the nearest neighbors and zero otherwise (in the following all parameters are measured in units of t). The second term represents the on-site Coulomb interaction between the d-band electrons with density $n_d=(1/L)\Sigma_i d_i^+ d_i$ and the localized f electrons with density $n_f=(1/L)\Sigma_i f_i^+ f_i$, where L is the number of lattice sites. The third term describes the hybridization between the itinerant and localized states, that can be local, $V_{ij}=V_0\delta_{ij}$, or nonlocal,[7,8] $V_{ij}=V(\delta_{j,i-1}-\delta_{j,i+1})$ (we assume that the crystal has inversion symmetry). The last term stands for the localized f electrons whose sharp energy level is E_f.

While the understanding of the ground-state properties of the FKM without hybridization has progressed considerably over the past decade,[9,10] the properties of the FKM with hybridization are still unclear. Even, in the existing literature on this model, different answers can be found on the fundamental question whether the nonzero hybridization can or cannot induce the insulator-metal transition. Depending on the type of methods used, both positive answers and negative answers have been found for the FKM with local hybridization. A hybridization induced insulator-metal transition has been obtained, for example, within so-called static approximation,[11] while no insulator-metal transitions are found by small-cluster exact-diagonalization calculations.[12] The same is true concerning the valence transition behavior of the model. It is well known that the FKM without hybridization shows a discontinuous valence transition as the f-level energy changes for both strong and intermediate interactions.[5] Some authors argue that this discontinuity still remains even for a small local hybridization.[13] Others, however, reported that there is no discontinuous transition in the FKM with local hybridization.[14] Only a few results are known about effects of nonlocal hybridization on ground-state properties of the FKM,[8,15] although for real systems with inversion symmetry this type of hybridization represents more realistic situation than the local hybridization.[7] Here we use the extrapolation of small-cluster exact-diagonalization calculations and the density matrix renormalization group (DMRG) method to resolve this problem. Special attention is devoted to the problem of hybridization induced insulator-metal transitions, and the behavior of the model with increasing E_f [such an analysis is very important since a parametrization of E_f with applied pressure p (Ref. 13) can, in principle, explain the behavior of the model with applied pressure].

Since the full Hilbert space of the FKM with hybridization (for given L) consists of 4^L quantum states the exact diagonalization calculations are strongly limited. Although

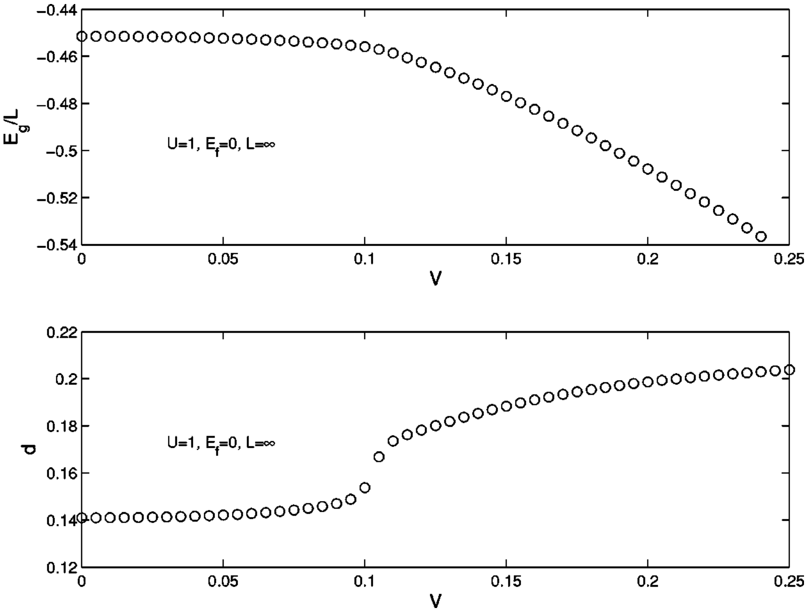

FIG. 1. The ground-state energy E_g and the density of doubly occupied sites d as functions of the nonlocal hybridization V obtained from extrapolation of small cluster exact diagonalization and DMRG results for $U=1$ and $E_f=0$.

the number of states can be reduced considerably by the use of symmetries of H, there is still a limit ($L\sim 12$) on the size of clusters that can be studied using small-cluster exact-diagonalization calculations. Therefore we combine this method with the DMRG method that allows one to treat several times larger clusters ($L\sim 60$) and still to keep the high accuracy of computations. We typically keep up to 200 states per block, although in the numerically more difficult cases, where the DMRG results converge slower, we keep up to 400 states. Truncation errors,[16] given by the sum of the density matrix eigenvalues of the discarded states, vary from 10^{-8} in the worse cases to zero in the best cases.

II. RESULTS AND DISCUSSION

To reveal effects of the nonlocal hybridization on the ground-state properties of the FKM we have started with the half-filled band case $E_f=0$ for which the nature of the ground state (at $V=0$), its energetic and structural properties are well understood at present. In this case the localized f-electrons fill up one of two sublattices of the hypercubic lattice [the charge-density-wave (CDW) state] and the corresponding ground state is insulating for all $U>0$. In Fig. 1 we present the extrapolated results (obtained from small cluster exact diagonalization and DMRG calculations) for the ground state energy of the FKM ($E_g=\langle H\rangle$) and for the density of doubly occupied sites [$d=(1/L)\Sigma_i\langle f_i^+ f_i d_i^+ d_i\rangle$]. It is seen that below some critical value of hybridization ($V_c\sim 0.1$) both quantities are almost independent of V, while in the opposite limit they strongly depend on V, indicating a phase transition at $V=V_c$.

This conjecture supports also the behavior of the f and d-electron density of states (with increasing V) presented in Fig. 2. One can easily recognize two different regimes (phases), and namely, $V<V_c$ and $V>V_c$ where the f and d electron spectra behave fully differently, however, within the given regime (phase) they exhibit qualitatively the same behavior. Analyzing spectra in these regimes, two others important statements can be made: (i) the CDW state has a dominant weight for all $V<V_c$, and (ii) the energy gap at the Fermi level is reduced with increasing hybridization indicating the insulator-metal transition.

To verify the first statement we have calculated explicitly (for $L=12$) the probabilities of all f-electron configurations by a projection of the ground-state wave function onto the subspace of states within a given equivalence class. We have found that for all $V<V_c$ the phase with the highest probability is just the CDW state. The dominant weight of the CDW state (the long-range order) for nonzero V can also be tested by calculating the Fourier transform of the f-electron density-density correlation function $S(q)$ defined by

$$S(q)=\frac{1}{L}\sum_{j,l} e^{iql}(\langle f_j^+ f_j f_{j+l}^+ f_{j+l}\rangle - \langle f_j^+ f_j\rangle\langle f_{j+l}^+ f_{j+l}\rangle). \qquad (2)$$

In the regimes of the long-range order $S(q)$ is constant and it scales linearly with L for $q=\pi$. The exhaustive numerical studies that we have performed for different finite clusters showed [see Fig. 3(a)] that below V_c the correlation function $S(q=\pi)$ is almost independent of V and it scales with the size of system L. Above this value $S(q=\pi)$ undergoes a rapid change that indicates the transition from the low hybridization ordered phase to the high hybridization homogeneous phase. This conclusion can be tested independently by calculating the f-electron site occupation $\langle f_i^+ f_i\rangle$ for different hybridization strength. Numerical results presented in Fig. 3(b) clearly demonstrate the transition from the inhomogeneous to homogeneous phase that takes place at $V\sim 0.1$.

To verify explicitly the second statement (the existence of the insulator-metal transition driven by hybridization) we have calculated the single particle excitation energy defined as $\Delta_s=E_g(L+1)+E_g(L-1)-2E_g(L)$, where $E_g(N)$ is the ground state energy for N electrons. The results of numerical calculations are displayed in Fig. 4(a). It is seen that Δ_s exhibits an unusual behavior that is apparently caused by the

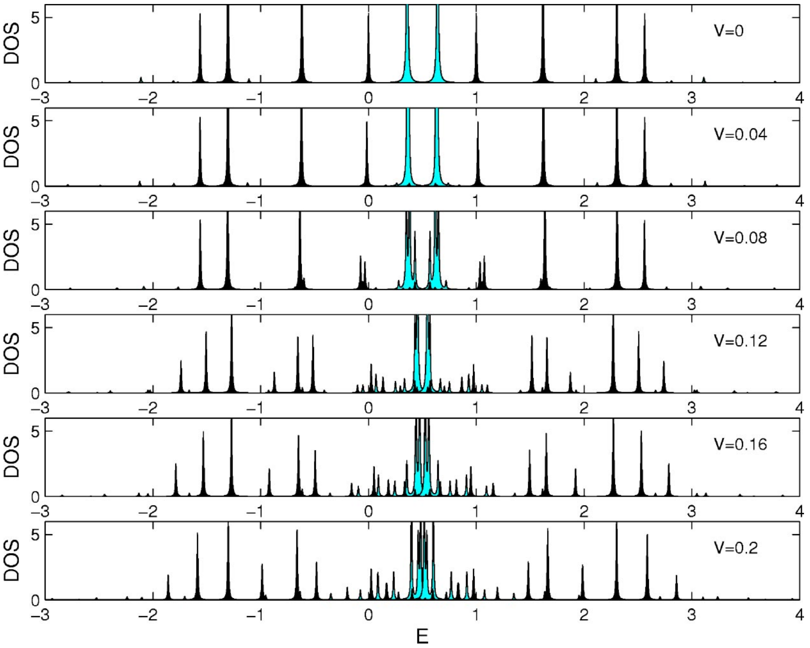

FIG. 2. (Color online) The f electron density of states (shaded regions) and the d electron density of states (black regions) of the FKM with nonlocal hybridization obtained for $U=1$, $E_f=0$ and several different values of V. The small cluster exact diagonalization results ($L=12$). The Fermi energy is located at $U/2$.

different nature of the ground state below and above V_c (the ordered and homogeneous phase). Below $V=V_c=0.103$ the single particle excitation energy is gradually reduced with increasing V. At $V=V_c$ the single particle excitation energy starts to increase rapidly, it reaches its local maximum at $V=0.107$, then continuously decreases and vanishes at $V\sim 0.2$, confirming an insulator-metal transition induced by nonlocal hybridization.

The fact that the nonlocal hybridization can induce the insulator-metal transition, even in the half-filled band case, shows how important a role the type of hybridization plays in description of ground-states properties of the FKM. Indeed, our recent studies of the FKM with local hybridization showed[12] that this type of hybridization cannot destroy the insulating ground state at half-filling (nor for small nor for large V), and even for large V this state is further stabilized (Δ_s increases). On the other hand the nonlocal hybridization is able to destroy fully the insulating ground state, even for relatively small values of V.

Moreover, the detailed analysis of the f and d-electron spectra revealed another important difference in the behavior of the FKM with local and nonlocal hybridization. While the energy gaps in the f and d-electron density of states at the Fermi level coincide ($\Delta_f=\Delta_d$) for the FKM with local hybridization,[12] the energy gaps in the FKM with nonlocal hybridization exhibit different behavior. As illustrated in Fig. 4(b) the energy gaps of the FKM with nonlocal hybridization coincide only for $V<V_c$, but they strongly differ in the op-

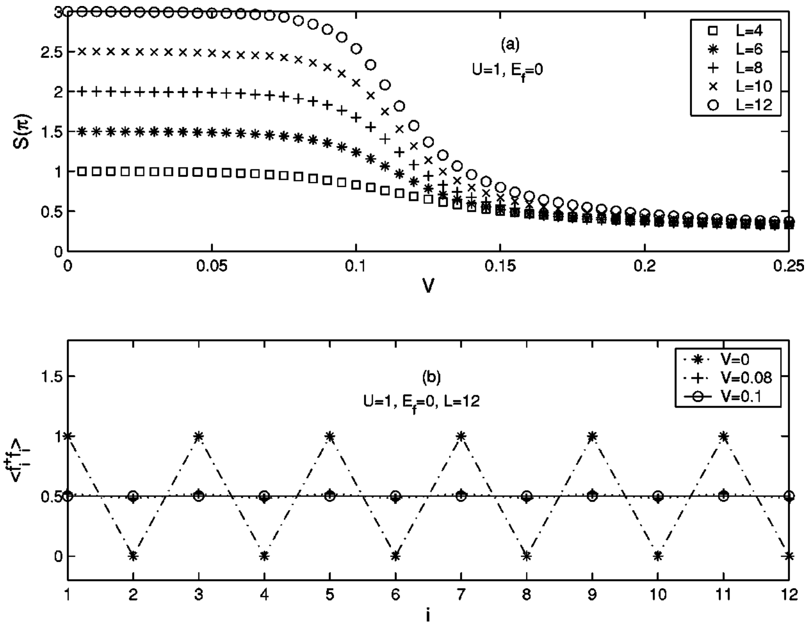

FIG. 3. (a) The Fourier transform of the f-electron density-density correlation function $S(\pi)$ as a function of nonlocal hybridization V calculated for $U=1$, $E_f=0$, and several different clusters. (b) The f-electron site occupation $\langle f_i^+ f_i\rangle$ as a function of i calculated for $U=1$, $E_f=0$, and several different values of nonlocal hybridization V.

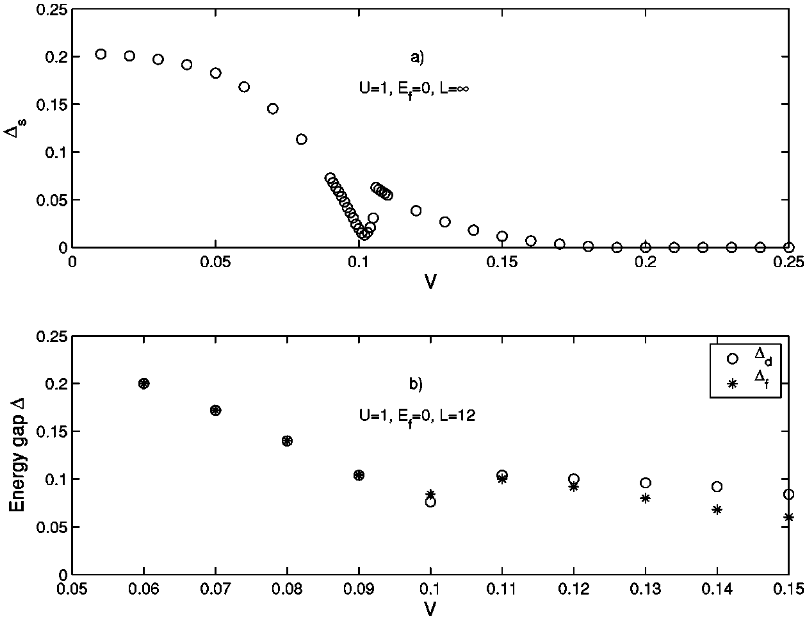

FIG. 4. (a) The single particle excitation energy Δ_s as a function of the nonlocal hybridization V obtained from extrapolation of DMRG results for $U=1$ and $E_f=0$. (b) The d-electron gap Δ_d and the f-electron gap Δ_f as functions of the nonlocal hybridization calculated from the f and d-electron density of states for $U=1$, $E_f=0$, and $L=12$. The small cluster exact diagonalization results.

posite limit. This again confirms the crucial role of hybridization (its type) in description of conducting properties of the FKM.

The strong effects of the nonlocal hybridization we have observed also for the unsymmetric case ($E_f \neq 0$). This is shown in Fig. 5(a), where the single particle excitation energy Δ_s is plotted as a function of the f-level energy E_f. It is seen that the metallic phase found for $V=0.2$ and $E_f=0$ persists up to relatively large values of $E_f(E_{fc}\sim 1.3)$, where the system undergoes the metal-insulator transition. Thus, in the pressure induced case (we remember the parametrization of E_f with applied pressure) the FKM with nonlocal hybridization can describe the metal-insulator transition driven by pressure. Furthermore, numerical computations that we have performed for $U=2$ showed that the FKM exhibits the same behavior also for larger values of U [see Fig. 5(b)]. This observation is very important from the theoretical as well as experimental point of view. Indeed, it is well-known[9] that the ground states of the FKM without hybridization (for all f-electron concentrations n_f) are insulating for Coulomb interactions $U > U_c \sim 1.2$. Thus, in the intermediate and strong coupling region the FKM can describe only one type of electronic transition observed experimentally in some rare-earth compounds,[17,18] and namely, the insulator-insulator transition driven by pressure (increasing E_f). Our results show that this deficiency of the model can be removed by including the term of nonlocal hybridization that can induce insulator-metal transitions also for stronger interactions, which is just the case of many rare-earth compounds.[17,18] For completeness we also present in Fig. 5(a) the E_f dependence of the

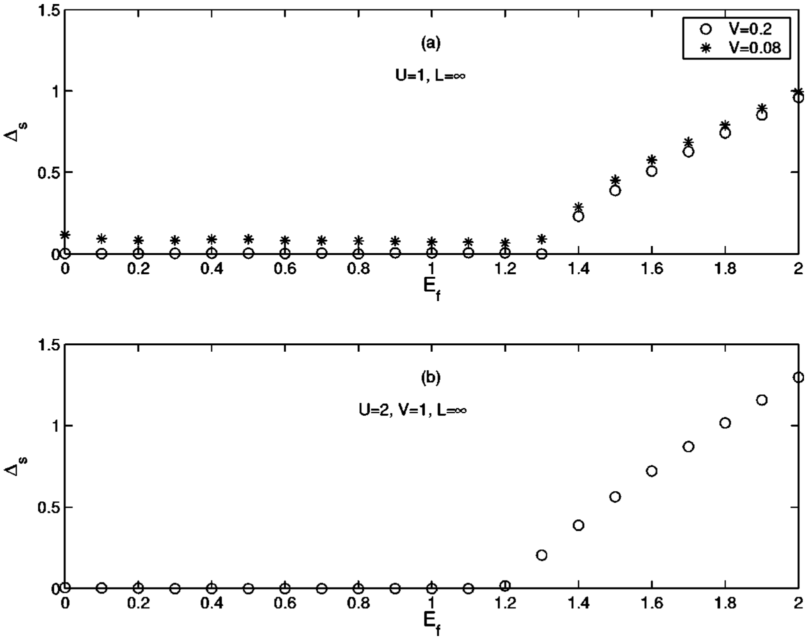

FIG. 5. The single particle excitation energy Δ_s as a function of the f-level energy E_f obtained from extrapolation of DMRG results. Case (a) corresponds to $U=1$ ($V=0.08$ and $V=0.2$) and case (b) corresponds to $U=2$ ($V=1$).

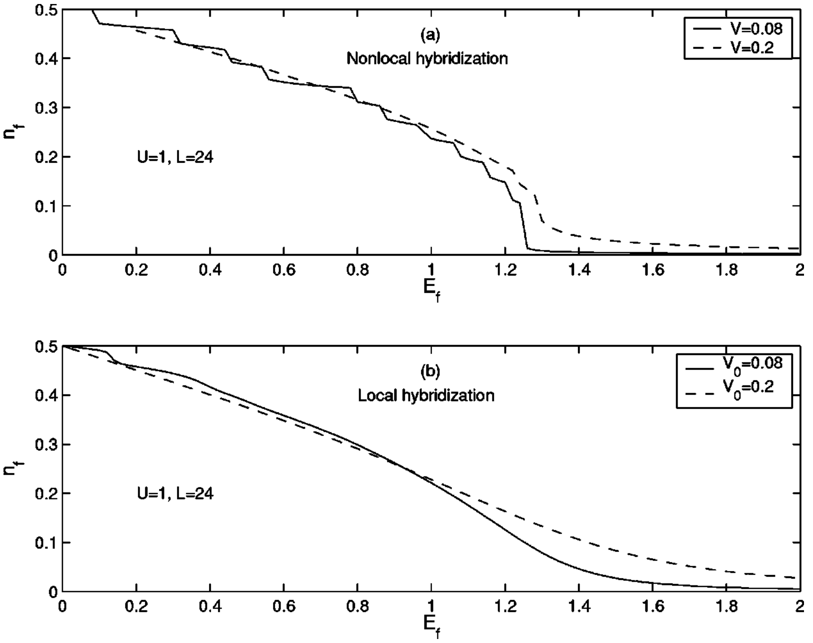

FIG. 6. Dependence of the f-electron occupation number n_f on the f-level position E_f calculated by DMRG method for two different values of nonlocal (a) and local (b) hybridization.

single particle excitation energy Δ_s for $V < V_c (V=0.08)$. In this case no insulator-metal transition driven by E_f is observed.

Finally, we have examined effects of the nonlocal hybridization V on the valence transition, i.e., the dependence of the f-electron occupation number n_f on the f-level energy E_f (pressure p) for nonzero V. The results of the DMRG calculations are summarized in Fig. 6. For a comparison we have displayed also the dependence of n_f on E_f for the local hybridization. Again one can see different effects of local and nonlocal hybridization. While already very small values of local hybridization ($V_0 \sim 0.08$) are able to destroy fully the staircase structure of the valence transition (found for zero hybridization[5]) the nonlocal hybridization has only a negligible influence on the valence transition for such small values of V. Obviously, this is a consequence of the fact discussed above, and namely, that the ground states found for $V=0$ have the dominant weight also for nonzero V (up to $V=V_c$). Above this value the nonlocal hybridization destroys the staircase structure of the valence transition similar to the local hybridization, but the n_f behavior still strongly differs (quantitatively) for these two types of hybridization.

In summary, our numerical study of the FKM with nonlocal hybridization showed that the nonlocal hybridization has strong effects on ground-state properties of the model. In particular, we have found that both the picture of insulator-metal transitions as well as the picture of valence transitions found for the FKM with nonlocal hybridization fully differ from corresponding pictures found for the FKM without hybridization (with local hybridization). The effect of nonlocal hybridization is so strong that it can induce the insulator-metal transition, even in the half-filled band case where the ground states of the FKM without hybridization are insulating for all finite Coulomb interactions. This metallic state persists also outside the half-filled band case (E_f finite) up to relative large E_f ($E_f > 1$), where the system undergoes a continuous transition to the insulating state. Thus in the pressure induced case the FKM with nonlocal hybridization can describe the metal-insulator transition, even at finite hybridization.

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[1] L.M. Falicov and J.C. Kimball, Phys. Rev. Lett. **22**, 997 (1969).
[2] J.K. Freericks and L.M. Falicov, Phys. Rev. B **41**, 2163 (1990).
[3] C. Gruber, J.L. Lebowitz, and N. Macris, Phys. Rev. B **48**, 4312 (1993); C. Gruber, D. Ueltschi, and J. Jedrzejewski, J. Stat. Phys. **76**, 125 (1994); J.K. Freericks, C. Gruber, and N. Macris, Phys. Rev. B **53**, 16189 (1996).
[4] K. Ramirez and L.M. Falicov, Phys. Rev. B **3**, 2425 (1971).
[5] P. Farkašovský, Phys. Rev. B **51**, 1507 (1995).
[6] P. Farkašovský, Phys. Rev. B **52**, R5463 (1995).
[7] G. Czycholl, Phys. Rep. **143**, 277 (1986).
[8] C.D. Batista, Phys. Rev. Lett. **89**, 166403 (2002).
[9] C. Gruber and N. Macris, Helv. Phys. Acta **69**, 851 (1996).
[10] J.K. Freericks and V. Zlatić, Rev. Mod. Phys. **75**, 1333 (2003)
[11] L. Craco, J. Phys.: Condens. Matter **13**, 263 (2001).
[12] P. Farkašovský, Phys. Rev. B **65**, 245119 (2002).
[13] M. Avignon and S.K. Ghatak, Solid State Commun. **16**, 1243

(1975); C.E.T. Goncalves da Silva and L.M. Falicov, *ibid.* **17**, 1521 (1975); K. Kanda, K. Machida, and T. Matsubara, *ibid.* **19**, 651 (1976); A. Giesekus and L.M. Falicov, Phys. Rev. B **44**, 10449 (1991).

[14] H.J. Leder, Solid State Commun. **27**, 579 (1978); E. Baeck and G. Czycholl, *ibid.* **43**, 89 (1982).

[15] T. Portengen, T. Östreich, and L.J. Sham, Phys. Rev. Lett. **76**, 3384 (1996).

[16] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993).

[17] A. Jayaraman, in *Handbook on the Physics and Chemistry of Rare Earth*, edited by K.A. Gschneider and L.R. Eyring (North-Holland, Amsterdam, 1979), Vol. 2.

[18] P. Wachter, in *Handbook on the Physics and Chemistry of Rare Earth*, edited by K.A. Gschneider and L.R. Eyring (North-Holland, Amsterdam, 1994), Vol. 19.