THE SPECTRAL PROPERTIES OF THE FALICOV–KIMBALL MODEL IN THE WEAK-COUPLING LIMIT

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The \( f \) and \( d \) electron density of states of the one-dimensional Falicov–Kimball model are studied in the weak-coupling limit by exact diagonalization calculations. The resultant behaviors are used to examine the \( d \) electron gap \( (\Delta_d) \), the \( f \) electron gap \( (\Delta_f) \), and the \( fd \) electron gap \( (\Delta_{fd}) \) as functions of the \( f \) level energy \( E_f \) and hybridization \( V \). It is shown that the spinless Falicov–Kimball model behaves fully differently for zero and finite hybridization between \( f \) and \( d \) states. At zero hybridization the energy gaps do not coincide \( (\Delta_d \neq \Delta_f \neq \Delta_{fd}) \), and the activation gap \( \Delta_{fd} \) vanishes discontinuously at some critical value of the \( f \) level energy \( E_{fc} \). On the other hand, at finite hybridization all energy gaps coincide and vanish continuously at the insulator-metal transition point \( E_f = E_{fc} \). The importance of these results for a description of real materials is discussed.

Keywords: Falicov–Kimball model; valence transitions; metal-insulator transitions.

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1. Introduction

Since its introduction in 1969 the Falicov–Kimball model (FKM) has become 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\(^4\). It is the latter language that we shall use here, considering a system of localized \( f \) electrons and itinerant \( d \) electrons coupled via the local interaction \( U \) and hybridization \( V \). The Hamiltonian of the spinless FKM is

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H = \sum_{ij} t_{ij} d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i + V \sum_i d_i^+ f_i + \text{h.c.},
\]

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 (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 $n_d = \frac{1}{L} \sum_i d_i^+ d_i$ and the localized $f$ electrons with density $n_f = \frac{1}{L} \sum_i f_i^+ f_i$, where $L$ is the number of lattice sites. The third term stands for the localized $f$ electrons whose sharp energy level is $E_f$. The last term represents the hybridization between the itinerant and localized states.

In this paper we perform exhaustive numerical studies of the spectral properties of the FKM with and without hybridization. While the static properties of the FKM are well understood at present\textsuperscript{5,6} (including the picture of valence transitions), the dynamical properties of the model are still unclear. Even then the spectral properties of the $f$ electrons are not satisfactorily understood, not even for $V = 0$, where only a few exact results are known for the infinite-dimensional systems.\textsuperscript{7,8} No exact results are known for nonzero hybridization and for $T = 0$, with the exception of numerical results obtained on very small clusters.\textsuperscript{9} The first systematic study of dynamical properties of the FKM with hybridization has been performed recently by Craco\textsuperscript{10} within the so called static approximation. He studied the model in the strong-coupling limit (large $U$) and found that the system is insulating for small values of hybridization (the size of the $f$ and $d$ electron gap coincides, including the case $V = 0$) and with increasing $V$ an insulator-metal transition takes place at some critical value of $V = V_c$. In our preceding paper we re-examined these strong-coupling results by exact-diagonalization calculations and obtained entirely different conclusions.\textsuperscript{11} In particular, we have found that for zero hybridization the gaps in the $f$ and $d$ electron density of states do not coincide, and almost all $f$ electron spectral weight is located outside the $d$ electron subbands. For nonzero hybridization, the $f$ and $d$ electron gaps coincide for both the symmetric and unsymmetric case but no insulator-metal transition driven by hybridization is observed in one as well as in two dimensions.

In this contribution we extend numerical calculations to the opposite limit (the weak-coupling limit). From this point of view the paper represents the first systematic (exact) study of dynamical properties of the FKM in the weak-coupling limit. Here, special attention is devoted to the behavior of the $f$ and $d$ electron density of states with increasing $E_f$. Such an analysis is very important since a parametrization of $E_f$ with applied pressure\textsuperscript{12} $P$ can, in principle, provide an interpretation of some experimental data, e.g. the behavior of the activation gap (the gap between the occupied and unoccupied states) with increasing $P$. In our previous paper\textsuperscript{6} the problem of pressure dependence of the activation gap was analyzed through the behavior of the energy gap in the $d$ electron spectrum of the FKM and many similarities with the experimental data on the valence fluctuating compound SmB$_6$ were found. These similarities are however only qualitative, since in
the correct analysis one should also take into account the behavior of the $f$ electron spectral functions. This was done by Park and Hong\textsuperscript{9} and a nice correspondence of theoretical and experimental results has been obtained. Unfortunately, these results have been obtained on a very small cluster (consisting of only eight sites) and thus cannot be considered as definite. Here we re-examine the behavior of the activation gap in the FKM for both $V = 0$ and $V > 0$. At zero hybridization we are able to present results on relatively large clusters for both the $d$ and $f$ electron density of states, and thus our results can be extrapolated satisfactorily to the thermodynamic limit. For nonzero hybridization we were able to perform small-cluster exact-diagonalization calculations on lattices only slightly larger than those used by Park and Hong\textsuperscript{9} ($L \sim 12$), however a fundamental different behavior of the model is observed already on such small clusters.

**Fig. 1.** The $f$ and $d$ electron density of states of the FKM obtained for $V = 0, U = 0.6$ at several different values of $E_f$. The results for the $f$ electron density of states are plotted for $L = 24$, while the results for the $d$ electron density of states are plotted for $L = 64000$. The corresponding $f$ electron concentrations are: \( n_f = 0.5 \) for $E_f = 0$, \( n_f = 4/10 \) for $E_f = 0.5$, \( n_f = 1/3 \) for $E_f = 0.8$, and \( n_f = 1/4 \) for $E_f = 1.2$. 

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\textsuperscript{9}Park and Hong.
Fig. 2. The $f$ electron density of states of the FKM obtained for $V = 0, U = 0.6$ at two different values of $L$ and $E_f$.

2. Results and Discussion

Let us start the discussion of our results with the case $V = 0$. In Fig. 1 we present numerical results for the $d$ and $f$ electron density of states obtained for $U = 0.6$ and several values of the $f$ level energy $E_f$. Since the ground state configurations of the FKM in the weak coupling limit are well-known ($6,13$) (the most homogeneous (insulating) configurations for $|E_f| < E_{fc} \approx 1.34$, and the phase separated (metallic) configurations for $|E_f| \geq E_{fc}$), the $d$-electron density of states can be calculated directly from the single particle spectrum of the FKM model for $V = 0$. For the periodic configurations this can be done analytically in the thermodynamic limit ($14$) and for an arbitrary $f$ electron concentration a numerical diagonalization is possible on very large clusters ($L = 64000$). Unlike this case, the $f$ electron density of states has to be calculated by exact diagonalization calculations (Lanczos method $15$), thereby the cluster sizes are strongly limited ($L \leq 24$). To minimize the finite-size effects on the $f$ electron spectra we have performed numerical calculations for several cluster sizes at each value of $E_f$. The typical behaviors are shown in Fig. 2 for two selected values of $E_f$. It is seen that finite-size effects are small and thus the results obtained for $L = 24$ can be used satisfactorily to represent the behavior of large systems. Although we have used in the numerical calculations the relatively large value of $\epsilon = 0.01$ for the resolution ($16$) the formation of the gap in the $f$ electron density of states at the Fermi level (in all examined cases the Fermi level is located between the first and the second peak) is apparent. It is also apparent that the gaps in the
$d$ and $f$ electron spectra do not coincide. Moreover, one can see (in accordance with results obtained in the strong-coupling limit\cite{11}) that practically all $f$ electron spectral weight is located inside the principal $d$ electron gap (the gap at the Fermi energy). With increasing $E_f$ both the principal gap as well as the $f$ electron spectrum shift to higher energies. Since the finite size effects on the $f$ electron spectra are negligible for the cluster sizes used in our numerical calculations ($L = 24$), and even the $d$ electron spectra can be obtained exactly on much larger clusters, one can try to construct the $E_f$ dependence of all relevant energy gaps. In particular, we have calculated the $d$ electron gap $\Delta_d$ (the gap in the $d$ electron spectrum at the Fermi energy), the $f$ electron gap $\Delta_f$ (the gap in the $f$ electron spectrum at the Fermi energy), and the $fd$ electron gap $\Delta_{fd}$ (the gap between the occupied $f$ subband and the empty $d$ subband (the activation gap). To obtain the $d$ electron gap $\Delta_d$ it is sufficient to know the $f$ electron distribution that minimizes the ground-state energy of the FKM for some given $E_f$ and $U$. As mentioned above, the ground-state configurations of the FKM in the weak-coupling limit are the most homogeneous configurations for $|E_f| < E_{fc}$, and the phase separated configurations for $|E_f| \geq E_{fc}$. While the most homogeneous distribution of $f$ electrons can be easily generated for arbitrary $E_f(n_f)$, the $f$ electron distribution in the phase separated configuration has to be determined numerically. This distribution can be found in principle exactly, as shown in Ref. 6, or approximately, as done in Ref. 13. Here we adopt the latter method, since it allows us to treat clusters ($L \sim 300$) which

![Graph](image.png)

Fig. 3. The $d$ electron gap $\Delta_d$, the $f$ electron gap $\Delta_f$, the $fd$ electron gap $\Delta_{fd}$, and the $d$ electron concentration $n_d$ as functions of the $f$ level energy $E_f$ calculated for $V = 0$ and $U = 0.6$. The solid lines are guides to the eye.
are several times larger and still to keep the high accuracy of computations. The results of numerical calculations for $\Delta_d$ obtained using this method on the cluster consisting of 240 sites are presented in Fig. 3. It is seen that $E_f$ dependence of the $d$ electron gap qualitatively mimics the pressure dependence of the activation gap in SmB$_6$ (we note a parametrization of $E_f$ with pressure). With increasing pressure (the $f$ level position $E_f$), the gap decreases and vanishes discontinuously at some critical pressure $P_c$ ($E_{fc}$). The finite-size scaling analysis that we have performed for a wide range of $L$ values ($L = 40, 60, \ldots, 240$) showed that $\Delta_d$ is practically independent of $L$ for all $|E_f| < E_{fc}$. On the other hand the same analysis performed for $|E_f| \geq E_{fc}$ revealed that the finite-size effects are still present in this region, but a disappearance of $\Delta_d$ can be satisfactorily confirmed by the extrapolation of results obtained for different $L$.

To determine the $E_f$ dependence of the $f$ electron gap $\Delta_f$ and the $fd$ electron gap $\Delta_{fd}$ we have performed exhaustive numerical studies of the $f$ electron density of states for a wide range of $E_f$ values. In particular, we have calculated the $f$ electron density of states for each $E_f$ from the interval $[0, 1.4]$ with the step $\Delta E_f = 0.05$, and with the step $\Delta E_f = 0.01$ for $E_f$ near the point of the insulator-metal transition. To reveal the finite-size effects on $\Delta_{fd}$ and $\Delta_f$ the calculations have been done for several cluster-sizes ($L = 12, 16, 20, 24$) at each $E_f$. It was found that finite-size effects on $\Delta_f$ and $\Delta_{fd}$ are negligible for $|E_f| < E_{fc}$, while small finite-size effects have been observed for $E_f > E_{fc}$. The resultant $E_f$ dependence of $\Delta_f$ and $\Delta_{fd}$ is presented in Fig. 3. It is seen that $\Delta_{fd}$ exhibits the same behavior as $\Delta_d$, of course with one exception, namely that $\Delta_{df} \sim \Delta_d/2$. Since $\Delta_{fd}$ is the gap between the occupied ($f$) and unoccupied ($d$) states (the activation gap) its behavior can be directly compared with the behavior of the activation gap in SmB$_6$. Although data for $\Delta_{fd}$ are more scattered, both activation gaps exhibit qualitatively the same behavior. This indicates that the spinless FKM, probably the simplest model of correlated electrons can, in principle, provide the correct physics for describing properties of real materials.

Let us now examine what happens if the hybridization is switched on. One could expect that just the hybridization will improve the accordance between the theoretical and experimental results for the activation gaps, since the hybridization generally smears behaviors. This conjecture also support results by Park and Hong, obtained for the FKM with hybridization on a very small cluster consisting of only eight sites. Their results obtained for the $E_f$ dependence of the activation gap and the $d$ electron concentration $n_d$ are summarized in Fig. 4. One can see a nice correspondence of theoretical and experimental data for both the activation gap as well as the $d$ electron concentration. Unfortunately, these results have been obtained on a very small cluster and so cannot be considered as definite. The actual behavior of the activation gap and the $d$ electron concentration $n_d$ on large lattices can be entirely different from one presented in Fig. 4. Indeed, a comparison of their results obtained for $n_d$ at $V = 0$ with our results presented in Fig. 3(b) reveals entirely different behavior of $n_d$. While $n_d$ calculated by Park and Hong for $L = 8$ is
constant for all values of $E_f$ from $E_f = 0.8$ to the insulator-metal transition point $E_{fc} = 1.34$, our results calculated on much larger clusters ($L = 240$) exhibit strong dependence on $E_f$. In the following we re-examine exactly the behavior of the FKM with hybridization on the cluster consisting of eight sites, as well as on slightly larger clusters ($L = 10, 12$). We present new results that significantly improve the findings obtained by Park and Hong.\textsuperscript{9}

To show the hybridization effects on $\Delta_d$, $\Delta_f$ and $\Delta_{fd}$ we have calculated exactly the $f$ and $d$ electron density of states for $V = 0$ and $V = 0.02$ on a small finite cluster consisting of $L = 8$ sites. We chose this cluster size to be compatible with the results of Park and Hong.\textsuperscript{9} The resultant behaviors are presented in Fig. 5. The most prominent difference between the results obtained for $V = 0$ and $V = 0.02$ is that a nonzero spectral weight appeared in the $d$ electron density of states at the Fermi level for finite hybridization. Of course, this fact will change dramatically the picture discussed above for $V = 0$. This is clearly demonstrated in Fig. 6(a), where the $E_f$ dependence of $\Delta_d$, $\Delta_f$ and $\Delta_{fd}$ is displayed for $V = 0.02$ and $L = 8$. It can be seen that all gaps coincide for nonzero $V$, which strongly contradicts the case of $V = 0$. For a comparison we have also displayed in Fig. 6(a) the behavior of 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. As one could expect (on the base of the strong-coupling results\textsuperscript{11}) the single particle excitation energy $\Delta_s$
Fig. 5. The $f$ and $d$ electron density of states of the FKM obtained for $U = 0.6, E_f = 1.2, L = 8$ at two different values of $V$. The arrow denotes the most prominent difference between the results obtained for $V = 0$ and $V = 0.02$.

Fig. 6. (a) The $d$ electron gap $\Delta_d$, the $f$ electron gap $\Delta_f$, the $fd$ electron gap $\Delta_{fd}$, and the single particle excitation energy $\Delta_s$ as functions of the $f$ level energy $E_f$ calculated for $V = 0.02, L = 8$ and $U = 0.6$. (b) The single particle excitation energy $\Delta_s$ as a function of the $f$ level energy $E_f$ calculated by DMRG method for the same values of $V$ and $U$. The solid and dashed lines are guides to the eye.
Fig. 7. The $f$ and $d$ electron density of states of the FKM obtained for $V = 0, U = 0.6$ and several different values of $E_f$. The results for the $f$ electron density of states are plotted for $L = 24$, while ones for the $d$ electron density of states are plotted for $L = 64000$. In all cases the $f$ electron concentration is equal to $n_f = 0.5$. To see clearly the $f$ electron gap, the $f$ electron density of states has been plotted with high resolution ($\epsilon = 0.001$).

coincides with $\Delta_d$, $\Delta_f$ and $\Delta_{fd}$ for nonzero hybridization. This result is very important from the numerical point of view since the single particle excitation energy can be calculated easily by other methods [that allow one to treat much larger clusters, e.g. the density matrix renormalization group method (DMRG)], and so it can be used satisfactorily for describing conducting properties of the model. As one can see from Fig. 6(a) the conducting properties of the FKM with hybridization are described very inaccurately within the small-cluster exact-diagonalization calculations. In the region where the metallic phase has been identified for $V = 0$, the single particle excitation energy increases and it is not clear if this is a consequence of finite hybridization or finite-size effects. Since calculations performed for $L = 10$ and $L = 12$ revealed relatively large finite-size effects we have decided to use DMRG method to verify the actual behavior of $\Delta_s$. In comparison to exact diagonalization calculations the DMRG method allows one to treat clusters which is several times larger ($L \sim 50$) and still to keep the high accuracy of computations. We typically keep up to 128 states per block, although in the numerically more difficult cases, where the DMRG results converge slower, we keep up to 400 states. Truncation errors, 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. The typical behavior of $\Delta_s$ is displayed in Fig. 6(b) for two finite clusters of $L = 32$ and $L = 36$ sites.
Although the finite-size effects are still present for cluster sizes treated by DMRG method the metallic region seems to be satisfactorily verified also for nonzero hybridization. However, there is one important difference between the case $V = 0$ and the case $V = 0.02$. Even though $V = 0$ both $\Delta_d$ and $\Delta_{fd}$ vanish discontinuously, they seem to vanish continuously for nonzero hybridization. This indicates that the spinless FKM behaves entirely differently for zero and non-zero hybridization, and so are the corresponding pictures of insulator-metal transitions. Since rare-earth compounds exhibit both types of insulator-metal transitions (discontinuous as well as continuous) their different behavior under the external pressure can be interpreted as a direct consequence of the absence (presence) of hybridization in a given material. According to this conjecture, e.g. SmB$_6$, that exhibits a discontinuous pressure-induced insulator-metal transition, should be a material with zero hybridization between $d$ and $f$ states. Indeed, SmB$_6$ is the highest symmetry of the $O_h$ point group and the on-site hybridization between $d$ and $f$ states is forbidden by inversion symmetry. This confirms that the spinless FKM, in spite of its relatively simplicity, can yield the correct physics in describing real materials (e.g. SmB$_6$). Besides a qualitative correspondence between the theoretical and experimental data for the activation gap, we can state another example that supports this conclusion. In Fig. 7 we have displayed in detail the $d$ and $f$ electron density of states near the Fermi level for several values of $E_f$ ($E_f = 0, 0.1, 0.2$). For this set of $E_f$ values the ground state is characterized by $n_f = 0.5$ which models very well the situation in SmB$_6$ at low temperatures. This electronic structure consisting of two wide and two narrow subbands strongly mimics the electronic structure that we have proposed several years ago for a description of low temperature resistivity data of SmB$_6$. The analysis of these data showed that they can be explained by introducing a fine structure (consisting of two narrow bands) into the principal gap, in accordance with our results presented in Fig. 7. Of course, all these comparisons are only qualitative since our results have been obtained for the one-dimensional system at $T = 0$, while the real experimental systems are three-dimensional and measurements are done at finite temperatures. In future work, we plan to perform a similar analysis in higher dimensions and $T \neq 0$. Moreover, we also want to examine the influence of other factors (the electron-phonon interaction, the orbital dynamics, etc.) that have been neglected in this version of the model.

In summary, the $f$ and $d$ electron density of states of the spinless Falicov–Kimball model were studied in the weak-coupling limit by exact diagonalization calculations. The resultant behaviors were used to examine the $d$ electron gap $\Delta_d$, the $f$ electron gap $\Delta_f$, and the $fd$ electron gap $\Delta_{fd}$ as functions of the $f$ level energy $E_f$ and hybridization $V$. It was shown that the spinless Falicov–Kimball model behaves completely differently for zero and finite hybridization between $f$ and $d$ states. At zero hybridization the energy gaps do not coincide ($\Delta_d \neq \Delta_f \neq \Delta_{fd}$), and the activation gap $\Delta_{fd}$ vanishes discontinuously at some critical value of the $f$ level energy $E_{fc}$. In all examined cases practically all $f$ electron spectral weight is located outside the $d$ electron subbands. On the other hand, at finite hybridization
all energy gaps coincide and vanish continuously at the insulator-metal transition point \( E_f = E_{fc} \). The results obtained are compared with experimental behaviors observed in SmB₆.

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References

16. \( \epsilon \) is a small (real) number introduced in the calculation of spectral properties to shift the poles of the Green's function into the complex plane (see Ref. 14 for details).