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Functional Integral Approach to the Falicov-Kimball Model

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Using the functional integral method of Hubbard-Stratonovich, we have studied the existence of first order phase transitions in the Falicov-Kimball model.
By means of two different approximation we have obtained results at variance. The first approximation, that we called uniform, is like a mean field one; and the second, a selfconsistent one, is similar to the coherent potential approximation.

Introduction

In order to describe the metal-insulator transitions observed in many transition metal oxides and rare earth compounds, Falicov and Kimball [1] have proposed a simple theoretical model, which has also been used to study the α-γ transition in metallic Ce [2, 3] and the semiconductor-metal transition in Samarium monochalcogenides [4]. In these cases, there are no changes in crystalline symmetry structure or magnetic order at the transition. The complications arising from such changes were not been included in the original model, which – within the rigid band approximation – allows to describe different situations according to the value of the model parameters. Thus, it is possible to describe systems which remain insulating or metallic at all temperatures, or that change from one phase to the other either continually or abruptly.

The existence of first-order-phase-transition has been challenged by Plischke [5] who has investigated the model by means of the coherent-potential-approximation (CPA). Goncalvez da Silva and Falicov [6] have made similar calculations for a different electronic density of states, obtaining results at variance with Plischke. Also Ghosh [7] has made an approximation similar to the CPA, obtaining results in agreement with Plischke.

In this work we have analyzed the existence of the first order phase transition by studying the model within the functional integral method, which in the context of statistical mechanics was introduced by Stratonovich and Hubbard [8], and has been extensively used to study the Anderson and Hubbard models [9, 10]. We have worked in the so called static approximation [9], in which the auxiliary fields are time independent. It can be shown that the partition function thus obtained reduces to the correct one in two limiting cases: zero bandwidth and zero interaction.

Within such scheme we have worked out two different approaches: the first one, that we call uniform approximation, is a kind of mean-field scheme; and secondly a selfconsistent approximation, analogous to the CPA. In what follows we present the functional integral scheme, the above referred approximations and a discussion of the results.

Functional Integral Scheme

We start from the following model Hamiltonian [2]

$$H=\sum_{k,\sigma}\varepsilon_{k\sigma}C^+_{k\sigma}C_{k\sigma}+\sum_{i,M}E_M b^+_{iM}b_{iM}$$
$$+U\sum_{i,M>M'}b^+_{iM'}b_{iM'}b^+_{iM}b_{iM}$$
$$+G\sum_{i,M,\sigma}b^+_{iM}b_{iM}C^+_{i\sigma}C_{i\sigma} \quad (1)$$

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where $C_{k\sigma}^+(C_{k\sigma})$ creates (annihilates) an electron in the band state with momentum "k" spin σ, energy $\varepsilon_{k\sigma}$, and $b_{iM}^+(b_{iM})$ creates (annihilates) an electron in the atomic shell of the atom at site i, spin projection M, and energy E_M. The third term corresponds to the Coulomb repulsion between localized electrons in the same atomic shell (we considered only one, and in the following we assume the limit $U\to\infty$, or in other words that we excluded configurations with more than one localized electron per site). The last term describes the localized-conduction quasiparticle interaction, G being the interaction parameter (we have assumed that such interactions are of short range, so that only intra-atomic terms need to be considered). The $C_{i\sigma}^+(C_{i\sigma})$ are Wannier creation (annihilation) operators corresponding to the band states, i.e.:

$$C_{j\sigma}^+=(1/\sqrt{N})\sum_k C_{k\sigma}^+\exp(ikR_j),$$

where N is the number of sites.

In order to apply the functional integral approach, we must write the last term in the following way.

$$H_1=-\frac{G}{4}\sum_i\{(n_i^{(l)}-n_i^{(c)})^2-(n_i^{(l)}+n_i^{(c)})^2\} \tag{2}$$

where $n_i^{(l)}=\sum_M b_{iM}^+ b_{iM}$, $n_i^{(c)}=\sum_\sigma C_{i\sigma}^+ C_{i\sigma}$.

A straightforward application of the Stratonovich-Hubbard method [8] gives the partition function Z as a multiple-functional integral

$$Z=\int\prod_i D\xi_i D\eta_i e^{-\beta\Omega(\xi,\eta)} \tag{3}$$

with

$$e^{-\beta\Omega(\xi,\eta)}=\operatorname{tr} Te^{-\beta\int_0^1\tilde{H}(\xi,\eta)d\tau}$$

where T is the time ordering operator, and

$$\tilde{H}(\xi,\eta)=\frac{\pi}{\beta}\sum_i\{\xi_i(\tau)^2+\eta_i(\tau)^2\}+\sum_{i,j,\sigma}\tilde{t}_{ij}^\sigma C_{i\sigma}^+ C_{j\sigma}^+$$
$$+\sum_{i,M}\tilde{E}_{iM}b_{iM}^+ b_{iM}+U\sum_{i,M>M'}n_{iM}n_{iM'} \tag{4}$$

$$\tilde{t}_{ij}^\sigma=t_{ij}^\sigma+\delta_{ij}\frac{C}{\beta}[\xi_i(\tau)-i\eta_i(\tau)];$$

$$t_{ij}^\sigma=\frac{1}{N}\sum_k\varepsilon_{k\sigma}e^{-ik(R_i-R_j)}$$

$$\tilde{E}_{iM}=E_M-\frac{C}{\beta}[\xi_i(\tau)+i\eta_i(\tau)];\quad C=\sqrt{\pi\beta G}.$$

We have thus reduced the partition function Z to an average of one-electron partition functions under the influence of two kinds of stochastic fields ξ_i and η_i. The field ξ_i is coupled to the difference between the occupation of localized and band states at site "i", while the field η_i is coupled to the total occupation at site "i". Following previous authors [9, 11], we treat the field η in the "stationary-point-approximation", that is: in $\tilde{H}(\xi,\eta)$ we take the value of $\eta_i(\tau)$ that makes it stationary

$$\frac{\partial\tilde{H}(\xi,\eta)}{\partial\eta_i(\tau)}=\frac{2\pi}{\beta}\eta_i(\tau)-i\frac{C}{\beta}[n_i^{(l)}(\tau)+n_i^{(c)}(\tau)]=0$$

$$\eta_i(\tau)=\frac{iC}{2\pi}[n_i^{(l)}(\tau)+n_i^{(c)}(\tau)].$$

At this point we fix the number of electrons per site. If we take $n_i^{(l)}+n_i^{(c)}=1$ (one electron per site), then:

$$\eta_i(\tau)=\eta_0=iC/2\pi. \tag{5}$$

Replacing this value for $\eta_i(\tau)$, we have:

$$\tilde{H}(\xi,\eta_0)=\frac{\pi}{\beta}\sum_i\xi_i(\tau)^2+\sum_{i,j,\sigma}\tilde{t}_{ij}^\sigma C_{i\sigma}^+ C_{j\sigma}$$
$$+\sum_{i,M}\tilde{E}_{iM}b_{iM}^+ b_{iM}+U\sum_{i,M>M'}n_{iM}n_{iM'}-\frac{NG}{4} \tag{6}$$

where $\tilde{t}_{ij}^\sigma=t_{ij}^\sigma+\delta_{ij}\left(\frac{c}{\beta}\xi_i(\tau)+\frac{G}{2}\right)$

$$\tilde{E}_{iM}=E_M+\frac{G}{2}-\frac{C}{\beta}\xi_i(\tau).$$

Going over to Fourier transforms on τ and using the fact that $\xi_i(\tau)$ is real, it is possible to write

$$\xi_i(\tau)=\sum_{\nu=-\infty}^{\infty}\xi_{i\nu}e^{-i\Omega_\nu\tau},\qquad \Omega_\nu=2\pi\nu \tag{7}$$

$$\xi_{i\nu}=\xi_{i-\nu}^*$$

and thus obtain the partition function in terms of the Fourier transformed fields.

In the very well known 'static approximation' we neglect the temporal dependence of ξ_i, or conversely all frequencies Ω_ν with $\nu\neq 0$. In this case the partition function further reduces to

$$Z=\int\prod_i d\xi_{i0}\,e^{-\pi\sum_i|\xi_{i0}|^2}\operatorname{Tr}e^{-\beta H(\xi)} \tag{8a}$$

with $H(\xi)$ given by (6), but replacing $\xi_i(\tau)$ by ξ_{i0}.

Although expression (8a) is notably simpler than the starting (3), we must resort to further approximations in order to get some results.

The first one, in the spirit of a mean-field-scheme, is 'The Uniform Approximation', which allows us to obtain results that resemble the rigid-band-approximation employed by Falicov and Kimball. The second one, 'The Self-Consistent-Approximation' is analogous to the Coherent Potential Approximation (CPA) [12].

The Uniform Approximation

This approximation consists of reducing the integral in (8a) over the complete ξ-space to another along a special path. This path corresponds to the "long-correlation-limit" between different sites, and is given by the line $\xi_i=\xi$ for all "i". In this case expression (8a) reduces to

$$Z=\int d\xi\, e^{-\pi N\xi^2}\operatorname{tr} e^{-\beta H(\xi)} \tag{8b}$$

Since the two parts of the Hamiltonian $H(\xi)$ (corresponding to conduction and localized states) commute with each other and both of them are diagonal (the first in the k-representation, and the second in the site-representation), we obtain (remind we assumed the limit $U\to\infty$):

$$Z=\int d\xi\, e^{-\beta N F(\xi)} \tag{9}$$

$$\begin{aligned}\beta F(\xi)=&\pi\xi^2-\sum_{\sigma}\int_{-\infty}^{\infty} d\varepsilon_\sigma\,\rho(\varepsilon_\sigma)\\ &\cdot\ln\{1+\exp[-\beta(\varepsilon_\sigma(\xi)-\mu)]\}\\ &-\ln\{1+\sum_M\exp[-\beta(E_M(\xi)-\mu)]\}-\beta\frac{G}{4},\end{aligned} \tag{10}$$

where $\varepsilon_\sigma(\xi)=\varepsilon_\sigma+G/2+C\xi/\beta$, $E_M(\xi)=E_M+G/2-\varepsilon\xi/\beta$, μ is the Fermi energy, and $\rho(\varepsilon)$ is the density of states of the unperturbed conduction band.

As an example, the expression of the magnetic susceptibility is given by

$$\chi=\frac{N}{3k_BT}\mu_B^2\{g_c^2\langle n_c(\xi)^2\rangle+g_L^2\langle n_L(\xi)\rangle\},$$

where g_c and g_L are the effective magneton number times the Landé factor for the conduction and localized states respectively, μ_B is the Bohr magneton, and

$$\langle n_L(\xi)\rangle=\frac{Q_L}{Z}\int d\xi\frac{e^{-\beta NF(\xi)}}{\{1+Q_L^{-1}\exp[-\beta(E(\xi)-\mu)]\}}.$$

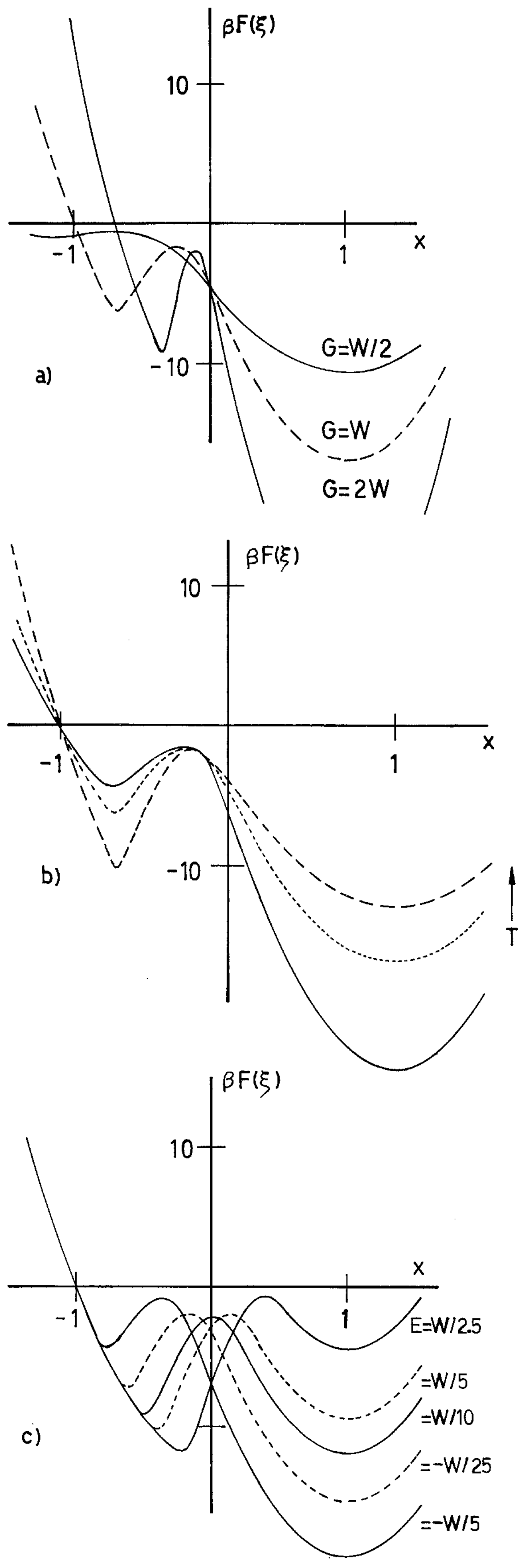

Fig. 1a–c. The curves corresponds to the free energy, given by the Eq. (10), as a function of $x=2\pi\xi/C$, for different physical situations. The interaction parameter G and the energy of the localized level E are given in unities of the band-width energy W. A constant density for the conduction states is assumed. **a** Different values of G, $E=-W/10$ and constant temperature. **b** Variation with temperature for $G=W$ and $E=-W/10$. **c** Dependence on the localized level's position (for instance it could be varied applying pressure), for constant temperature and $G=W$

Q_L is the multiplicity of the level. A similar expression holds for $\langle n_c(\xi)^2\rangle$. If we assume a Pauli behaviour for the contribution of the conduction states, the expression for the magnetic susceptibility results to be equivalent to the one obtained by Ramirez and Falicov [3].
Even though it is possible to obtain the full phase diagram, such calculation is out of the scope of this work. Nevertheless, we can reach some conclusions about the possibility of first order phase transitions by analyzing the free-energy (10) for different values of the physical parameters. In Fig. 1 we show three sets of curves of the free energy as a function of ξ. It is apparent that by varying the temperature or the position of the localized level it is possible to find first-order phase-transitions. This is a consequence of the abrupt change that the relevant point of integration suffers (for instance in a steepest descent method), under such variations.

Self-Consistent Approximation

From the point of view of the conduction states, the problem defined by (8) is analogous to those considered for disordered systems. At each lattice site "i" we have a static stochastic field ξ_i, and we must perform an average over such fields. To perform the averaging we use a scheme similar to the CPA, in whose derivation we have followed the analysis of Weller [11] for the Hubbard model.
We rewrite (8) as:

$$Z=\int\prod_i d\xi_i\, e^{-\beta\Omega(\xi_i)} \tag{8c}$$

and

$$\beta\Omega(\xi_i)=\pi\sum_i \xi_i^2 - \int_{-\infty}^{\infty} d\omega\,\rho(\omega,\xi_i)\ln\left[1+e^{-\beta(\omega-\mu)}\right]-\frac{\beta NG}{4} \tag{11}$$

The density of states $\rho(\omega,\xi_i)$ is given by

$$\rho(\omega,\xi_i)=-\frac{1}{\pi}\operatorname{Im}\left\{\sum_{i,\sigma} G_{ii}^{\sigma}(\omega+is,\xi_i)+\sum_{i,M} G_{ii}^{M}(\omega+is,\xi_i)\right\} \tag{12}$$

where G_{ii}^{σ} and G_{ii}^{M} are the conduction and localized one-particle Green functions respectively. The second term gives as before:

$$\sum_i \ln\left\{1+\sum_M \exp\left[-\beta(E_M+G/2-C\xi_i/\beta-\mu)\right]\right\}. \tag{13}$$

In order to obtain the conduction-electron Green function we write Dyson's equation:

$$G_{ij}^{\sigma}(\omega,\xi_i)=\tilde{G}_{ij}^{\sigma}(\omega)+\sum_{lm}\tilde{G}_{il}^{\sigma}(\omega)\,\Upsilon_{lm}^{\sigma}(\omega,\xi_i)\,\tilde{G}_{mj}(\omega) \tag{14}$$

where, following Ref. [11], we have defined the renormalized zero order Green function $\tilde{G}^{\sigma}$ as:

$$(\tilde{G}^{\sigma^{-1}})_{ij}=(G^{(0)\sigma^{-1}}(\omega))_{ij}-\delta_{ij}\,\Sigma_{i\sigma}(\omega) \tag{15}$$

where $G^{(0)\sigma}$ is the Green function corresponding to the unperturbed band, $\Sigma_{i\sigma}$ is the self-energy operator, and Υ is the scattering matrix given by

$$\Upsilon_{sm}^{\sigma}=\Upsilon_{s,\sigma}^{(1)}\delta_{sm}+\Upsilon_{s,\sigma}^{(1)}(N\tilde{G}^{\sigma})_{sm}\Upsilon_{m,\sigma}^{(1)} +\sum_{S}\Upsilon_{s,\sigma}^{(1)}(N\tilde{G}^{\sigma})_{ss'}\Upsilon_{s',\sigma}^{(1)}(N\tilde{G}^{\sigma})_{s',m}\Upsilon_{m,\sigma}^{(1)}+\dots. \tag{16}$$

The single-site-scattering-matrix is given by:

$$\Upsilon_{s,\sigma}^{(1)}(\omega,\xi_s)=\frac{c\,\xi_s/\beta-\Sigma_{s\sigma}(\omega)}{1-(c\,\xi_s/\beta-\Sigma_{s\sigma}(\omega))\,\tilde{G}_{ss}^{\sigma}(\omega)} \tag{17}$$

where $(N\tilde{G}^{\sigma})$ is the non-diagonal part of the matrix $\tilde{G}^{\sigma}$. In deriving (14) to (17) no further approximation has been used.
Now we write

$$\Upsilon_{l,\sigma}^{(1)}(\omega,\xi_s)=\langle\Upsilon_{l,\sigma}^{(1)}\rangle_{\xi}+\{\Upsilon_{\xi,\sigma}^{(1)}(\omega,\xi_l)-\langle\Upsilon_{\xi,\sigma}^{(1)}\rangle_{\xi}\} \tag{18}$$

where in the first term we have used the average $\langle\ \rangle_{\xi}$ of the $\Upsilon^{(1)}$-matrix over the ξ_l and the second term corresponds to the fluctuating part. Substituing (18) in (16), and neglecting powers of the fluctuating part higher than the first, we obtain

$$\begin{aligned}\Upsilon_{ss'}^{\sigma}=&\langle\Upsilon_{ss'}^{\sigma}\rangle_{\xi}+[\Upsilon_{s,\sigma}^{(1)}-\langle\Upsilon_{s,\sigma}^{(1)}\rangle_{\xi}]\,\delta_{ss'}\\&+\sum_{s_1}[\Upsilon_{s,\sigma}^{(1)}-\langle\Upsilon_{s,\sigma}^{(1)}\rangle_{\xi}](N\tilde{G}^{\sigma})_{ss_1}\langle\Upsilon_{s',\sigma}^{(1)}\rangle_{\xi}\\&+\sum_{s_1}\langle\Upsilon_{s,\sigma}^{(1)}\rangle_{\xi}(N\tilde{G}^{\sigma})_{ss_1}[\Upsilon_{s',\sigma}^{(1)}-\langle\Upsilon_{s',\sigma}^{(1)}\rangle_{\xi}]\\&+\sum_{s_1s_2s_3}\langle\Upsilon_{ss_1}^{\sigma}\rangle_{\xi}(N\tilde{G}^{\sigma})_{s_1s_2}[\Upsilon_{s_2,\sigma}^{(1)}-\langle\Upsilon_{s_2,\sigma}^{(1)}\rangle_{\xi}]\\&\cdot(N\tilde{G}^{\sigma})_{s_2s_3}\langle\Upsilon_{s_3,s}^{\sigma}\rangle_{\xi}\end{aligned} \tag{19}$$

where $\langle\Upsilon_{ss'}^{\sigma}\rangle_{\xi}$ results of replacing $\Upsilon_{s,\sigma}^{(1)}\to\langle\Upsilon_{s,\sigma}^{(1)}\rangle_{\xi}$ everywhere. By means of the condition:

$$\langle\Upsilon_{s,\sigma}^{(1)}(\omega,\xi_s)\rangle_{\xi}=0 \tag{20}$$

we determine the operator $\Sigma_{s\sigma}(\omega)$. This is consistent with a CPA procedure [12], and (19) reduces to

$$\Upsilon_{ss'}^{\sigma}=\Upsilon_{s\sigma}^{(1)}\delta_{ss'}. \tag{21}$$

The result for the Gibbs potential is:

$$e^{-\beta\Omega}=\int\prod_i d\xi_i\, e^{-\beta\sum_i \Omega_i(\xi_i)} \tag{22}$$

with:

$$\beta\Omega_i(\xi_i)=\pi\xi_i^2$$
$$+\frac{1}{\pi}\sum_\sigma\int_{-\infty}^{\infty} d\omega \ln[1+e^{-\beta(\omega-\mu)}]\,\mathrm{Im}\{\tilde{G}_{ii}^{\sigma}+(\tilde{G}^{\sigma 2})_{ii}\,\Upsilon_{i,\sigma}^{(1)}\}$$
$$+\ln\left\{1+\sum_M \exp\left[-\beta\left(E_M+G/2-\frac{C\xi i}{\beta}-\mu\right)\right]\right\}-\frac{\beta G}{4} \tag{23}$$

The self-consistent problem to be solved is that given by (20), (22), (23) and the average:

$$\langle \Upsilon_{s,\sigma}^{(1)}(w,\xi_s)\rangle_\xi=\frac{\int d\xi_s\,\Upsilon_{s,\sigma}^{(1)}(\omega,\xi_s)\,e^{-\beta\Omega_s(\xi_s)}}{\int d\xi_s\,e^{-\beta\Omega_s(\xi_s)}}. \tag{24}$$

We can reach direct conclusions about the existence of first-order phase-transitions without explicitly solving the self-consistent problem. Expression (22) can be factorized in the following way.

$$=\{\int d\xi_i\,e^{-\beta\Omega_i(\xi_i)}\}^N \tag{25}$$

where N indicates the number of lattice sites. Since the partition function factorizes into uncoupled one-site partition functions, there is no possibility of cooperative effects which could lead to a first order phase transition.

Discussion

We have investigated the existence of first-order phase-transitions in the Falicov-Kimball model, within the functional integral approach.

In first place, we considered the uniform approximation. This is a kind of mean field approach, and therefore leads to the possibility of such transitions within the Falicov-Kimball model. On the other hand, the self-consistent approximation gives a negative answer, yielding an explanation for the inexistence of first-order transitions within a CPA scheme. This is a result of the inherent factorization of the partition function within a self-consistent approach, which is a consequence of the single-site-scattering approximation used in the method.

The results at variance obtained by two different approximations stress the importance of the method used in problems involving first-order phase transitions. In this context, we feel the approach of [6] is more adequate, since it is a mean-field scheme improved by including a self-consistent like description of the conduction band shift.

An improvement on the uniform-approximation obtained by taking into account the spatial and temporal fluctuations beyond the static-approximation within a method similar to the random-phase-approximation [10] is in progress.

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