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QUASI PARTICLE ENERGY OF 4F-STATES IN THE RAMIREZ-FALICOV-KIMBALL (RFK) MODEL: MEMORY FUNCTION FORMALISM

I. C. da Cunha Lima (1), C. E. Leal (1), E. A. de Andrade e Silva (1) and A. Troper (2)

(1) Instituto de Pesquisas Espaciais, av. dos Astronautas, 1758, 12.200 São Jose dos Campos, SP, Brazil
(2) Centro Brasileiro de Pesquisas Fisicas - CBPF, Rua Dr. Xavier Sigaud, 150, 22290 Rio de Janeiro, RJ, Brazil

Abstract. - A new formalism is developed, based on the memory function approach, to treat many particle systems. The formalism is applied to the Ramirez-Faliquov-Kimball (RFK) Hamiltonian, suitable to describe photo-emission spectra in many light rare earth intermetallics. We obtain a quasi particle 4f-energy in the weak correlation regime and we discuss the bimodal structure of the f-f propagator in this regime comparing with the Hubbard-type structure in the strong correlation regime.

It is well known that many experiments concerning the photo-emission of 4f-electrons in light rare-earth elements, e.g., Ce, show a double peak structure: one localized at the Fermi level and another approximately 2.5 eV below it.

Parks et al. [1] and Wieliczka et al. [2] have shown that this bimodal structure of the 4f-spectra occurs in many other metallic systems containing light rare earths such as Pr and Nd.

Many works [3, 4, 5] have been proposed in order to explain the 4f-double structure, based, for example, on the rare earth magnetic properties [3] or on screening effects [4, 5]. Nunez-Regueiro and Aivignon [6] have calculated the 4f-spectral density, based on the Falicov-Kimball model, adopting Hubbard's "resonance broadening approximation". This strong correlation regime approximation, yields one or two peaks depending on the ratio between the Coulomb correlation U between the f-localized states and the d-itinerant states and the d-bandwidth Δ. Moreover, f-d hybridization plays no significant role in the broadening of the two peaks.

In this work, adopting the Ramirez-Falicov-Kimball (RFK) Hamiltonian, we calculate the f-f Green's function in the weak correlation regime, i.e., U/W < 1. We develop here a Memory Function matrix formalism, which enables us to describe the weak correlation regime beyond the usual Hartree-Fock approximation.

For the sake of simplicity, we discuss here only the RFK Hamiltonian in the one-impurity case:

\[
H = \sum_\sigma \epsilon_\sigma f_\sigma^+ f_\sigma + \sum_\sigma k \epsilon_\sigma^* d_\sigma^+ d_\sigma +
\sum_\sigma V \left( f_\sigma^+ d_\sigma^+ f_\sigma f_\sigma \right) + \sum_{\sigma' \sigma} U n_{\sigma \sigma'} n_{\sigma' \sigma} \ ;
\]

\[
\sum_\sigma \alpha_\sigma = \alpha_\sigma^* \ ; \\
\sum_\sigma n_{\sigma \sigma'} = n_{\sigma \sigma'} \ ; \quad (\alpha = f \text{ or } d).
\]

The local f-f Green function is given by

\[
G_{ff}^{\alpha \alpha'} (t) = i \theta (t) \left( \left[ f_\sigma^+ f_\sigma (t) \right]_{\alpha \alpha'} \right) \quad (\alpha = f \text{ or } d).
\]

Now we introduce the self-consistent many body theory developed by Pedro and Wilson [7], Kishore [8] and Chao et al. [9]. Let us consider two sets of Heisenberg fermion operators \( A_\alpha \) and \( B_\beta \) forming a complete space:

\[
\{ A_\alpha \} = \{ f_\sigma^+, d_\sigma^* \}
\]
\[
\{ B_\beta \} = \{ f_\sigma^+, d_\sigma^* \}
\]

and a projection operator \( P \) defined as

\[
P \Psi = \sum_j P_j \Psi = \sum_j B_j \left( [A_j, \Psi]_+ \right).
\]

Using the sets given by equation (3), we have:

\[
P \Psi = f_\sigma^+ \left( [f_\sigma^+, \Psi]_+ \right) + \sum_k d_\sigma^* \left( [d_\sigma^*, \Psi]_+ \right).
\]

An equation of motion for the matrix \( G (w) \):

\[
G_{\alpha \beta} (t) = i \theta (t) \left( [A_\alpha, B_\beta (t)]_+ \right)
\]

can be worked out:

\[
\tilde{G} (w) = \left[ \tilde{\alpha} \tilde{\Omega} - \tilde{\gamma} (w) \right]^{-1} \tilde{\chi}
\]

where

\[
\tilde{\Omega}_{\alpha \beta} = \left( [A_\alpha, L B_\beta]_+ \right)
\]

and

\[
\tilde{\gamma}_{\alpha \beta} = \left( [A_\alpha, B_\beta]_+ \right) \delta_{\alpha \beta}
\]

\[
\tilde{\chi}_{\alpha \beta} = \left( [A_\alpha, B_\beta]_+ \right) \tilde{\delta}_{\alpha \beta}
\]

\[
\tilde{G}_{00}^{ff} (w) = \left[ w \tilde{\Omega} - \tilde{\gamma} (w) \right]^{-1} \tilde{\chi}_{11}.
\]

Equation (11) can be solved in several levels of approximations for the matrix \( \tilde{\gamma} (w) \). In the lowest level of approximation we use the linearized f-d Coulomb term in the Hamiltonian. Then we find: \( \tilde{\gamma} (w) = 0 \). The f-f propagator becomes:

\[
G_{00}^{ff} (w) = \frac{1}{w - \tilde{\epsilon}_f - U \langle n_0^d \rangle - V^2 F (w)}
\]

where

\[
F (w) = \sum_k \frac{1}{w - \epsilon_k - U \langle n_0^d \rangle}.
\]

and we recover the Hartree-Fock approximation.
In the next step, we use a recursion formula for the self-energy $\gamma(w)$ [9, 10].

The hierarchy of the Green's function is truncated by approximating conveniently the self-energy $\gamma^f(n+1:w)$. Thus, in the first order approximation, we linearize the Hamiltonian for $\gamma^f(2:w)$, which will give us again $\gamma^f(2:w) = 0$. Then we obtain from the recursion formula:

$$E_{\pm} = \frac{V^2 F(w)}{2} \pm \frac{1}{2} \sqrt{2 \varepsilon_0 + 2U \langle n_0^d \rangle + V^2 F(w)^2} + 4U^2 \langle n_0^d \rangle (\langle n_0^d \rangle + \epsilon_0 + U \langle n_0^d \rangle).$$

The f-f propagator, exhibiting a n-modal structure is obtained by linearizing again the Coulomb interaction contribution for higher $\gamma^f(n+1:w)$ terms in the recursion formula. As an illustration of this peculiar feature, we perform the calculation up to a higher level of approximation, truncating the expansion terms in $\gamma^f(3:w)$, giving rise to terms in $U^3$. Then, we have:

$$\gamma^f(w) = \frac{w U^2 \langle n_0^d \rangle (\langle n_0^d \rangle + \epsilon_0 + U) + V^2 U \langle n_0^d \rangle + \epsilon_0 + U) + V^2 U \langle n_0^d \rangle}{w^2 + \epsilon_0 + \langle n_0^d \rangle + \epsilon_0^2 + 2\epsilon_0 U \langle n_0^d \rangle + V^2 U \langle n_0^d \rangle + \epsilon_0^2 + V^2}.$$

Introducing the above result in equation (11) the f-f Green function which exhibits a tri-modal structure for the 4f-spectral density of states, associated to the higher order of the approximations on the self-energy $\gamma^f(w)$.

If one goes back in our perturbative treatment one can obtain, in principle, a n-modal structure for the f-f propagator. However, for the physical situation which we are interested in, one needs only to go up to second order in $U$, where the main features of the 4f-states structures are already present (cf. Eq. (19)).

Finally, it should be mentioned, that this approach can also be applied in the case of strong correlation limit, i.e., $U/\Delta \gg 1$. In this case, the choice of the starting set of operators is a different one, namely:

$$\langle A^f_+ \rangle = \langle f_{\sigma} n_{0}^{d+}, d_{k\sigma} \rangle$$
$$\langle A^-_+ \rangle = \langle f_{\sigma} n_{0}^{d-}, d_{k\sigma} \rangle$$
$$\langle B_i \rangle = \langle f_{\sigma} n_{0}^{d}, d_{k\sigma} \rangle$$

where:

$$n_{0}^{d+} = n_{0}^{d}$$
$$n_{0}^{d-} = 1 - n_{0}^{d}.$$

With this choice, the f-f propagator can be written as:

$$\eta_{00}^f(w) = G_{00}^{f+}(w) + G_{00}^{f-}(w)$$

where

$$G_{00}^{f+}(w) = i\theta(t) \left[ f_{\sigma} n_{0}^{d+}, f_{\sigma} \right].$$

In the lowest approximation and assuming $V = 0$ (i.e., a Falicov-Kimball model), one gets the usual Hubbard-type bimodal structure

$$G_{00}^{f+}(w) = \frac{1 - n_{0}^{d}}{w - \epsilon_0 + \langle n_0^d \rangle},$$

which is completely different from the bimodal structure derived in this work, in the weak correlation regime.