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

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Abstract. - A new formalism is developed, based on the memory function approach, to treat many particle systems. The formalism is applied to the Ramirez-Falicov-Kimball (RFK) Hamiltonian, suitable to describe photoemission spectra in many light rare earth intermetalics. 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 Avignon [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 $\Delta$. 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:

$$H = \sum_{\sigma \sigma'} \varepsilon_{f, \sigma, \sigma'} f_{\sigma, \sigma'}^+ f_{\sigma, \sigma'} + \sum_{\mathbf{k}, \mathbf{k}' \sigma \sigma'} V_{\mathbf{k}, \mathbf{k}'} f_{\mathbf{k}, \mathbf{k}', \sigma} d_{\mathbf{k}, \sigma}^+ d_{\mathbf{k}, \sigma}$$

$$+ \sum_{\sigma \sigma'} \sum_{\mathbf{k}} V (f_{\mathbf{k}, \sigma} d_{\mathbf{k}, \sigma'}^+ + d_{\mathbf{k}, \sigma'}^+ f_{\mathbf{k}, \sigma}) + \sum_{\sigma \sigma'} \sum_{\mathbf{k}, \mathbf{k}'} U_{\mathbf{k}, \mathbf{k}'} n_{\mathbf{k}, \sigma}^0 n_{\mathbf{k}', \sigma}\,;$$

$$n_{\mathbf{k}, \sigma}^0 = \alpha_{\sigma}, \alpha_{\sigma}, \quad \sum_{\sigma} n_{\mathbf{k}, \sigma}^0 = n_{\mathbf{k}}^0, \quad (\alpha = f \text{ or } d). \quad (1)$$

The local f-f Green function is given by

$$G_{00\sigma\sigma}(t) = \theta(t) \left[ f_{\sigma, \sigma'}(t) f_{\sigma, \sigma'}^+(t) \right]_+ . \quad (2)$$

Now we introduce the self-consistent many body theory developed by Fedro 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:

$${\{A_\alpha\}} = \{f_{0, \sigma}, d_{K, \sigma}\}$$

$${\{B_\beta\}} = \{f_{0, \sigma}^+, d_{K, \sigma}^+\}$$

and a projection operator $P$ defined as

$$P\Psi = \sum_{\beta} P_j \Psi = \sum_{\beta} B_j \left[ [A_j, \Psi]_+ \right] \left[ [B_j, \Psi]_+ \right] . \quad (4)$$

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

$$P\Psi = f_{00} \left[ [f_{00}, \Psi]_+ \right] + \sum_{\mathbf{k}} d_{K, \sigma}^+ d_{K, \sigma} \left[ [d_{K, \sigma}, \Psi]_+ \right] . \quad (5)$$

An equation of motion for the matrix $\tilde{G}(w)$:

$$G_{\alpha\beta}(t) = i \theta(t) \left[ [A_{\alpha}, B_{\beta}(t)]_+ \right] \quad (6)$$

can be worked out:

$$\tilde{G}(w) = \left[ xI - \tilde{\Omega} - \tilde{\gamma}(w) \right]^{-1} \tilde{\chi} \quad (7)$$

where

$$\Omega_{\alpha\beta} = \left[ [A_{\alpha}, B_{\beta}]_+ \right]$$

$$\chi_{\alpha\beta} = \left[ [A_{\alpha}, B_{\beta}]_+ \right] \delta_{\alpha\beta}$$

and

$$\gamma_{\alpha\beta}(w) = \left[ [A_{\alpha}, L + \frac{1}{w} f_{00} \left( \frac{1}{1 - P} f_{00} \right) L B_{\beta}]_+ \right] , \quad (8)$$

$L$ being the Liouvillian operators: $L\Psi = [H, \Psi]$.

If we identify our first matrix element with the f-state, we have:

$$G_{00\sigma\sigma}(w) = \left[ wI - \tilde{\Omega} - \tilde{\gamma}(w) \right]^{-1} \chi_{11} . \quad (11)$$

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:

$$G_{00\sigma\sigma}(w) = \frac{1}{w - \varepsilon_0 - U \left( n_{0}^d \right) - V^2 F(w)} \quad (12)$$

where

$$F(w) = \sum_{\mathbf{k}} \frac{1}{w - \varepsilon_0 - U \left( n_{k}^f \right)} . \quad (13)$$

and we recover the Hartree-Fock approximation.
In the next step, we use a recursion formula for the self-energy $\gamma (w)$ \cite{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:

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

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:

$$\gamma^f (w) = \frac{\langle f_{0\nu}, L (1 - P) Pf_{0\nu} \rangle + \langle f_{0\nu}, L^2 (1 - P) Pf_{0\nu} \rangle + \langle f_{0\nu}, L^2 Pf_{0\nu} \rangle + \langle f_{0\nu}, Pf_{0\nu} \rangle_{+}}{w^2 + w \langle f_{0\nu}, Lf_{0\nu} \rangle_{+} + \langle f_{0\nu}, Pf_{0\nu} \rangle_{+} + \langle f_{0\nu}, Pf_{0\nu} \rangle_{+} + \langle f_{0\nu}, Pf_{0\nu} \rangle_{+}}$$

and after some algebra we obtain:

$$\gamma^f (w) = \frac{wU^2 \langle n_0^d \rangle (1 - \langle n_0^d \rangle) + U^2 \langle n_0^d \rangle (1 - \langle n_0^d \rangle) (2\varepsilon_0 + U) + V^2 \langle n_0^d \rangle - \langle n_0^d \rangle)}{w^2 + \langle \varepsilon_0 + U \rangle_0^\nu + \langle \varepsilon_0 + 2\varepsilon_0 U \rangle_0^\nu + U^2 \langle \varepsilon_0 \rangle + V^2}.$$  

Introducing the above result in equation (11) the $f$-$f$ Green function which exhibits a tri-modal structure in the weak correlation regime. This tri-modal structure is 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:

$$G_{00\nu}^f (w) = \frac{w - \varepsilon_0}{w - \varepsilon_0} + \frac{\langle n_0^d \rangle}{w - \varepsilon_0 - U},$$

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