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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:

$$H = \sum_{\sigma} \varepsilon_0 f_{0\sigma}^\dagger f_{0\sigma} + \sum_{k \sigma} \varepsilon_k d_{k\sigma}^\dagger d_{k\sigma} + \frac{V}{2} \sum_{k \sigma} \left( f_{0\sigma}^\dagger d_{k\sigma} + d_{k\sigma}^\dagger f_{0\sigma} \right) + \sum_{\sigma \sigma'} U n_{0\sigma} n_{0\sigma'} \; ;$$

$$n_{0\sigma} = n_{0\sigma}^a = n_{0\sigma}^b \; ; \quad \sum_{\sigma} n_{0\sigma} = n_0 \; , \quad (\alpha = f \text{ or } d). \quad (1)$$

The local f-f Green function is given by

$$G_{00\sigma}^f (t) = i\theta (t) \left\langle [f_{0\sigma}^\dagger, f_{0\sigma}^\dagger (t) ]_+ \right\rangle \cdot (2)$$

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:

$$\{A_\alpha\} = \left\{ f_{0\sigma}, d_{k\sigma}^\dagger \right\}$$

$$\{B_\beta\} = \left\{ f_{0\sigma}^\dagger, d_{k\sigma} \right\}$$

and a projection operator $P$ defined as

$$P\Psi = \sum_j P_j \Psi = \sum_j B_j \left\langle [A_j, \Psi]_+ \right\rangle \cdot (3)$$

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

$$P\Psi = f_{0\sigma}^\dagger \left\langle [f_{0\sigma}, \Psi]_+ \right\rangle + \sum_k d_{k\sigma}^\dagger \left\langle [d_{k\sigma}, \Psi]_+ \right\rangle \cdot (4)$$

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

$$G_{\alpha\beta} (t) = i\theta (t) \left\langle [A_\alpha, B_\beta (t)]_+ \right\rangle \cdot (5)$$

can be worked out:

$$\tilde{G} (w) = \left[ \tilde{\Sigma} - \tilde{\Omega} - \tilde{\gamma} (w) \right]^{-1} \tilde{\chi} \cdot (6)$$

where

$$\Omega_{\alpha\beta} = \left\langle [A_\alpha, LB_\beta]_+ \right\rangle \cdot (7)$$

$$\chi_{\alpha\beta} = \left\langle [A_\alpha, B_\beta]_+ \delta_{\alpha\beta} \right\rangle \cdot (8)$$

and

$$\gamma_{\alpha\beta} (w) = \left\langle [A_\alpha, L - \frac{1}{w - (1 - P) E (1 - P) LB_\beta}]_+ \right\rangle \cdot (9)$$

$L$ being the Liouvillean operators: $L\Psi \equiv [H, \Psi]$.

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

$$G_{00\alpha}^f (w) = \left[ w \tilde{\Sigma} - \tilde{\Omega} - \tilde{\gamma} (w) \right]^{-1}_{11} \chi_{11} \cdot (10)$$

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:

$$G_{00\alpha}^f (w) = \frac{1}{w - \varepsilon_0 - U \left\langle n_0^d \right\rangle - V^2 F (w)} \cdot (11)$$

where

$$F (w) = \sum_k \frac{1}{w - \varepsilon_k - U \left\langle n_k^f \right\rangle} \cdot (12)$$

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 \( \gamma^R(n+1 : w) \). Thus, in the first order approximation, we linearize the Hamiltonian for \( \gamma^R(2 : w) \), which will give us again \( \gamma^R(2 : w) = 0 \). Then we obtain from the recursion formula:

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

The f-f propagator, exhibiting a n-modal structure is obtained by linearizing again the Coulomb interaction contribution for higher \( \gamma^R(n+1 : w) \) 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 \( \gamma^R(n : w) \), giving rise to terms in \( U^3 \). Then, we have:

\[
\gamma^R (w) = \frac{\left\langle f_{\sigma \theta} \begin{pmatrix} L (1 - P) L f^{\theta}_{\sigma} \end{pmatrix} \right\rangle_{1+} + \left\langle f_{\sigma \theta} \begin{pmatrix} L^2 (1 - P) L f^{\theta}_{\sigma} \end{pmatrix} \right\rangle_{2+}}{w^2 + w \left\langle f_{\sigma \theta} \begin{pmatrix} L f^{\theta}_{\sigma} \end{pmatrix} \right\rangle_{1+} + \left\langle f_{\sigma \theta} \begin{pmatrix} L^2 f^{\theta}_{\sigma} \end{pmatrix} \right\rangle_{2+}}
\]

and after some algebra we obtain:

\[
\gamma^R (w) = \frac{w U^2 \left\langle n_0^d \right\rangle \left( 1 - \left\langle n_0^d \right\rangle \right)}{w^2 + \left( \varepsilon_0 + U \left\langle n_0^d \right\rangle \right)} + \left( \varepsilon_0^2 + 2\varepsilon_0 U \left\langle n_0^d \right\rangle + U^2 \left\langle n_0^d \right\rangle + V^2 \right).
\]

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 approximation on the self-energy \( \gamma^R(w) \).

If one goes further 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:

\[
\begin{align*}
\langle A_+ \rangle &= \{ f_{\sigma \theta} n_0^{d+} \}, \quad d_{K_\sigma} \\
\langle a^- \rangle &= \{ f_{\sigma \theta} n_0^{d-} \}, \quad \langle d_{K_\sigma} \rangle \\
\langle b \rangle &= \{ f_{\sigma \theta} \}
\end{align*}
\]

where:

\[
\begin{align*}
n_0^{d+} &= n_0^1 \\
n_0^{d-} &= 1 - n_0^1
\end{align*}
\]

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

\[
G_{00\theta}^{\pm} (w) = G_{00\theta}^{d+} (w) + G_{00\theta}^{d-} (w)
\]

where

\[
G_{00\theta}^{d\pm} (w) = \delta (t) \left\langle \left[ f_{\sigma \theta} n_0^{d\pm} \right] \right\rangle.
\]

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

\[
G_{00\theta}^{d\pm} (w) = \frac{1 - \left\langle n_0^d \right\rangle}{w - \varepsilon_0} + \frac{\left\langle n_0^d \right\rangle}{w - \varepsilon_0 - U},
\]

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