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ABSTRACT

We show that the Green's function solution of the Anderson model calculated by the functional derivative method developed earlier yields the density of states having the three-peak structure proposed by Grüner and Zawadowski and that the central peak indeed introduces the $\ell n T$ dependence.

INTRODUCTION

It is generally accepted that the problem of localized moments in metals may be discussed more naturally by the Anderson model[1] than by the s-d model, although the Kondo effect[2] has been formulated solely by the s-d model. The Schrieffer-Wolff transformation[3] can convert the Anderson model to the s-d model, but this is possible only in the limit where the density of states for d electrons is negligible at the Fermi surface. To circumvent the difficulties, Grüner and Zawadowski[4] have proposed the density of states exhibiting a three-peak structure. At high temperatures where many body corrections are not strong enough to modify the Hartree-Fock results, two broad but well-separated peaks corresponding to the majority- and minority-spin electrons appears. The conduction electron scattering is then described with two phase shifts. At zero temperature, on the other hand, the system is in the singlet ground state with a well-defined single phase shift, introducing a narrow third peak. They have assumed that this narrow resonance is responsible for the Kondo effect. Zlatic et al[5] have constructed a scattering amplitude by adding this narrow resonance but did not find the $\ell n T$ dependence.

THE CALCULATION OF THE GREEN'S FUNCTION

In this paper, we shall show that the Green's function solution of the nondegenerate Anderson model calculated by the functional derivative method developed earlier[6] yields the density of states having the three-peak structure and that the central peak indeed introduce the $\ell n T$ dependence. Let us consider the equations of motion for the two types of Green's

functions $\Gamma^{(+)}_{k\lambda\sigma} \equiv \langle\langle C_{d\sigma}(t) N^{(+)}_{d\bar{\sigma}}(t)\ C^{\dagger}_{\lambda\sigma}(t')\rangle\rangle$, where $N^{(+)}_{d\sigma}(t) \equiv N_{d\sigma}(t) = C^{\dagger}_{d\sigma}(t)\ C_{d\sigma}(t)$, $N^{(-)}_{d\sigma}(t) = 1 - N_{d\sigma}(t)$, and λ = d or k. Here, in line with the Hubbard treatment[7] of narrow bands, the projection operators $N^{(\pm)}$ are inserted so that the intra-atomic interaction U is correctly calculated whenever an electron with opposite spin $\bar{\sigma}$ appears at the impurity site. The one-electron Green's function is then given by $G = \Gamma^{(+)} + \Gamma^{(-)}$.

The equations of motion involve the following two types of terms

$$g_1 = \sum_k V_{dk} \langle\langle C_{k\sigma}(t)[N_{d\bar{\sigma}}(t) - \langle N_{d\bar{\sigma}}\rangle] C^{\dagger}_{\lambda\sigma}(t')\rangle\rangle \quad , \tag{1}$$

$$g_2 = \sum_k \{V_{dk} \langle\langle C_{d\sigma}(t)[C^{\dagger}_{d\bar{\sigma}}(t) C_{k\bar{\sigma}}(t) - \langle C^{\dagger}_{d\bar{\sigma}} C_{k\bar{\sigma}}\rangle] C^{\dagger}_{\lambda\sigma}(t')\rangle\rangle$$

$$- V_{kd} \langle\langle C_{d\sigma}(t)[C^{\dagger}_{k\bar{\sigma}}(t) C_{d\bar{\sigma}}(t) - \langle C^{\dagger}_{k\bar{\sigma}} C_{d\bar{\sigma}}\rangle] C^{\dagger}_{\lambda\sigma}(t')\rangle\rangle\}, \tag{2}$$

where V_{kd} is the hopping matrix element between conduction electron k and localized electron d. If one neglects g_1 and g_2, the equations can be solved immediately, yielding G_o. Since g_1 and g_2 can be reduced to functional derivatives of G, they can be calculated iteratively by inserting G_o. The reason why, instead of the Hartree-Fock solution, G_o is used as the zeroth order approximation is that the intra-atomic interaction U is included rigorously in each step of perturbation calculation, making our result distinctly different from any other existing calculation. The result is

$$2\pi G^{-1}_{dd\sigma}(\omega) = \frac{(\omega - \varepsilon_d)(\omega - \varepsilon_d - U) - iG_{dd\sigma}(\omega) Y(\omega)}{\omega - \varepsilon_d - (1 - n_{d\bar{\sigma}})U}$$

$$- \sum_k \frac{|V_{dk}|^2}{\omega - \varepsilon_k} \frac{[\omega - \varepsilon_d - (\frac{3}{4} - \frac{n_{d\bar{\sigma}}}{2})U]^2}{(\omega - \omega_a)(\omega - \omega_b) - iG_{dd\sigma}(\omega) Y(\omega)}, \tag{3}$$

where ε_d and ε_k are the energies of electrons k and d; $n_{d\sigma} = \langle N_{d\sigma}\rangle$, and

$$Y(\omega) = (U/2)^2 M_{\bar{\sigma}} [\omega - \varepsilon_d - (1 - n_{d\bar{\sigma}})U](\omega - \omega_{-x})^{-1}(\omega - \omega_x)^{-1},$$

$$\omega_{a,b} = \varepsilon_d + (\frac{3}{4} - \frac{n_{d\bar{\sigma}}}{2})U \mp \sqrt{n_{d\bar{\sigma}}(1 - n_{d\bar{\sigma}})U},$$

$$\omega_{\pm x} = \varepsilon_d + (\frac{3}{4} - \frac{n_{d\bar{\sigma}}}{2})U \pm [iG_{dd\sigma}(\omega)](U/4), \tag{4}$$

$$M_{\bar{\sigma}} = \frac{1}{2} \sum_k [V_{dk} \langle C^{\dagger}_{d\bar{\sigma}} C_{k\bar{\sigma}}\rangle + V_{kd} \langle C^{\dagger}_{k\bar{\sigma}} C_{d\bar{\sigma}}\rangle] \ .$$

If $\sum_k |V_{dk}|^2/(\omega-\varepsilon_k)$ is replaced by ε_k, the structure of above expression becomes exactly the same as that of the Hubbard model obtained in Ref. 8 . The value of $\sum_k |V_{dk}|^2/(\omega-\varepsilon_k)$ may be evaluated as $\Gamma-i\Delta$, where $\Gamma(<0)$ and Δ are the effective energy shift and the width parameter of the d states, respectively. However, the term involving $iG_{dd\sigma}(\omega)Y(\omega)$ in the summation $\Sigma_k\ldots$ should be handled with care, since $iG_{dd\sigma}(\omega) = [1-f(\omega)]A(\omega)$ where $f(\omega)$ is the Fermi-Dirac distribution function and $A(\omega)$ the spectral function. In this particular term, $\sum_k |V_{dk}|^2/(\omega-\varepsilon_k)$ cannot be reduced to $\Gamma-i\Delta$, and instead the relation

$$\sum_k |V_{dk}|^2 f(\omega)/(\omega-\varepsilon_k) = \kappa(\omega)-i\mathscr{K}(\omega) \quad , \tag{5}$$

should be used where $\kappa(\omega)$ is the Kondo integral responsible for the $\ell n T$ dependence of the resistivity and $\mathscr{K}(\omega) = f(\omega)\Delta$. Then

$$2\pi G^{-1}_{dd\sigma}(\omega) = \frac{(\omega-\varepsilon_d)(\varepsilon-\varepsilon_d-U) - [1-f(\omega)]A(\omega)Y(\omega)}{\omega-\varepsilon_d-(1-n_{d\bar{\sigma}})U}$$
$$- \frac{(\Gamma-i\Delta)[\omega-\varepsilon_d-(\frac{3}{4}-\frac{n_{d\bar{\sigma}}}{2})U]^2}{(\omega-\omega_a)(\omega-\omega_b)-(1-k+i\ell)A(\omega)Y(\omega)+\ldots} \quad , \tag{6}$$

where $k = (\kappa\Gamma+\mathscr{K}\Delta)/(\Gamma^2+\Delta^2)$ and $\ell = (\mathscr{K}\Gamma-\kappa\Delta)/(\Gamma^2+\Delta^2)$.

THE RESULTS AND DISCUSSIONS

Since $M_{\bar{\sigma}}$, Γ and Δ are all proportional to $|V^2|$, the Kondo term $(k-i\ell)$ is of order $|V^4|$ in $G_{dd\sigma}(\omega)$ and of order $|V^6|$ in the conduction electron Green's function $G_{kk\sigma}(\omega)$ in agreement with the result of the Schrieffer-Wolff transformation. However, the $\ell n T$ dependence will appear only if the density of d electrons, $A(\omega)$, is finite at the Fermi level. We shall show this by solving the polynomial equation $G^{-1}_{dd\sigma}(\omega) = 0$ graphically. Since the method is completely parallel to that used in the Hubbard model,[8] we shall only outline the procedure and the results.

In the limit of $\Gamma=\Delta=0$, the poles of G is calculated by solving the quartic equation in ω:

$$(\omega-\varepsilon_d)(\omega-\varepsilon_d-U) - [1-f(\omega)]Y(\omega) = 0 \quad , \tag{7}$$

where $f(\omega) \neq 0$ since we are calculating the scattering amplitude of conduction electron k traveling right above the Fermi level; $G_{dd\sigma}(\omega)$ is a part of $G_{kk\sigma}(\omega)$ for this electron. The term $Y(\omega)$ is generated by the correction term g_2 and tends to introduce magnetism.

In fact, the solution calculated by Eq. (7) satisfies the condition for magnetism $\delta n_{d\sigma}(n_{d\bar{\sigma}})/\delta n_{d\bar{\sigma}} < -1$. As long as $n_{d\bar{\sigma}}$ is small, however, the poles ω_1' and ω_2' will not deviate drastically from the isolated atomic levels ε_d and $\varepsilon_d + U$ while the additional poles $\omega'_{\pm x}$ are physically unimportant since they are nearly equal to $\omega_{\pm x}$ and the spectral weights are vanishingly small.

The solutions of

$$(\omega-\omega_a)(\omega-\omega_b)-(1-k+i\ell)A(\omega)Y(\omega) = 0 \qquad (8)$$

can be calculated similarly. At high temperature where $K(\omega)$ is small, $k \gtrsim f(\omega)$ and $\ell \gtrsim 0$. In the nonmagnetic limit $n_{d\sigma} = n_{d\bar{\sigma}} \gtrsim 1/2$, $\omega_a = \varepsilon_d$ and $\omega_b = \varepsilon_d+U$ and hence Eq. (8) becomes identical to Eq. (7), yielding $\omega_a' = \omega_1'$ and $\omega_b' = \omega_2'$. In the fully magnetic limit $n_{d\sigma} \cong 1$ and $n_{d\bar{\sigma}} \cong 0$, on the other hand, $\omega_a = \omega_b = \varepsilon_d + (3/4)U$. As the magnetization $n_{d\sigma} - n_{d\bar{\sigma}}$ decreases, the value of ω_a decreases from $\varepsilon_d+(3/4)U$ to ε_d while the value ω_b increases from $\phi_d+(3/4)U$ to ϕ_d+U. Note that the difference between ω_1 and ω_a remains large as long as the difference $n_{d\sigma} - n_{d\bar{\sigma}}$ is appreciable.

The complete solutions $\bar{\omega}_1$, $\bar{\omega}_a$ etc. of Eq. (6) can now be obtained graphically by assuming $\Delta = \ell = 0$. The contribution from the imaginary parts of the equation can then be estimated perturbationally. For the nonmagnetic case, however, the calculation is trivial since $\omega_1' = \omega_a'$ and $\omega_2' = \omega_b'$. $\bar{\omega}_1$ and $\bar{\omega}_a$ (or $\bar{\omega}_2$ and $\bar{\omega}_b$) will split into two and the separation, being proportional to $\sqrt{|\Gamma|}$, would be small as compared with the width parameter Δ of ω and the two peaks $\bar{\omega}_1$ and $\bar{\omega}_a$ (or $\bar{\omega}_2$ and $\bar{\omega}_b$) will look like a broad single peak. As the magnetization $n_{d\sigma} - n_{d\bar{\sigma}}$ increases from zero to one, the difference $\omega_a' - \omega_1'$ increases, yielding two distinct solutions $\bar{\omega}_1$ and $\bar{\omega}_a$. Although $\bar{\omega}_1$ remains more or less constant, $\bar{\omega}_a$ increases from $\sim\varepsilon_d$ to $\sim\varepsilon_d + (3/4)U$. $\bar{\omega}_2$ and $\bar{\omega}_b$ will remain exhibiting a single peak.

As temperature is lowered, $K(\omega)$ and hence $(1-k)$ and ℓ increase, making ω_a' and $\bar{\omega}_a$ larger. The calculated value of $n_{d\sigma}$ will then decrease and, to maintain the self-consistent requirement $\delta n_{d\sigma}(n_{d\bar{\sigma}})/\delta n_{d\bar{\sigma}} < -1$, $n_{d\bar{\sigma}}$ has to increase, resulting in the reduction of the magnetization $n_{d\sigma} - n_{d\bar{\sigma}}$ as well as ω_a.

Let us now summarize the foregoing results. At high temperature where the Kondo integral is negligible, magnetic solution with the three-peak structure appears as long as the term $Y(\omega)$ which enhances magnetism dominates over the term which is proportional to $\Gamma-i\Delta$ and generated from the correction term g, and which tends to suppress magnetism. As long as

there exists a small density of d states at the Fermi level ε_F, the value of (1-k) increases as T decreases, tending to make $\bar{\omega}_a$ larger. If the third peak $\bar{\omega}_a$ lies below ε_F, the peak $\bar{\omega}_a$ will be shifted ε_F, increasing the density of d states and enhancing the ℓnT dependence. As T is lowered further, the magnetization $n_{d\sigma} - n_{d\bar{\sigma}}$ will decrease, making ω_a smaller. Consequently $\bar{\omega}_a$ will not increase and instead remain constant near ε_F. If, on the other hand, the third peak ω_a appears above the Fermi level, the tendency to increase $\bar{\omega}_a$ again introduces two competing procedures. One is the tendency to reduce the density of d states at ε_F and hence the tendency to increase $\bar{\omega}_a$ will be suppressed greatly. The second effect is to reduce the magnetization $n_{d\sigma} - n_{d\bar{\sigma}}$, making ω_a' and hence $\bar{\omega}_a$ smaller. If $\bar{\omega}_a$ becomes smaller and approaches to ε_F, the density of d states at ε_F increases, enhancing the ℓnT dependence in (1-k). Hence the third peak $\bar{\omega}_a$ will be shifted towards ε_F and remains there.

As the magnetization $n_{d\sigma} - n_{d\bar{\sigma}}$ becomes small, however, ω_a' becomes nearly equal to ω_1' and will not decrease further. Then the mechanism to keep ω_a around ε_F will disappear and ω_a starts to increase, thus reducing the density of d states at ε_F and hence reducing the ℓnT dependence. The system will then behave like spin fluctuations. This is possible because the imaginary parts of Eq. (6) are proportional to $[\omega-\varepsilon_d-(3/4-n_{d\bar{\sigma}}/2)U]^2$ or $[\omega-\varepsilon_d-(1-n_{d\bar{\sigma}})U]$, and hence the width of the third peak remains narrow.

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