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Seebeck coefficient for the Anderson model

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The single-site Anderson model with degeneracy N_f is solved for the case in which the lowest eigenstate contains L electrons in the f orbital, where $0<L<N_f$. The noncrossing approximation is used to find the density of states including the Kondo resonance. The Seebeck coefficient is calculated as a function of temperature for every value of L. We find that the Seebeck coefficient is largest for $L=1$ and declines in value as L increases. This suggests that large Seebeck coefficients are not possible in mixed-valent systems besides those of cerium or ytterbium. [S0163-1829(97)02742-2]

I. INTRODUCTION

There is great interest in finding materials suitable for thermoelectric applications.[1–5] Present materials are good at room temperature and above, but there is a lack of good materials at low temperatures. Generally the material must have high values of the electrical conductivity and Seebeck coefficient, while having a small value of the thermal conductivity.

Metals are generally unsuitable for thermoelectric applications because they have a small Seebeck coefficient.[6] An exception are mixed-valent materials where the Seebeck coefficient can obtain high values.[7,8] An alloy of copper and nickel called constantan is a well-known thermocouple. The highest values of Seebeck coefficient are obtained in rare-earth metallic compounds[5,8] such as YbAl_3 or CePd_3 where $|S|\sim 100$ μV/K. Many other compounds containing Ce or Yb have been found to have values of the Seebeck coefficient which are slightly lower.[8]

A few mixed-valent materials have been found which contain other rare-earth compounds. None have a Seebeck coefficient as high as 100 μV/K. This raises the theoretical question of whether these other rare-earth elements can have a high Seebeck coefficient.

Numerous theoretical calculations of the Seebeck coefficient for Ce or Yb predict the value of 100 μV/K, in agreement with the observed maximum.[9–22] These values are obtained by four different methods: Gunnarsson and Schönhammer,[9,10] the noncrossing approximation[11,13–15,23] slave-boson techniques,[12] and renormalization-group techniques.[21,22] Here we have used the noncrossing approximation to extend these calculations to other values of the f-orbital occupancy. We solve the single-site Anderson model[27] for the case of a level with degeneracy N_f. We find the Kondo resonance and Seebeck coefficient for the case that the ground state has L electrons in the f orbital, where $0<L<N_f$.

Generally we find that the Kondo resonance becomes smaller when L is increased. We present a series of calculations where we keep fixed the important values of $\Delta_\pm = E_{L\pm1}-E_L$, while varying ε_f to change L. Since the Kondo resonance becomes smaller, the Seebeck coefficient also becomes smaller. The largest value we get is for $L=1$. This corresponds to the case of Ce or Yb, and our values of $S\sim 100$ μV/K are in agreement with other workers[11,22] for the case that the orbital degeneracy is $N_f=6$. When we increase the value of L then the maximum value of S declines, as does the Kondo temperature. This is a calculation of these properties for general values of L.

A realistic calculation of the Seebeck for the configuration $(4f)^n$ requires that one include the various splittings of the f levels due to spin orbit and other interactions. This has only been done for Ce,[10,11,24–26] which has $L=1$. We are in the process of doing this calculation for $L=2$ which corresponds to Pr. However, we expect the Anderson model results to be a guide to what will be found when we split the levels. We expect that splitting the levels and lowering the degeneracy will only make the Seebeck smaller. Thus it is unlikely that splitting the levels will increase the Seebeck, nor change our qualitative conclusions.

II. SINGLE-SITE ANDERSON MODEL

The standard theoretical model for discussing rare-earth compounds was introduced by Anderson[27]

$$H=H_0+V, \tag{2.1}$$

$$H_0=\sum_{k\nu} \varepsilon_k C^\dagger_{k\nu} C_{k\nu} + \varepsilon_f \sum_\mu n_\mu + U\sum_{\mu>\nu} n_\mu n_\nu, \tag{2.2}$$

$$n_\mu = f^\dagger_\mu f_\mu, \tag{2.3}$$

$$V=\frac{1}{\sqrt{N}}\sum_{k\nu} V_{k\nu}[f^\dagger_\nu C_{k\nu} + C^\dagger_{k\nu} f_\nu], \tag{2.4}$$

where V is the hybridization interaction between the band electrons (k) and the localized electrons f_μ. The on-site Coulomb repulsion is U and ε_f is the eigenvalue for a single f electron. The eigenvalue and degeneracy factor Z_n for the f electrons, in the absence of hybridization are

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$$E_n = n\varepsilon_f + \frac{n(n-1)}{2}U, \qquad (2.5)$$

$$Z_n = \binom{N_f}{n}. \qquad (2.6)$$

The ground-state degeneracy of a rare-earth ion is given according to Hund's rules. The Anderson model ignores the splittings of the f orbital due to spin orbit and other factors, and gives the wrong degeneracy. In a future paper we will include these realistic splittings of the f levels. The present calculation is intended to be a solution of the Anderson model as given in Eqs. (1)–(4).

The eigenvalue expression (2.5) is parabolic in the level occupancy n. Since $\varepsilon_f < 0$ then the minimum energy is found near to $n \sim 1/2 - \varepsilon_f/U$. Denote as L the value of n which has the lowest value of E_n. We can increase L by increasing the value of ε_f towards larger negative values, while keeping U fixed.

A mixed valence is when the number of f electrons can vary between n and $n \pm 1$. The hybridization interaction causes mixing whenever $|E_L - E_{L\pm1}|$ is a small energy. The standard nomenclature[28] is to define the two excitation energies out of the ground state as

$$\Delta_- = E_{L-1} - E_L = -[\varepsilon_f + (L-1)U], \qquad (2.7)$$

$$\Delta_+ = E_{L+1} - E_L = \varepsilon_f + LU, \qquad (2.8)$$

$$U = \Delta_+ + \Delta_- . \qquad (2.9)$$

Values of $\Delta_\pm$ have been calculated for the rare-earth metals in Ref. 28. Generally they find one value which is small ($\Delta \sim 1.0$ eV), while the other is larger so that $U \sim 6-8$ eV. We assume that similar values apply to the rare earths when they are in metallic compounds.

Next we discuss the properties of the Hamiltonian H_0 without the hybridization V. This interaction is included in the following section. The Green's function for the f states in the absense of the hybridization term is

$$\mathcal{G}_f(i\omega_m) = -\sum_\mu \int_0^\beta d\tau e^{i\omega_m\tau}\langle T_\tau f_\mu(\tau) f_\mu^\dagger\rangle. \qquad (2.10)$$

This can be written exactly for the nonintracting states. We employ the notation $N_f = 14$ to denote the number of states for a single f electron. The degeneracy of the having n electrons in the f state is Z_n as defined above:

$$\mathcal{G}_f(i\omega_m) = \frac{1}{Z}\sum_{n=0}^{N_f} Z_n e^{-\beta E_n}\left\{\frac{N_f - n}{i\omega_m + E_n - E_{n+1}} + \frac{n}{i\omega_m + E_{n-1} - E_n}\right\}, \qquad (2.11)$$

$$A_f(\omega) = -2\Im[G_f(\omega)], \qquad (2.12)$$

$$A_f(\omega) = \frac{2\pi}{Z}\sum_{n=0}^{N_f} Z_n e^{-\beta E_n}\{(N_f - n)\delta(\omega + E_n - E_{n+1}) + n\delta(\omega + E_{n-1} - E_n)\}, \qquad (2.13)$$

$$Z = \sum_0^{N_f} Z_n e^{-\beta E_n}. \qquad (2.14)$$

The spectral function $A_f(\omega)$ is obtained by the analytic continuation $i\omega_m \to \omega + i\eta$ and then taking twice the imaginary part.

Let E_L be the lowest eigenvalue ($n = L$) and assume that L is neither 0 nor N_f. The most important terms in the summation is when $n = L-1, L, L+1$ which gives the approximation

$$Z = Z_L \mathcal{Z} e^{-\beta E_L}, \qquad (2.15)$$

$$\mathcal{Z} = 1 + \frac{L}{N_f + 1 - L}e^{-\beta\Delta_-} + \frac{N_f - L}{L+1}e^{-\beta\Delta_+}, \qquad (2.16)$$

$$A_f(\omega) = \frac{2\pi}{\mathcal{Z}}\left[L\delta(\omega + \Delta_-)(1 + e^{-\beta\Delta_-}) + (N_f - L)\delta(\omega - \Delta_+)(1 + e^{-\beta\Delta_+}) + e^{-\beta\Delta_-}\frac{L(L-1)}{N_f + 1 - L}\delta(\omega + E_{L-2} - E_{L-1}) + e^{-\beta\Delta_+}\frac{(N_f - L)(N_f - L - 1)}{L+1}\delta(\omega + E_{L+1} - E_{L+2})\right]. \qquad (2.17)$$

The spectra has four peaks. Two are below the chemical potential and two above. We follow custom and ignore the last two terms in $A_f(\omega)$ and include only the peaks at $\omega = -\Delta_-, \Delta_+$. For the case that $L = 1$ then the third term is missing anyway since there is no state $L-2$.

III. SELF-ENERGY OF ELECTRONS

The hybridization interaction V in Eq. (4) describes the processes whereby a conduction electron can hop on or off the f shell of the local atom. This process leads to several important effects. The first is an energy parameter defined as

$$\Gamma(E) = \frac{\pi}{N}\sum_k V_k^2 \delta(E - \varepsilon_k). \qquad (3.1)$$

This function is assumed to be a constant, independent of energy. Its value for the rare earths is about 0.1 eV. The second effect is that the resonance lines at $\omega = -\Delta_-, \Delta_+$

become broadened by an amount proportional to Γ. The third effect is that a resonance peak appears in $A_f(\omega)$ near to zero energy. This is the Kondo resonance, and it is the important feature for the calculation of the Seebeck coefficient.

In the prior section we showed that there were energy levels associated with having n electrons in the f state. We introduce a Green's function for this state

$$G_n(\omega)=\frac{1}{\omega-E_n-\Sigma_n(\omega)}. \tag{3.2}$$

The hybridization interaction causes the self-energy $\Sigma_n(\omega)$. We calculate this function using the method of Ref. 11. First consider the result for the self-energy in the second order of perturbation theory

$$\Sigma_n(\omega)=nS'^{(0)}_{n-1}(\omega)+(N_f-n)S^{(0)}_{n+1}(\omega), \tag{3.3}$$

$$S^{(0)}_{n+1}(\omega)=\frac{1}{N}\sum_k \frac{V_k^2 n_k}{\omega-(E_{n+1}-\varepsilon_k)+i\eta}, \tag{3.4}$$

$$S'^{(0)}_{n-1}(\omega)=\frac{1}{N}\sum_k \frac{V_k^2(1-n_k)}{\omega-(E_{n-1}+\varepsilon_k)+i\eta}. \tag{3.5}$$

There are two terms. The first term $(f^\dagger C_k)$ in V adds an electron to the f levels, which changes n to $n+1$, while destroying a band electron in the state k. This process is proportional to the occupation number n_k of the band electrons. The second term $(C_k^\dagger f)$ in V takes an electron away from the f level, which changes n to $n-1$, while adding an electron to the band. This process is proportional to the probability $(1-n_k)$ that the band state is unoccupied.

Arguments of $S^{(0)}$ are Green's functions G_n without the self-energies:

$$S_n^{(0)}(\omega)=\frac{1}{N}\sum_k V_k^2 n_k G_n^{(0)}(\omega+\varepsilon_k). \tag{3.6}$$

The noncrossing approximation[11,25,26] (NCA) is to evaluate these Green's functions while including these self-energies. Setting the self-energies in the denominators

$$\Sigma_n(\omega)=nS'_{n-1}(\omega)+(N_f-n)S_{n+1}(\omega), \tag{3.7}$$

$$S_{n+1}(\omega)=\frac{1}{N}\sum_k V_k^2 n_k G_{n+1}(\omega+\varepsilon_k), \tag{3.8}$$

$$S'_{n-1}(\omega)=\frac{1}{N}\sum_k V_k^2(1-n_k)G_{n-1}(\omega-\varepsilon_k). \tag{3.9}$$

The above equations comprise a self-consistent definition for the self-energies. They are solved by iteration on the computer. We assume a density of states

$$g(\varepsilon)=\frac{2D}{\varepsilon^2+D^2}, \tag{3.10}$$

and place the chemical potential at $\varepsilon=0$. The parameter D is an effective bandwidth and $\Gamma=\pi g(0)V(0)^2=2\pi V(0)^2/D$. In $S'_n(\omega)$ we can change variables $\varepsilon\to-\varepsilon$ which now makes $S'_n=S_n$. In effect, we evaluate the integral

$$S_n(\omega)=\frac{\Gamma}{\pi}\int\frac{d\varepsilon}{1+(\varepsilon/D)^2}n_F(\varepsilon)G_n(\omega+\varepsilon). \tag{3.11}$$

Some authors[15,16] argue that when one includes finite U then one should also include vertex corrections. Of course, it always better to include as many terms as possible in the self-energy and correlation functions. However, the inclusion of vertex terms increases significantly the numerical effort. We have examined these terms carefully and concluded that they are all smaller than $O(\Gamma/U)$ than the important terms that we keep in the calculation. Furthermore, the important feature, the Kondo resonance, is unaffected by vertex corrections. In the end we followed others[25,26] and left them out.

IV. *f*-ELECTRON GREEN'S FUNCTION

The final step is to calculate the spectral function of the f electron in the NCA. We must also include in the thermal averages the feature that the interactions give a spread in energy. Our result is

$$A_f(\omega)=\frac{1}{Z}\sum_{n=0}^{N_f} Z_n\int\frac{dE}{2\pi}e^{-\beta E}A_n(E)\{nA_{n-1}(E-\omega)+(N_f-n)A_{n+1}(E+\omega)\}, \tag{4.1}$$

$$Z=\sum_{n=0}^{N_f} Z_n\int\frac{dE}{2\pi}e^{-\beta E}A_n(E). \tag{4.2}$$

A detailed derivation of this result is provided in the Appendix. These results are similar in spirit to those of Ref. 11. They took the limit that $U\to\infty$ which eliminated all states with $n>1$. They only had the two states of $n=0,1$ in their system and $L=1$. Here we include all of the states with different values of n. We fix the value $U=6$ eV. We choose $\varepsilon_f=-0.5-U(L-1)$ (in units of electron Volts) to have a variety of values so that we have different occupancies L in the f state, while keeping fixed the values of $\Delta_-=-0.5$ eV, $\Delta_+=5.5$ eV. We make an approximation in our numerical solution of retaining only the states with $n=L-1,L,L+1$ in our self-consistent solution. We also choose $N_f=6$ and $\Gamma=0.1$ eV in order to compare with previous calculations.

It is convenient to introduce the notation

$$B_n(\omega)=e^{-\beta(\omega-E_L)}A_n(\omega). \tag{4.3}$$

This factor will account for the exponential factor of exp $(-\beta E)$ in Eq. (4.1). We added the factor of $\exp(\beta E_L)$ to provide convenient normalization, since the interesting structure in these functions is in the vicinity of $\omega\sim E_L$. This factor cancels between numerator and denominator. So we actually evaluate

$$\mathcal{Z}=\int\frac{dE}{2\pi}\left[B_L(E)+\frac{L}{N_f+1-L}B_{L-1}(E)+\frac{N_f-L}{L+1}B_{L+1}(E)\right], \tag{4.4}$$

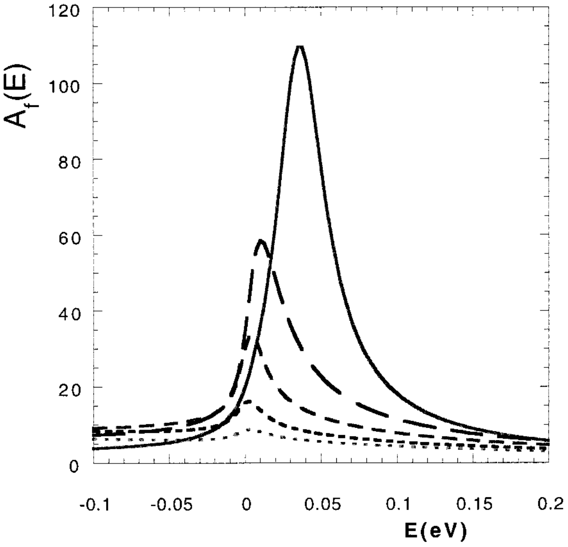

FIG. 1. The Kondo resonance at $T=50$ K for different values of L while $N_f=6, U=6, \Delta_-=-0.5, \Delta+=5.5$ remained fixed. The largest peak is for $L=1$ and the smallest is for $L=5$. Peak decreases steadily for increasing L.

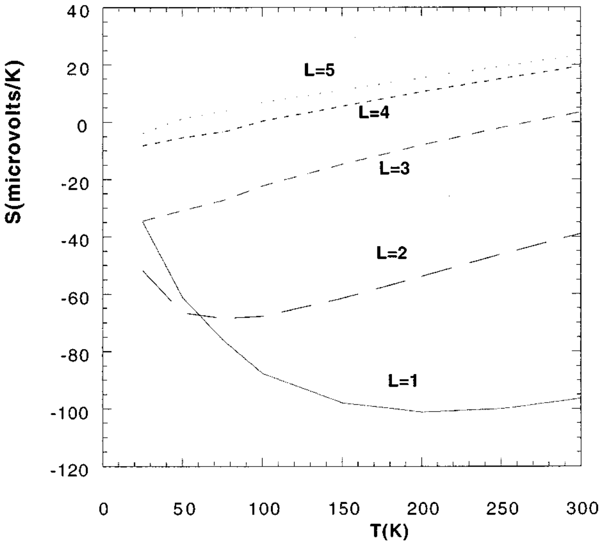

FIG. 2. Seebeck coefficient as a function of temperature between 50 and 300 K. The maximum value of the Seebeck coefficient occurs near to the Kondo temperature T_K. The maximum value of the Seebeck coefficient, and T_K, both decline with increasing values of L. Other parameters are the same as in Fig. 1.

$$A_f(\omega)=\frac{1}{\mathcal{Z}}\int\frac{dE}{2\pi}\{L[B_L(E)A_{L-1}(E-\omega)+A_L(E)B_{L-1}\times(E-\omega)]+(N_f-L)[B_L(E)A_{L+1}(E+\omega)+A_L(E)B_{L+1}(E+\omega)]\}. \tag{4.5}$$

As discussed in Ref. 11, the $B_n(E)$ functions cannot be obtained with numerical accuracy by just multiplying $A_n(E)$ by the exponential factor. Instead, one must obtain them by iteration along with the $A_n(E)$ functions. The latter functions have a width $\Gamma_n(E)=\Im[\Sigma_n(E)]$ and we introduce the similar function $\gamma_n(E)$ for the numerator of the $B_n(E)$ function:

$$\gamma_n(\omega)=e^{-\beta(\omega-E_L)}\Gamma_n(\omega), \tag{4.6}$$

$$B_n(\omega)=\frac{2\gamma_n(\omega)}{(\omega-E_n-\Re[\Sigma_n(\omega)])^2+\Gamma_n(\omega)^2}, \tag{4.7}$$

$$\gamma_n(\omega)=nT_{n-1}(\omega)+(N_f-n)T_{n+1}(\omega) \tag{4.8}$$

$$T_n(\omega)=e^{-\beta(\omega-E_L)}\frac{\Gamma}{2\pi}\int\frac{D^2d\varepsilon}{D^2+\varepsilon^2}n_F(\varepsilon)A_n(\omega+\varepsilon) \tag{4.9}$$

$$=\frac{\Gamma}{2\pi}\int\frac{D^2d\varepsilon}{D^2+\varepsilon^2}n_F(-\varepsilon)B_n(\omega+\varepsilon). \tag{4.10}$$

The latter equation provides a definition of $T_n(\omega)$ in terms of integrals over the function $B_n(E)$. This set of equations self-consistently defines $B_n(E)$ and are solved by iteration. Thus there are two iterations: one for $A_n(E)$ and another for $B_n(E)$.

V. RESULTS AND SUMMARY

Figure 1 shows the Kondo resonance at $T=50$ K as a function of energy in electron volts. We fixed U,Δ_-, and Δ_+, as described above, and varied the value of L: here L denotes the value of n at which E_n has the minimum value. The size of the Kondo resonance decreases in value as L increases. The largest Kondo resonance is the case $L=1$ and the smallest is the case with $L=5$. In these calculations, the only factors which is changing are (n,N_f-n) or (L,N_f-L) in Eqs. (3.7,4.5). These factors relate to the degeneracy of the various levels as given by the factor of Z_n. If we do a more realistic calculation for f electrons, with the factors which split the levels into sublevels, then we will reduce these factors.[25,26] This reduction can only make the Seebeck coefficient smaller.

The Seebeck coefficient for these cases is shown in Fig. 2 as a function of temperature. The largest Seebeck value is for $L=1$, and the values decrease in size when L increases. This is in accord with the observation that the Kondo resonance is getting smaller. The Kondo resonance causes the large values of the Seebeck.[11,5] The Seebeck coefficient peaks at a temperature near to the Kondo temperature. The peak in our calculated Seebeck coefficients declines with increasing values of L. For $L\geqslant 3$ it is below 50 K and the peak is off the figure to the left. However, one can see that even at the peak value the Seebeck will be small for these cases. Note that we choose to plot the result as a linear function of temperature, rather than as $\ln(T/T_K)$ as is customary. That is because we are primarily interested in applications where materials are needed over the range of temperatures in Fig. 2.

The Seebeck coefficient has a large value when the

Kondo resonance is large and asymmetric. The largest asymmetry is when $L, N_f - L$ differ by as much as possible. This happens when $L=1$, or when $L=5$ in the case of $N_f=6$. However, because of our choice that Δ_- is smaller than Δ_+, the large Kondo resonance happens for $L=1$. If we reverse the magnitudes of Δ_- and Δ_+ then the largest result is for $L=5$. In fact, the mapping of $\Delta_- \rightarrow \Delta_+, \Delta_+ \rightarrow \Delta_-, L \rightarrow N_f - L$ leaves the results unchanged. The case for Yb corresponds to $N_f=8, \Delta_+$ small and Δ_- large. That will give values similar to those for $N_f=6, L=1$ shown in the figures.

Our main conclusion is that the Seebeck and Kondo temperature decline in value as one considers values L of f-level occupancy larger than one. The same conclusion applies to f holes. Of course, in mixed-valence systems, the ground-state configuration $(4f)^L$ will change has the occupancy fluctuates. Here we denote L as the principle valence. These results suggest that Ce and Yb will have the largest values of the Seebeck coefficient among all of the rare-earth compounds. This theoretical conclusion is in accord with the experimental observations.[8]

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APPENDIX

Here we discuss in more detail the derivation of Eqs. (4.1–4.2). Define $|n\rangle$ as the exact eigenstate of H_0, while $|\alpha)$ is the exact eigenstate of $H=H_0+V$. In terms of these states, we define the spectral and Green's functions as

$$H|\alpha)=\mathcal{E}_\alpha|\alpha), \tag{A1}$$

$$A_n(\omega)=2\pi\langle n|\delta(\omega-H)|n\rangle \tag{A2}$$

$$=2\pi\sum_\alpha \delta(\omega-\mathcal{E}_\alpha)|(\alpha|n\rangle|^2, \tag{A3}$$

$$G_n(\omega)=\sum_\alpha \frac{|(\alpha|n\rangle|^2}{\omega-\mathcal{E}_\alpha+i\eta}. \tag{A4}$$

In terms of these quantities, we can define the self-energy as

$$\Sigma_n(\omega)=\sum_I \frac{|(I|V|n\rangle|^2}{\omega-\mathcal{E}_I} \tag{A5}$$

$$=\frac{1}{N}\sum_{k\alpha} V_k^2\left\{\frac{n_k|(\alpha|f^\dagger|n\rangle|^2}{\omega-(\mathcal{E}_\alpha-\varepsilon_k)}+\frac{(1-n_k)|(\alpha|f|n\rangle|^2}{\omega-(\mathcal{E}_\alpha+\varepsilon_k)}\right\} \tag{A6}$$

$$=\frac{1}{N}\sum_{k\alpha} V_k^2\left\{\frac{n_k|(\alpha|n+1\rangle\langle n+1|f^\dagger|n\rangle|^2}{\omega-(\mathcal{E}_\alpha-\varepsilon_k)}+\frac{(1-n_k)|(\alpha|n-1\rangle\langle n-1|f|n\rangle|^2}{\omega-(\mathcal{E}_\alpha+\varepsilon_k)}\right\} \tag{A7}$$

$$=\frac{1}{N}\sum_k V_k^2\{(N_f-n)n_kG_{n+1}(\omega+\varepsilon_k)+n(1-n_k)G_{n-1}(\omega-\varepsilon_k)\}. \tag{A8}$$

The summation over intermediate states $(I|$ includes the exact states $(\alpha|$ and the eigenstates of the band electrons. They are summed explicitly in the second line. The two terms correspond to the processes in V of adding or removing an electron from the local f level. The last equation, in the above set, is the expression for the self-energy in the noncrossing approximation. In terms of these functions, expression (4.2) for Z can be derived in a few lines

$$Z=\sum_n Z_n\langle n|e^{-\beta H}|n\rangle \tag{A9}$$

$$=\sum_n Z_n\sum_\alpha e^{-\beta\mathcal{E}_\alpha}|(\alpha|n\rangle|^2 \tag{A10}$$

$$=\sum_n Z_n\int\frac{d\varepsilon}{2\pi}e^{-\beta\varepsilon}A_n(\varepsilon). \tag{A11}$$

A similar technique can be used to derive the spectral function $A_f(\omega)$.

$$\mathcal{G}_f(ik_n)=-\frac{1}{Z}\sum_n Z_n\int_0^\beta d\tau e^{ik_n\tau}\langle n|e^{-(\beta-\tau)H}fe^{-\tau H}f^\dagger|n\rangle.$$

The expression in brackets can be written exactly as

$$\sum_{\alpha\lambda n'}\langle n|\alpha)e^{-(\beta-\tau)\mathcal{E}_\alpha}(\alpha|n'\rangle\langle n'|f|n'+1\rangle \times\langle n'+1|\lambda)e^{-\tau\mathcal{E}_\lambda}(\lambda|n+1\rangle\langle n+1|f^\dagger|n\rangle. \qquad \text{(A12)}$$

We adopt the approximation of Refs. 25,26 and restrict the summation to the terms with $n'=n$. Gunnarsson and Schönhammer[9,10] consider the terms with $n'=n\pm1$ and find they make a small contribution. These are vertex corrections. This approximation simplifies the expression. After performing the integral over τ we find .

$$\mathcal{G}_f(ik_n)=\frac{1}{Z}\sum_n Z_n(N_f-n)\sum_{\alpha\lambda}|(\alpha|n\rangle|^2|(\lambda|n+1\rangle|^2 \times\frac{e^{-\beta\mathcal{E}_\alpha}+e^{-\beta\mathcal{E}_\lambda}}{ik_n+\mathcal{E}_\alpha-\mathcal{E}_\lambda}. \qquad \text{(A13)}$$

The summations over α and λ can be expressed in terms of the spectral functions A_n and A_{n+1} which immediately produces the result (4.1) for the spectral function $A_f(\omega)$.

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