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RESONANCE FORMATION IN THE SYMMETRIC ANDERSON MODEL

M. Salomaa*

Department of Physics, University of California, Los Angeles, CA 90024, U.S.A.

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We discuss the temperature dependence of the local *d*-electron spectral density function for the symmetric Anderson model in the local spin fluctuation limit. The present calculation provides a description of the rapid but continuous transition of the quasi-particle between the high and low temperature regimes.

THE ANDERSON HAMILTONIAN, first proposed in 1961 to describe magnetic impurities in metals [1], proved notoriously difficult in regard to extracting pure numbers to be compared with experimental data. Only quite recently two important advances were made to obtain relevant quantitative results from this deceivingly simple-appearing model:

(i) Wilson's numerical renormalization group (RNG) technique, which was originally devised for the Kondo model [2], was generalized to the Anderson Hamiltonian by Krishna-murthy, Wilkins and Wilson [3]. Their work provided the static susceptibility of magnetic impurities in metals for any parameters of the Anderson model. However, no calculations of any dynamic properties of the Anderson model have been reported in the framework of the RNG approach.

(ii) Yosida and Yamada developed a convergent perturbation theory [4] in terms of the Coulomb repulsion energy in the local spin fluctuation (LSF) limit. The latter authors employed a complicated machinery involving Pfaffian determinants to derive some static and dynamic properties of the Anderson Hamiltonian. In particular, they were able to calculate the local density of *d*-electron states and to show that at zero temperature it has a triple peaked structure.

The basic Anderson Hamiltonian is presently understood to model the underlying physics of a large variety of different systems of great interest. There thus appears to exist ample reason to try and find simpler methods than the above ones in order to obtain at least qualitatively the correct basic properties of this important model. In this communication we want to present a short derivation of the second-order self-energy for the *d*-electron propagator using an equation of motion method pioneered by Götze and Wölfle [5] in connection with the *s*–*d* model. At zero temperature our calculation agrees with that of Yosida and Yamada, but ours has the advantage of being applicable at any temperature, not only at $T = 0$. This facilitates discussion of the rapid but smooth change in the nature of the impurity complex as temperature is varied.

In order to illustrate our approach, let us consider the Anderson Hamiltonian [1]

$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} (V_k c^\dagger_{k\sigma} d_\sigma + V^*_k d^\dagger_\sigma c_{k\sigma}) + \sum_\sigma E_\sigma d^\dagger_\sigma d_\sigma + U d^\dagger_\sigma d_\sigma d^\dagger_{-\sigma} d_{-\sigma}. \tag{1}$$

The $c^\dagger_{k\sigma}$ and $d^\dagger_\sigma$ are creation operators for the conduction and *d*-electrons, respectively, and σ is the spin index. We employ standard notation [1–4], we shall assume here the symmetric situation $2E + U = 0$ for simplicity and work in zero external field. It is convenient to measure the strength of the admixture interaction whose matrix element is V_k by $\Gamma = \pi N(0)\langle |V_k|^2\rangle$, where $N(0)$ is the density of conduction band states at the Fermi level and the angular brackets denote averaging over the Fermi surface.

We shall use $\langle\langle A; B\rangle\rangle^\pm_z$ to denote double-time anticommutator and commutator Zubarev functions [6]. They represent the linear response of an operator A to a perturbation which has been coupled to B; they obey the Heisenberg equations of motion:

$$z\langle\langle A; B\rangle\rangle^\pm_z = \langle [A, B]_\pm\rangle + \langle\langle [A, H]; B\rangle\rangle^\pm_z, \tag{2a}$$

$$= \langle [A, B]_\pm\rangle - \langle\langle A; [B, H]\rangle\rangle^\pm_z. \tag{2b}$$

An important quantity to consider is the *d*-electron anticommutator Green's function

$$G_\sigma(z) = -\langle\langle d_\sigma; d^\dagger_\sigma\rangle\rangle^+_z. \tag{3}$$

We may introduce a holomorphic self-energy function $\Sigma_\sigma(\omega \pm i0) = \Sigma'_\sigma(\omega) \pm i\Sigma''_\sigma(\omega)$, to represent G_σ as follows

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*Permanent address: Department of Theoretical Physics, University of Helsinki, SF-00170 Helsinki 17, Finland.

$$\langle\langle d_\sigma ; d_\sigma^\dagger \rangle\rangle_z^+ = \frac{1}{z + i\Gamma + \Sigma_\sigma(z)} . \tag{4}$$

To derive the d-electron self-energy in the leading second order in U, we employ the equation of motion (2a) for the anticommutator function, which yields

$$(z - E_\sigma + i\Gamma)\langle\langle d_\sigma ; d_\sigma^\dagger \rangle\rangle_z^+ = 1 + U\langle\langle n_{-\sigma} d_\sigma ; d_\sigma^\dagger \rangle\rangle_z^+ , \tag{5a}$$

and equation (2b) for the new anticommutator function introduced on the r.h.s. of equation (5a):

$$\begin{aligned}\langle\langle n_{-\sigma} d_\sigma ; d_\sigma^\dagger \rangle\rangle_z^+ (z - E_\sigma + i\Gamma) &= \langle n_{-\sigma} \rangle \\ &+ U\langle\langle n_{-\sigma} d_\sigma ; d_\sigma^\dagger n_{-\sigma} \rangle\rangle_z^+ .\end{aligned} \tag{5b}$$

Comparing the high frequency expansions of equations (5a) and (5b) with that of equation (4) and noting that $\langle n \rangle = 1/2$ identically, in the symmetric case, one finds for the second-order self-energy

$$\Sigma_\sigma(z) = - U^2 \langle\langle n_{-\sigma} d_\sigma ; d_\sigma^\dagger n_{-\sigma} \rangle\rangle_z^+ . \tag{6}$$

Since equation (6) is explicitly of the order U^2, we may to this order in perturbation theory calculate it neglecting correlations. Factorizing in the Fourier transform (time) space yields the absorptive (imaginary) part of the self-energy as

$$\begin{aligned}\Sigma_\sigma''(\omega) = U^2 \int \frac{d\omega'}{2\pi} &\left[\coth \frac{\omega - \omega'}{2T} + \tanh \frac{\omega'}{2T}\right] \\ &\times \chi_{-\sigma}''(\omega - \omega') G_\sigma''(\omega') .\end{aligned} \tag{7}$$

This formula describes the relaxation of d-electron excitations with spin σ due to localized spin fluctuations with spin $-\sigma$. Above G_σ'' may be substituted from equation (4) neglecting Σ, i.e. $G_\sigma''(\omega) = \Gamma/(\omega^2 + \Gamma^2)$, and the commutator function $\chi_{-\sigma}'' = -\langle\langle n_{-\sigma} ; n_{-\sigma} \rangle\rangle_\omega^{-\prime\prime}$, the absorptive part of the local d-spin susceptibility, may be obtained from our previous calculation [7] as

$$\begin{aligned}\chi_{-\sigma}''(\omega) = \frac{1}{\pi\omega} \operatorname{Re} &\left\{ \frac{2i\Gamma}{\omega + 2i\Gamma} \left[\psi\left(\frac{1}{2} + \frac{\Gamma}{2\pi T} - i\frac{\omega}{2\pi T}\right) \right.\right. \\ &\left.\left. - \psi_r\left(\frac{1}{2} + \frac{\Gamma}{2\pi T}\right)\right]\right\} .\end{aligned} \tag{8}$$

Here $\psi(z) = \psi_r(z) + i\psi_i(z)$ denotes the digamma function [8];

The integral in equation (7) cannot be calculated analytically for an arbitrary temperature. We have therefore resorted to the numerical Gauss' integration formula [8]. Note that all figures in this paper were calculated for just one representative value $U/\pi\Gamma = 2$, for brevity.

The absorptive part of the self-energy $\Sigma''(\omega)$ is displayed in Fig. 1(a). At high temperatures ($T = 10\Gamma$ and $T = \Gamma$), $\Sigma''(\omega)$ has a large value at zero frequency and it decreases monotonically for increasing ω. At intermediate temperatures ($T = 0.316\Gamma$ and $T = 0.1\Gamma$), the intercept $\Sigma''(\omega = 0)$ rapidly decreases while the maximum in $\Sigma''(\omega)$ moves out to a finite frequency, roughly $\omega \approx U$. In the low temperature limit (represented by $T = 0.01\Gamma$), low frequency relaxation is inhibited, $\Sigma''(\omega = 0)$ tends towards zero, and in this limit our calculation coincides with that of Yamada [4] (except for a different sign convention: our self-energy function is positive definite, while that of [4] is negative definite).

Since $\Sigma(z)$ is holomorphic and decreases asymptotically as $1/z$, its real (dispersive) part Σ' is connected to the imaginary part Σ'' through a Kramer–Kronig relation. Since $\Sigma''(\omega)$ is even $\Sigma'(\omega)$ is odd and we may express it as an integral over positive frequencies only:

$$\Sigma'(\omega) = 2\omega \int_0^\infty \frac{d\omega'}{\pi} \frac{\Sigma''(\omega')}{(\omega')^2 - \omega^2} . \tag{9}$$

This function was again computed numerically by Gauss' integration formula; it is displayed in Fig. 1(b) for the same parameters as were used in Fig. 1(a) for $\Sigma''(\omega)$. At high temperatures ($T = 10\Gamma$ and $T = \Gamma$), $\Sigma'(\omega)$ decreases linearly for small ω, passes through a minimum for increasing ω and approaches the ω-axis asymptotically from below as $1/\omega$. At intermediate and especially at low temperatures there occurs a positive frequency shift: $\Sigma'(\omega)$ first increases with ω, it reaches a maximum value and then starts to decrease until a minimum is attained and $\Sigma'(\omega)$ gradually tends to the asymptotic $1/\omega$ behaviour.

Using equation (4) we obtain the following representation for the d-electron spectral density function (in zero field there is no spin dependence):

$$G''(\omega) = \frac{\Gamma + \Sigma''(\omega)}{[\omega + \Sigma'(\omega)]^2 + [\Gamma + \Sigma''(\omega)]^2} . \tag{10}$$

Inserting the self-energy of Fig. 1 into equation (10), we have produced the curves displayed in Fig. 2. Note that since $G''(\omega)$ is symmetric it suffices to consider positive frequencies only. In the high temperature ($T = 10\Gamma$) regime one just finds two lifetime broadened resonances at $\omega = \pm U/2$. For decreasing temperature ($T = \Gamma$) the low frequency spectral weight starts to grow at the expense of large frequencies. In the intermediate temperature regime ($T = 0.316\Gamma$ and $T = 0.1\Gamma$) there rapidly forms a third peak at zero frequency, which narrows further with decreasing temperature. At the lowest temperatures the central peak approaches the unitary limiting value and we exactly reproduce the $T = 0$ triple peaked structure obtained by Yamada [4].

The XPS lineshape of $3d$-metal ions dissolved in aluminium [9] is believed to probe the local d-electron

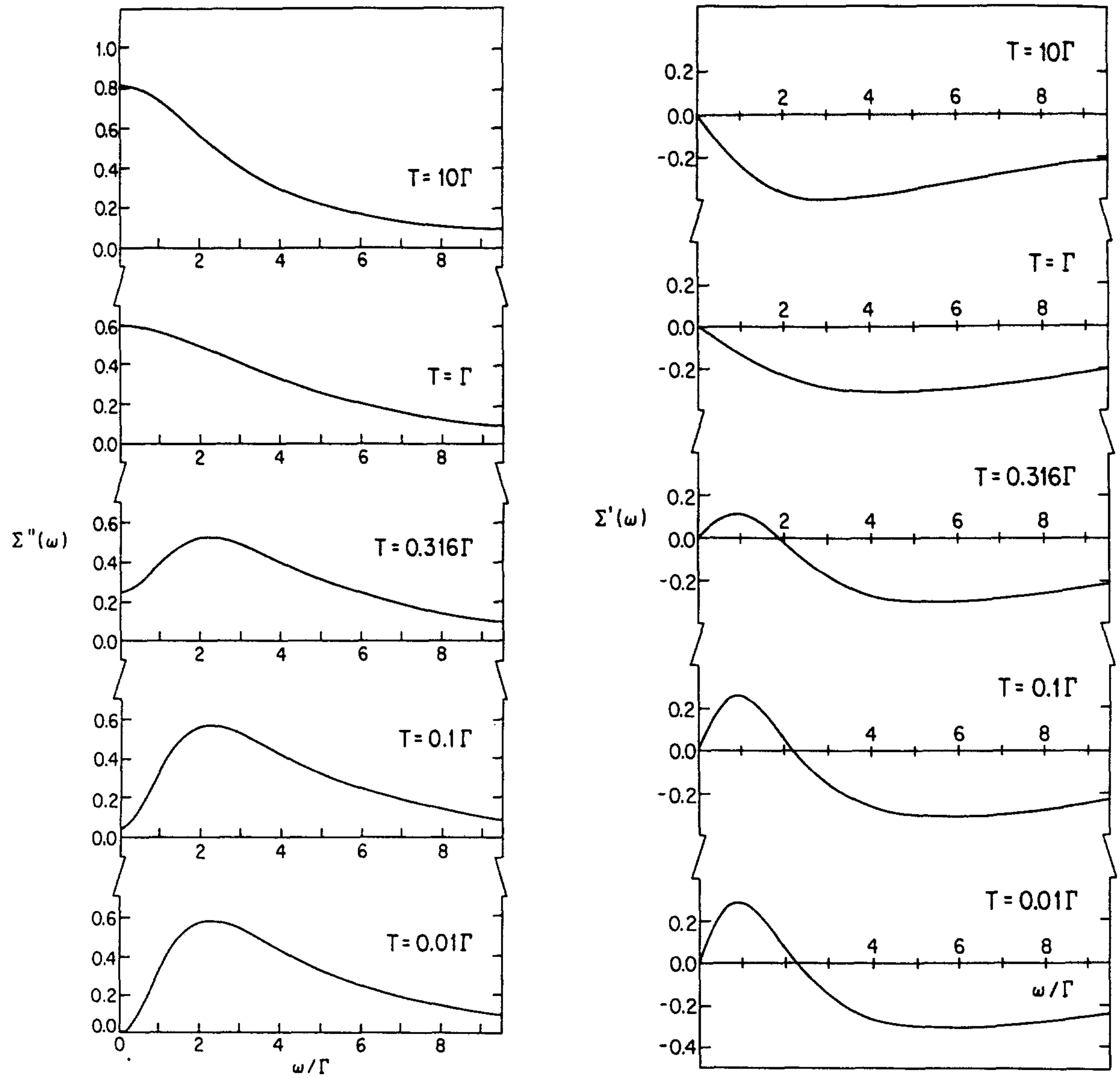

Fig. 1. The second-order d-electron self-energy $\Sigma(\omega) = \Sigma'(\omega) + i\Sigma''(\omega)$ [equation (6), measured in units of $U^2/\pi\Gamma$] as a function of frequency for representative temperatures. (a) The imaginary part of the self-energy $\Sigma''(\omega)$, as obtained from equation (7). (b) The real part of the self-energy $\Sigma'(\omega)$ calculated from $\Sigma''(\omega)$ using the Kramers–Kronig equation (9).

spectral function. It would be interesting to look for a temperature variation in such spectra.

Owing to its simplicity, the present approach is easily extended to encompass the asymmetric and finite field situations, too. Details of these calculations as well as generalizations to more complicated Hamiltonians will be presented elsewhere.

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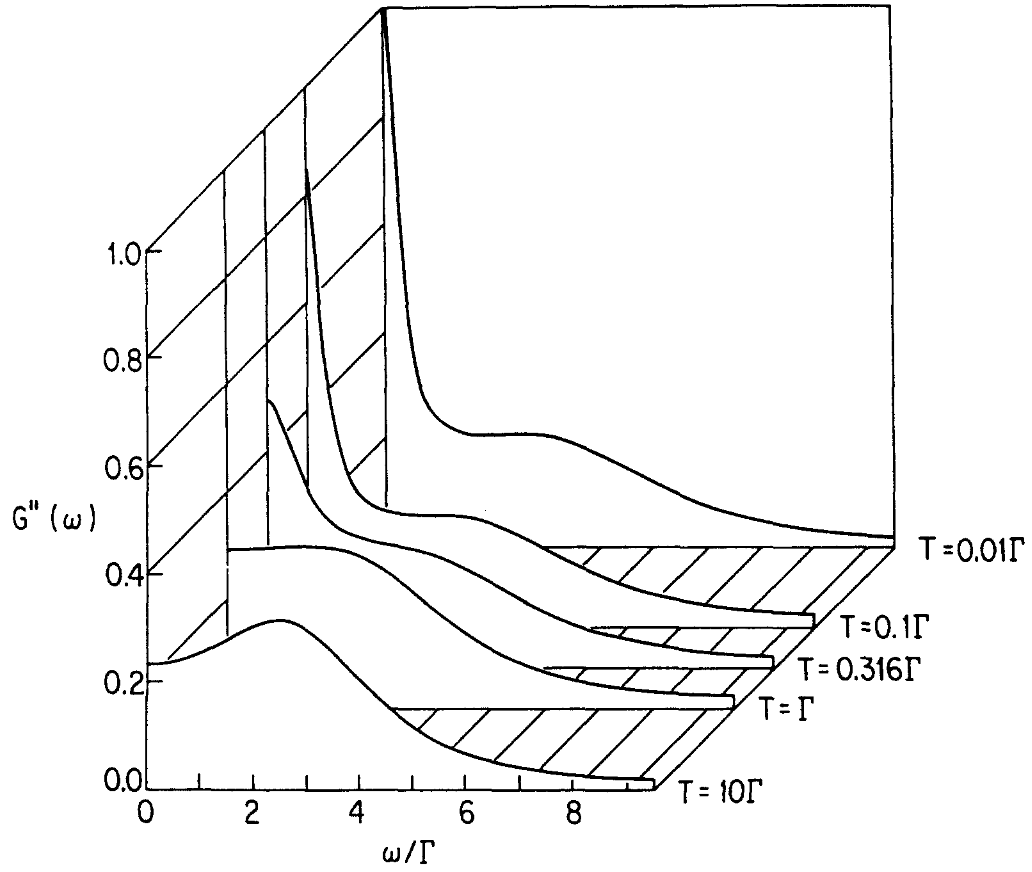

Fig. 2. Temperature variation of the local frequency-dependent *d*-electron spectral density, as obtained from equation (10) using the self-energy displayed in Fig. 1. The spectral function is measured in units of Γ and we used the value $U/\pi\Gamma = 2$.

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