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Specific heat of a localized magnetic impurity in a non-magnetic host: A spectral density method for the Anderson–Holstein model

Ch. Narasimha Raju, Ashok Chatterjee *

School of Physics, University of Hyderabad, Hyderabad 500046, India

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ABSTRACT

The effect of electron–phonon interaction on the spectral function of a magnetic impurity in a non-magnetic host metal is studied within the framework of the Anderson–Holstein model using a spectral density method. The impurity contribution to the specific heat of the host metal is also calculated.

1. Introduction

Several investigations were made in the past on the properties of dilute magnetic alloys. One of the most interesting phenomena that attracted a lot of attention in this context was the appearance of a broad minimum in their resistivity at low temperature. This effect, known as the Kondo effect [1], was first explained by Kondo and can be captured through the single-impurity Anderson model [2–5]. In strongly correlated systems, impurity vibrations do also couple to the local charge on the impurity leading to an electron–phonon (*el–ph*) interaction. Thus in recent years, a few investigations have also been reported on the influence of *el–ph* interaction on the Kondo effect [6–8]. In the present work we shall study the effect of *el–ph* interaction on the spectral function of the impurity and determine its contribution to the specific heat of the non-magnetic host metal.

We shall model a dilute magnetic alloy by the single-impurity Anderson–Holstein (AH) Hamiltonian [9] which is obtained by adding the well-known Holstein *el–ph* interaction term to the Anderson Hamiltonian to describe the linear *el–ph* coupling present on the impurity. This model was first introduced to describe negative-*U* tunneling centers in superconductors [10]. In recent years this model has also been used to study a few other systems like heavy fermionic systems [11] and quantum transport in single molecular transistors [12, 13]. In the present paper we are interested in the contribution of the magnetic impurity to the specific heat of the system. This can be obtained from the double-time-temperature Green functions using the equation of motion method. However, in these methods, one has to use some decoupling approximations for the higher-order Green functions, which restrict the validity of the method. Indeed in a recent paper [14], we have calculated the spectral function and the specific heat of the impurity atom using the equation of motion (EOM) Green function method within the framework of a mean-field decoupling scheme which obviously ignores the fluctuations. The spectral density method (SDM), proposed by Kalashnikov and Fradkin [15] and later used by others [16–23] circumvents this problem. In this method, instead of Green's functions one considers the corresponding spectral densities and writes closed equations between them to calculate the spectral density (SD) function. Once the SD function is calculated, it becomes quite straight-forward to calculate the specific heat of the impurity atom. In the present paper we employ SDM to the AH model to calculate the spectral density of the impurity atom and the corresponding specific heat.

2. Model

The AH model can be expressed as

$$H = \sum_{k,\sigma} \epsilon_{k\sigma} n_{k\sigma} + \sum_{\sigma} \epsilon_d n_{d\sigma} + U n_{d,\sigma} n_{d,-\sigma} + \sum_{k,\sigma} \left(V_k c^{\dagger}_{k\sigma} c_{d\sigma} + h.\, c \right) + \hbar\omega_0 b^{\dagger} b + \lambda\hbar\omega_0 \sum_{\sigma} n_{d\sigma} \left(b^{\dagger} + b \right), \quad (1)$$

* Corresponding author.
E-mail address: acsp@uohyd.ernet.in (A. Chatterjee).

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where $n_{k\sigma}(=c^{\dagger}_{k\sigma}c_{k\sigma})$ stands for the number operator for electrons in the continuum momentum state k and spin σ with energy $\epsilon_{k\sigma}$, $c^{\dagger}_{k\sigma}$ $(c_{k\sigma})$ being the creation (annihilation) operator for the electrons, while $n_{d\sigma}(=c^{\dagger}_{d\sigma}c_{d\sigma})$ stands for the number operator for the electrons of spin σ in the localized non-degenerate level d with energy $\epsilon_{d\sigma}$, $c^{\dagger}_{d\sigma}(c_{d\sigma})$ being the creation (annihilation) operator for these electrons. Thus the first and the second terms in Eq. (1) describe respectively the electrons in the conduction band of the host metal and that on the impurity atom. The third term gives the on-site electron–electron (*el–el*) interaction at the impurity site, U being the strength of the interaction. The fourth term describes the interaction between the impurity and the conduction band electrons with V_k as the strength of the interaction. This term can also be referred to as the s–d interaction with V_k giving a measure of the probability of hopping of an electron from the conduction band to the impurity level. The fifth term denotes the free phonon Hamiltonian with $b^{\dagger}(b)$ as the creation (annihilation) operator for a local phonon of frequency ω_0. The last term describes the local *el–ph* interaction on the impurity with the dimensionless coupling strength λ. Here all the energies are measured from chemical potential.

3. Elimination of phonons

The *el–ph* interaction term in the Hamiltonian is first eliminated by using the well-known Lang–Firsov [24] canonical transformation with a generator

$$S = \lambda\left(b^{\dagger} - b\right)\sum_{\sigma} n_{d\sigma}. \tag{2}$$

followed by a zero-phonon averaging. The effective Anderson Hamiltonian H_{eff} reads

$$H_{eff} = \sum_{k,\sigma}\epsilon_{k\sigma}n_{k\sigma} + \sum_{\sigma}\tilde{\epsilon}_d n_{d\sigma} + \tilde{U}\, n_{d,\sigma}\, n_{d,-\sigma} + \sum_{k,\sigma}\tilde{V}_k\left(c^{\dagger}_{k\sigma}c_{d\sigma} + c^{\dagger}_{d\sigma}c_{k\sigma}\right), \tag{3}$$

where $\tilde{\epsilon}_d = \left(\epsilon_d - \lambda^2\hbar\omega_0\right)$, $\tilde{U} = \left(U - 2\lambda^2\hbar\omega_0\right)$ and $\tilde{V}_k = Ve^{-(\lambda^2/2)}$ which is reminiscent of the well-known Holstein reduction factor. Due to the polaronic effect, ϵ_d and U are renormalized. When the phonon-mediated attractive *el–el* interaction overcomes the *el–el* Coulomb repulsion, the formation of bipolaron at the impurity atom becomes possible [25]. The exponential reduction of the s–d interaction implies that the electron hopping is accompanied by a phonon cloud. Here we assume V_k to be independent of k i.e. we consider $V_k = V$. In the long wavelength limit this is a good enough approximation. Furthermore, we have considered for the conduction band of the host metal a constant density of states. In the present work, we closely follow the approach of Gavrilenko and Fedyanin [26].

4. Spectral density method

This method is based on the choice of a physically motivated single-particle spectral density (SD) function with some parameters. In this work we use a modified Gaussian ansatz for the SD function to consider the damping effect of quasi-particles on the impurity. Thus we choose

$$\Lambda_{d\sigma}(\omega) = \frac{f(\omega)}{M^{(0)}_{d\sigma}(\omega)}e^{-(\omega-\alpha)^2/\Gamma^2}, \tag{4}$$

where $M^{(0)}_{d\sigma}(\omega)$ is the normalization constant, $f(\omega)$ is the Fermi distribution and α and Γ are the free parameters denoting the position and width of the peak of SD function, respectively. The free parameters are calculated self-consistently using the spectral moment relation given by

$$M^{(m)}_{d\sigma}(\omega) = \frac{1}{\hbar}\int \omega^m \Lambda_{d\sigma}(\omega)d\omega = \left\{\left[c_{d\sigma}, H_{eff}\right]_m, c^{\dagger}_{d\sigma}\right\}, \tag{5}$$

where $M^{(m)}_{d\sigma}(\omega)$ is the mth moment of the SD function $\Lambda_{d\sigma}(\omega)$ and

$$\left[c_{d\sigma}, H_{eff}\right]_0 = c_{d\sigma}, \tag{6a}$$

$$\left[c_{d\sigma}, H_{eff}\right]_1 = \left[c_{d\sigma}, H_{eff}\right], \tag{6b}$$

$$\left[c_{d\sigma}, H_{eff}\right]_2 = \left[\left[c_{d\sigma}, H_{eff}\right], H_{eff}\right], \tag{6c}$$

and so on. After solving the spectral moment relation in Eq. (5) for $m = 0, 1, 2$, we obtain

$$M^{(0)}_{d\sigma}(\omega) = \Gamma\sqrt{\pi}, \tag{7a}$$

$$M^{(1)}_{d\sigma}(\omega) = \alpha = \tilde{\epsilon}_d + \tilde{U}n_{d,-\sigma}, \tag{7b}$$

$$M^{(2)}_{d\sigma}(\omega) = \alpha^2 + \Gamma^2/2 = 2\tilde{\epsilon}_d\tilde{U}n_{d,-\sigma} + \tilde{\epsilon}^2_d + \tilde{U}^2 n_{d,-\sigma} + \sum_k \tilde{V}^2, \tag{7c}$$

which yield

$$\Gamma = \sqrt{2}\left[\tilde{U}^2\left(n_{d,-\sigma} - n_{d,-\sigma^2}\right) + \sum_k \tilde{V}^2\right]^{1/2}. \tag{8}$$

Once the SD function is obtained, the average occupancy of the impurity can be determined in a self-consistent way at finite temperature. We obtain

$$n_{d\sigma} = \int_{-\infty}^{\infty}\Lambda_{d\sigma}(\omega)d\omega = \frac{1}{2}erfc\left(\frac{\alpha-\mu}{\Gamma}\right) + \frac{(\pi k_B T)^2\alpha}{3\sqrt{\pi}\Gamma^3}e^{-(\alpha/\Gamma)^2}. \tag{9}$$

To solve the above integral we use the Sommerfeld expansion and retain terms up to quadratic in k_BT. The contribution to the specific heat C from the impurity electron [27] can be obtained using the expression as

$$C = \frac{1}{3}(\pi k_B)^2 T\sum_{\sigma}\Lambda_{d\sigma}(0). \tag{10}$$

5. Results and discussion

Here we consider a three-dimensional symmetric AH model i.e. $\epsilon_d = -U/2$ and make a flat band approximation for the electron density of states $g(0)$. It is a good enough approximation in many cases, as a small variation in the density of states does not significantly alter the physical properties. We fix $\hbar = \omega_0 = 1$ and measure energies in units of $\hbar\omega_0$. In Figs. 1 and 2 we study the SD function as a function of ω for different values of the *el–ph* interaction strength λ for $U = 2$ and $U = 5$, respectively. Comparison of Figs. 1 and 2 shows that as the *el–el* interaction strength increases, the height of the peak of the SD function also increases. The effect of the *el–ph* interaction on the SD function is also clearly visible from both the figures. In the absence of the *el–ph* interaction i.e., for $\lambda = 0$, the SD function has a peak at $\omega = 0$. As the *el–ph* interaction increases, the peak position of the SD function shifts towards the left. It indicates the formation of polaron at the