A theory of resistivity in Kondo lattice materials: memory function approach

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Abstract
We have theoretically analysed DC resistivity ($\rho$) in the Kondo-lattice materials using the powerful memory function formalism. The complete temperature evolution of $\rho$ is investigated using the Wölfle–Götze expansion of the memory function. The resistivity in this model originates from spin–f\textsubscript{l}ip magnetic scattering of conduction s-electrons off the quasi-localized d or f electron spins. We find the famous resistivity upturn in lower temperature regime ($k_B T < \mu_d$), where $\mu_d$ is the effective chemical potential of d-electrons. In the high temperature regime ($\mu_d < k_B T$) we discover that resistivity scales as cube root of $T$ ($\rho \propto T^{3/2}$).

Our results are in reasonable agreement with the experimental results reported in the literature.

Keywords: Kondo effect, Kondo resistivity, scattering mechanism, memory function formalism, heavy-fermion systems

1. Introduction

In heavy fermion materials such as CeCu\textsubscript{2}Si\textsubscript{2}, CeCu\textsubscript{2}Ge\textsubscript{2}, UR\textsubscript{2}Si\textsubscript{2}, UPd\textsubscript{2}Al\textsubscript{3} etc \cite{1, 2} at sufficiently high temperatures ($T > T_K$) where $T_K$ is the Kondo temperature, it becomes possible to divide the electronic system into two components: (1) mobile or conduction s-electrons, and (2) localized d or f moments. The localized moments lead to the typical curie susceptibility ($\chi \propto \frac{1}{T}$) and the itinerant s-electrons provide the electrical conduction. As temperature is lowered the conduction electron spins start to quantum mechanically hybridize with the localized d or f-moments. At sufficiently low temperature $T_K$, conduction electrons and localized f moments form what is known as Kondo singlets. The process of hybridization is gradual one starting from higher temperature, where f-moments are free, to very low temperature ($T < T_K$) where f-moments form spin singlets with conduction s electrons. In this very low temperature regime ‘hybridized electrons’ emerges. These ‘hybridized electrons’ are very heavy (their mass is many order of magnitude larger than free electron mass). That why these systems are called heavy Fermion systems. It turns out that the Fermi volume contains both the conduction s-electrons and the ‘localized’ f or d electrons in the low temperature regime, $T < T_K$. However, in the high temperature regime Fermi volume contains the conduction electrons only not the localized f or d-moments \cite{1, 2}.

The current investigation, however, is devoted to a different problem of electrical conduction in related systems. In the current investigation which is valid for $T > T_K$ we study the scattering of conduction s-electrons via the quasi-localized f-moments. Our aim is to calculate the temperature dependence of the electrical resistivity originating from magnetic scattering.

Resistivity from magnetic scattering is a well known phenomena \cite{7–15}. The Kondo effect of resistivity minima in materials containing magnetic impurities such as AuFe is a well known phenomena \cite{3–5}. It occurs due to spin flip scattering of conduction electrons via spin flips of localized magnetic impurity spin. Kondo explained it using second order perturbation theory \cite{3–5}. In other words it takes into account the spin flip of the impurity and scattering electron as an intermediate state:

$$\sum_{k'\epsilon'} J(k\downarrow, \uparrow \rightarrow k'\epsilon\uparrow, \downarrow) J(k'\epsilon\uparrow, \downarrow \rightarrow k'\epsilon\uparrow, \uparrow) \left(1 - f_{\epsilon'} \right),$$

where the factor $1 - f_{\epsilon'}$ represents the probability that the state $|k'\epsilon\rangle$ is empty. The above term represents the scattering of an
electron with wavevector \( k \) in spin down state \( | \downarrow \rangle \) and the impurity in spin up state \( | \uparrow \rangle \) into an intermediate state having electron with wavevector \( k' \) but flipped spins for both the impurity and the electron. Then from this intermediate state electron scatters to a final state with wavevector \( k'' \) with one more flips of electron and impurity spins, such that the spin states returns back to its original form. As is well known the resistivity due to above Kondo term scales as \( \log(T) \) \cite{3-6}. However, this calculation does not capture full temperature evolution of resistivity. Our calculation using memory function formalism incorporates the above Kondo term and we analytically obtain the full temperature dependence of the resistivity including the high temperature behaviour, \( \rho \propto T^2 \). In the present treatment the coupling of \( s \)-electrons with quasi-localized \( d \) or \( f \)-moments is taken to be the Kondo coupling. We treat \( d \) or \( f \) electrons as quasi-localized instead of perfectly localized ones as considered in the standard Kondo problem. Perfect localization of \( f \) or \( d \) electrons occurs in the integer valence compounds (at half filling) \cite{1}. Due to integer valence and strong onsite Coulomb repulsion (Hubbard \( U \)) double occupancy at a given site is prohibited. In our calculation we consider systems away from integer valence and \( d \) or \( f \) electrons are treated as quasi-localized, and they form a small Fermi surface (see section 2 and appendix A). The coupling Hamiltonian is the Kondo lattice Hamiltonian also known in the literature as \( s-d \) Hamiltonian:

\[
H_{sd} = \frac{J}{N} \sum_{k'k} \left\{ a_{k'\uparrow}^\dagger a_{k\uparrow} S^-(k' - k) + a_{k\downarrow}^\dagger a_{k'\downarrow} S^+(k' - k) \\
+ (a_{k'\uparrow}^\dagger a_{k\uparrow} - a_{k\downarrow}^\dagger a_{k'\downarrow}) S^0(k' - k) \right\} \tag{2}
\]

Here \( a_{k\sigma}^\dagger, a_{k\sigma} \) are the operators of \( s \)-electrons and \( S^-(k' - k) \) is the spin lowering operator of \( d \)-or \( f \) electrons (\( S^0(q) = \sum_x a_{x\sigma}^\dagger a_{x\sigma} \)).

Another novelty of our calculation over the published calculations of electrical resistivity \cite{7-13, 17} is that it is manifestly beyond the relaxation time approximation (RTA) which is taken into account in the memory function formalism \cite{19-23} (our main tool in the current investigation) and full temperature evolution of the resistivity can be calculated whereas in the references \cite{7-13, 17} resistivity is calculated either using the variational solution of the Bloch–Boltzmann equation or the iterative approximate method \cite{16, 19}. The problem with the Bloch–Boltzmann approach is that the full temperature evolution of resistivity is difficult to obtain analytically (only in low and high temperature limits (with respect to the Debye temperature), the collision integral can be analytically simplified). Within the memory function formalism, we could analyse the full temperature evolution of resistivity rigorously and point out two regimes of interest: in the low temperature regime (\( k_B T \ll \mu_d \)), we find an upturn in the resistivity and in the high temperature regime (\( k_B T \gg \mu_d \)), we find that \( \rho \propto T^2 \). We also find that when some mobility is allowed for \( d \) electrons Kondo logarithmic (\( \rho \propto -\log(T) \)) is replaced by a power law \( \rho \propto \frac{1}{T} f(\frac{T}{\mu_d}) \) (where scaling form \( \frac{1}{T} \) is weak function of \( T \)) in the low temperature limit.

2. Computational procedure: MF formalism

In Kubo’s linear response theory, the dynamical conductivity is given by

\[
\sigma_{\mu\nu}(\omega) = V \int_0^\infty dt e^{\omega t} \int_0^\beta d\lambda \langle J_{\mu}(s) (-i\hbar \lambda) J_{\nu}(t) \rangle. \tag{3}
\]

This is called the Kubo formula \cite{18, 19, 23}. By using the Mori–Zwanzig projection operator technique the above Kubo formula can be rewritten in the following form \cite{19, 23}

\[
\sigma_{\mu\nu}(\omega) = \frac{i}{4\pi} \frac{\omega}{z + \mu \nu} \tag{4}
\]

Here \( M_{\mu\nu}(z) \) is called the memory function and \( z \) is the complex frequency \((z = \omega + i\delta)\). Thus, the problem of computation of the dynamical conductivity boils down to the computation of the memory function \( M_{\mu\nu}(z) \). Within the Götze–Wölfle approach the memory function is computed using the equation of motion method and a perturbative expansion of the memory function. All the technical details are available in references \cite{19, 23} here we outline the approach. It turns out that

\[
M(z) \approx \frac{1}{z} \left( \frac{ne^2}{m} \right) \left[ \langle \langle J_1; J_\tau \rangle \rangle - \langle \langle J_\tau; J_1 \rangle \rangle \right] \tag{5}
\]

where

\[
J_1 = -\frac{i}{\hbar}[J_1, H]. \tag{6}
\]

The total Hamiltonian is \( H = H_0 + H_{sd} \) and \( H_0 \) is the free electron unperturbed part and \( H_{sd} \) is defined in equation (2). The double brackets are defined as

\[
\langle \langle \hat{O}_1; \hat{O}_2 \rangle \rangle = \frac{V}{h} \int_0^\infty d\tau e^{\omega \tau} \langle \langle \hat{O}_1(t); \hat{O}_2(0) \rangle \rangle \tag{7}
\]

Here \( \langle \cdot \cdot \cdot \rangle \) means canonical ensemble average. The operator \( \hat{O}(t) \) is in the Heisenberg representation \( \hat{O}(t) = e^{iH_0t} \hat{O}(0) e^{-iH_0t} \). The current density operator is \( J_1 = \frac{e}{V} \sum_{k, \sigma} v_{1\sigma} a_{k\sigma}^\dagger a_{k\sigma} \) with \( v_1 = \frac{\hbar \delta}{eV} \) and \( V \) is the volume of the sample. With this information equation (6) takes the form:

\[
\dot{J}_1 = -\frac{e}{V} \sum_x \sum_{k'k} \left\{ v_1(\lambda) a_{k'\sigma}^\dagger a_{k\sigma} \right\} \sum_{k, k'} \left[ a_{k'\sigma}^\dagger a_{k\sigma} \right] S^0(k' - k) + (a_{k'\sigma}^\dagger a_{k\sigma} - a_{k\sigma}^\dagger a_{k'\sigma}) S^0(k' - k) \right\} \tag{8}
\]

The current operator commutes with the unperturbed Hamiltonian, hence we are left with terms containing \( H_{sd} \) which is treated as a perturbation. Using Leibniz’s bracket rule \([ab, c] = a[b, c] - [a, c]b\), the above expression reduces to
\[ \hat{J}_1 = -i \frac{e \ell_j}{2N\hbar V} \sum_{k,k'} (v_1(k') - v_1(k)) \times \left( a_{k'\uparrow}^\dagger a_{k\uparrow} S'(k' - k) + a_{k'\downarrow}^\dagger a_{k\downarrow} S^+(k' - k) \right). \]  

(9)

Define the correlator \( \phi(z) = \langle \langle \hat{J}_1; \hat{J}_1 \rangle \rangle : \)

\[ \phi(z) = -\frac{e^2 \hbar^2}{N^2 \hbar^2 V^2} \sum_{k,k'} \sum_{p,p'} \left( v_1(k') - v_1(k) \right) \left( v_1(p) - v_1(p') \right) \times \left\{ \langle a_{k'\uparrow}^\dagger a_{k\uparrow} S'(k' - k) \rangle + a_{k'\downarrow}^\dagger a_{k\downarrow} S^+(k' - k) ; a_{p'\uparrow}^\dagger a_{p\uparrow} S'(p - p') + a_{p'\downarrow}^\dagger a_{p\downarrow} S^+(p - p') \right\}. \]  

(10)

Then the memory function (5) can be written as \( \mathcal{M}(z) \simeq \frac{1}{\sqrt{N^2 V^2}} \phi(z) - \phi(0) \). This is called the Götze–Wölfle memory function approximation [19, 23]. Now for the computation of memory function we need to compute the correlator \( \phi(z) \):

\[ \phi(z) = \langle \langle \hat{J}_1; \hat{J}_1 \rangle \rangle = i \frac{\hbar}{N^2 V^2} \int_0^\infty \text{d} \tau \text{d} \zeta \langle \langle \hat{J}_1(t); \hat{J}_1(0) \rangle \rangle \text{d} t. \]  

(11)

The correlation function \( \phi(z) \) can be simplified to

\[ \phi(z) = -\frac{e^2 \hbar^2}{N^2 \hbar^2 V^2} \sum_{k,k'} \sum_{p,p'} \left( v_1(k') - v_1(k) \right) \left( v_1(p) - v_1(p') \right) \times \left\{ \langle a_{k'\uparrow}^\dagger a_{k\uparrow} S'(k' - k) ; a_{p'\uparrow}^\dagger a_{p\uparrow} S^+(p - p') \rangle + \langle a_{k'\downarrow}^\dagger a_{k\downarrow} S^+(k' - k) ; a_{p'\downarrow}^\dagger a_{p\downarrow} S^+(p - p') \rangle \right\}, \]  

(12)

as the cross-terms of the form \( \langle a_{k'\uparrow}^\dagger a_{k\uparrow} S'(k' - k) ; a_{p'\downarrow}^\dagger a_{p\downarrow} S^+(p - p') \rangle \) vanish [19, 23]. We separate the function \( \phi(z) \) into two sub functions \( \phi_1(z) \) and \( \phi_2(z) \) for simplification. The first function takes the form:

\[ \phi_1(z) = -i \frac{e^2 \hbar^2}{N^2 \hbar^2 V^2} \sum_{k,k'} \sum_{p,p'} \left( v_1(k') - v_1(k) \right) \left( v_1(p) - v_1(p') \right) \times \int_0^\infty \text{d} \tau \text{d} \zeta \left\{ a_{k'\uparrow}^\dagger(t) a_{k\uparrow}(t) S'(k' - k, t), a_{p'\uparrow}^\dagger(t) a_{p\uparrow}(t) S^+(p - p', t) \right\}. \]  

(13)

It is to be noted the impurity and conduction electron spin flip terms of the form of equation (2) are incorporated in the commutator in the above equation (13) that is \( a_{k'\uparrow}^\dagger(t) a_{k\uparrow}(t) S'(k' - k, t), a_{p'\uparrow}^\dagger(t) a_{p\uparrow}(t) S^+(p - p', t) \) etc. as we write the time dependence of operators explicitly as \( a_{k'\uparrow}(t) = e^{i\omega_{k'} t} a_{k'\uparrow}(0) \) for s-band mobile electrons. For d-band density operators we write

\[ S^-(k' - k, t) = e^{-i\omega_{k'} t} S'(k' - k, t, 0). \]  

In the present case \( \hbar \omega_{k' - k} \) represents the spin flip energy of an excitation of the quasi localized of d or f electrons. Dispersion of the magnetic excitation created by operators \( S'(q) \) and \( S^+(q) \) is assumed to be of the form \( \hbar \omega_q \approx \hbar^2 q^2 \) in the long wavelength limit which we use in the present calculation [8]. Next on performing the time integration and applying anticommutating Leibniz rule\(^5\) to the Fermion operators in equation (13) we obtain

\[ \phi_1(z) = C_1 \sum_{k,k} \sum_{p,p'} \left( \frac{1}{\frac{\omega_{k' - k} - \omega_k}{\hbar} - \frac{\omega_{k' - k} + \omega}{\hbar}} \right) \left( v_1(k') - v_1(k) \right) \times \left\{ \langle a_{k'\uparrow}^\dagger a_{k\uparrow} S'(k' - k) ; a_{p'\uparrow}^\dagger a_{p\uparrow} S^+(p - p') \rangle + \langle a_{k'\downarrow}^\dagger a_{k\downarrow} S^+(k' - k) ; a_{p'\downarrow}^\dagger a_{p\downarrow} S^+(p - p') \rangle \right\}. \]  

(14)

Here \( C_1 = \frac{e^2 \hbar^2}{N^2 \hbar^2 V^2} \). We write \( \langle a_{k'\uparrow}^\dagger a_{k\uparrow} a_{p'\uparrow}^\dagger a_{p\uparrow} \rangle = \langle a_{k'\uparrow}^\dagger (\delta_{k \uparrow} - a_{p'\downarrow}^\dagger a_{p\downarrow}) \rangle \) and use bracket rule\(^4\) to solve factor \( \langle a_{k'\downarrow}^\dagger a_{k\downarrow} a_{p'\downarrow}^\dagger a_{p\downarrow} \rangle \). On simplifying, using the properties of delta functions \( \delta_{k \uparrow} \) and \( \delta_{k' \downarrow} \), we get:

\[ \phi_1(z) = -C_1 \sum_{k,k} \left( \frac{1}{\frac{\omega_{k' - k} - \omega_k}{\hbar} - \frac{\omega_{k' - k} + \omega}{\hbar}} \right) \left( v_1(k') - v_1(k) \right)^2 \times \left\{ f_{k'\uparrow}^d (1 - f_{k'\uparrow}^d) \langle [S'(k' - k), S^+(k - k')] \rangle \right. \]  

\[ + \left. (f_{k'\uparrow}^d - f_{k'\uparrow}^d) \langle S^+(k - k') S^{-}(k' - k) \rangle \right\}. \]  

(15)

Here \( f_{k'\uparrow}^d = \langle a_{k'\uparrow}^\dagger a_{k\uparrow} \rangle \) is the Fermi function of the s-band electrons. The spin density operators of d-band transforms the expression (15) to (refer to appendix A)

\[ \phi_1(z) = -C_1 \sum_{k,k} \left( \frac{1}{\frac{\omega_{k' - k} - \omega_k}{\hbar} - \frac{\omega_{k' - k} + \omega}{\hbar}} \right) \left( v_1(k') - v_1(k) \right)^2 \times \left\{ f_{k'\uparrow}^d (1 - f_{k'\uparrow}^d) \sum_{k'_\uparrow, k''_\uparrow} \left( f_{k'\uparrow}^d - f_{k''_\uparrow}^d \right) \right. \]  

\[ - \left. (f_{k'\uparrow}^d - f_{k''_\uparrow}^d) \sum_{k'_\downarrow, k''_\downarrow} \left( f_{k'\downarrow}^d - f_{k''_\downarrow}^d \right) \right\}. \]  

(16)

Similarly write \( \phi_2(z) \) part from equation (12):

\[ \phi_2(z) = -\frac{e^2 \hbar^2}{N^2 \hbar^2 V^2} \sum_{k,k'} \sum_{p,p'} \left( v_1(k') - v_1(k) \right) \left( v_1(p) - v_1(p') \right) \times \left\{ \langle a_{k'\uparrow}^\dagger a_{k\uparrow} S^{-}(k' - k) ; a_{p'\uparrow}^\dagger a_{p\uparrow} S^+(p - p') \rangle \right\}. \]  

(17)

Again following the similar steps that are followed for the calculation of \( \phi_1(z) \), we obtain expression for \( \phi_2(z) \) as:

\[ {\{a, b, c\}d} = a_{\{b, c\}d} - a_{\{b, d\}c} + a_{\{c, d\}b} - c_{\{a, d\}b}. \]
\[ \phi(z) = -C_1 \sum_{k'k} \left( \frac{1}{\frac{\hbar}{k} - \frac{\hbar}{k'} - \omega_{k'-k} - z} \right) (v_1(k') - v_1(k))^2 \]
\[ \times \left[ f'_{k'} (1 - f'_{k'}) \sum_{k_d k_d'} (f'_{k_d'} - f'_{k_d}) \right] \]
\[ - (f'_{k_d} - f'_{k_d'}) \sum_{k_d k_d'} (1 - f'_{k_d'}) \right]. \tag{18} \]

We drop the spin notation in Fermi functions as there is no Zeeman splitting (no external and internal magnetic fields present). The total \( \phi(z) \) takes the form:
\[ \phi(z) = -\frac{e^2 f^2}{N^2 \hbar^3 V} \sum_{k'k} (v_1(k') - v_1(k))^2 \left\{ f'_{k'} (1 - f'_{k'}) \right. \]
\[ \times \left[ (f'_{k_d'} - f'_{k_d}) - (f'_{k_d} - f'_{k_d'}) \sum_{k_d k_d'} (1 - f'_{k_d'}) \right] \]
\[ \left. \times \left[ \frac{1}{\frac{\hbar}{k} - \frac{\hbar}{k'} - \omega_{k'-k} - z} + \frac{1}{\frac{\hbar}{k} - \frac{\hbar}{k'} - \omega_{k'-k} - z} \right]. \tag{19} \]

### 3. Computation of the memory function in the DC limit

Our aim is to determine the dynamical conductivity \( \sigma(z) \) that depends on the memory function, therefore writing \( \phi(z) \) in terms of \( M(z) \) using formula \( M(z) = \frac{i}{\hbar} \frac{d}{dz} (\phi(z) - \phi(0)) \), we obtain
\[ M(z) = -\frac{f^2 m}{N^2 \hbar^3 n V} \omega \sum_{k'k} (v_1(k') - v_1(k))^2 \left\{ f'_{k'} (1 - f'_{k'}) \right. \]
\[ \times \left[ (f'_{k_d'} - f'_{k_d}) - (f'_{k_d} - f'_{k_d'}) \sum_{k_d k_d'} (1 - f'_{k_d'}) \right] \]
\[ \left. \times \left[ \frac{1}{\frac{\hbar}{k} - \frac{\hbar}{k'} - \omega_{k'-k} - z} + \frac{1}{\frac{\hbar}{k} - \frac{\hbar}{k'} - \omega_{k'-k} - z} \right]. \tag{20} \]

where \( M(z) = M(\omega \pm i0) = M(\omega) \pm iM'(\omega) \). Here we are interested in the imaginary part of the memory function \([19, 23]\). The use of identity \( \lim_{\omega \rightarrow 0} \frac{1}{\omega} = \frac{1}{\pi} \Im \delta(\omega) \) transforms the expression (20) into delta function form. On comparing imaginary part of the above expression, we get
\[ \lim_{\omega \rightarrow 0} \frac{1}{\omega} = \frac{1}{\pi} \Im \delta(\omega) = \frac{1}{\pi} \Im \delta(\omega) + \pi \delta(\omega - \epsilon - i\omega + \omega) \]

Using the momentum conservation \( \vec{k} - \vec{k'} = \vec{k}_d - \vec{k}_d = \vec{q} \). Write \( \vec{k} - \vec{k'} \) in terms of \( \vec{k} + \vec{q} \) and \( \vec{k}_d + \vec{q} \). Also write \( (v_1(k') - v_1(k))^2 = \frac{2m}{\hbar^2} (\vec{k} - \vec{k'})^2 \). To deal with the magnitude of \( (\vec{k} - \vec{k'}) \), insert an integral \( dq \delta(\vec{q} - |\vec{k} - \vec{k'}|) \) over \( \vec{q} \) into equation (21) which simplifies the calculation greatly. Using the spatial isotropy in the present free electron case we can write \( \nu'' = (\nu''_1 + \nu''_2 + \nu''_3) = 3\nu'' \). Converting sums into integrals for \( k \) and \( k' \) using \( \frac{1}{\nu''} \sum_{\nu''} \int \frac{d^3k}{(2\pi)^3} \), the above equation can be written as
\[ M''(\omega) = -\frac{f^2 m \pi}{3N^2 \hbar^3 mn \omega} \int_0^\infty \frac{dq}{q^2} \int_0^\infty \frac{d^3k}{(2\pi)^3} \int_0^\infty \frac{d^3k'}{(2\pi)^3} \delta(\vec{q} - |\vec{k} - \vec{k'}|) \]
\[ \times F(f'_{k_d'}, f'_{k_d}, f'_{k_d'}, f'_{k_d}) \left[ \delta(\epsilon_{k+q} - \epsilon_k - \hbar\omega_q + \omega) \right. \]
\[ \left. - \delta(\epsilon_{k+q} - \epsilon_k - \hbar\omega_q - \omega) \right]. \tag{22} \]

Here, we write \( F(f'_{k_d'}, f'_{k_d}, f'_{k_d'}, f'_{k_d}) \) as short hand notation for Fermi distribution function inside the curly braces. Write \( \int d^3k = 4\pi \int k^2 dk \), \( \int d^3k' = 2\pi \int k^2 dk' \int_0^\pi \sin \theta d\theta \) (take \( k = k' \) as pointing along the -direction). Therefore \( M''(\omega) \) takes the form
\[ M''(\omega) = -\frac{f^2 m \pi}{3N^2 \hbar^3 mn \omega} \int_0^\infty \frac{dq}{q^2} \int_0^\infty k^2 dk \int_0^\infty k^2 dk' \]
\[ \times \int_0^\pi \sin \theta \, d\theta \, d\theta \delta(q - \sqrt{(k^2 + k'^2 - 2kk' \cos \theta)}) \]
\[ \times \sum_{k_d k_d'} F(f'_{k_d'}, f'_{k_d}, f'_{k_d'}, f'_{k_d}) \left[ \delta(\epsilon_{k+q} - \epsilon_k - \hbar\omega_q + \omega) \right. \]
\[ \left. - \delta(\epsilon_{k+q} - \epsilon_k - \hbar\omega_q - \omega) \right]. \tag{23} \]

To simplify further, we shift momentum integral variables into energy variables \( k^2 = \frac{2m}{\hbar^2} \omega_q \) and \( dk = \sqrt{k \omega_q} \, d\omega_q \). On writing \( \epsilon_k \) as \( \epsilon' \) and \( \epsilon_k \) as \( \epsilon' \), changes the expression to
\[ M''(\omega) = -\frac{2f^2 m \pi \omega_q}{3N^2 \hbar^3 mn} \int_0^\infty \sqrt{q} \int_0^\infty \sqrt{q} d\omega_q \int_0^\infty \sqrt{q} d\omega_q' \]
\[ \times \int_0^\pi \sin \theta \, d\theta \, d\omega_q \delta(q - \sqrt{\epsilon' + 2\sqrt{\epsilon' \cos \theta}}) \]
\[ \times \sum_{k_d k_d'} F(f'_{k_d'}, f'_{k_d}, f'_{k_d'}, f'_{k_d}) \left[ \delta(\epsilon_{k+q} - \epsilon_k - \hbar\omega_q + \omega) \right. \]
\[ \left. - \delta(\epsilon_{k+q} - \epsilon_k - \hbar\omega_q - \omega) \right]. \tag{24} \]
On performing the $\theta$ integral the above expression (appendix B) reduces to the form

$$M''(\omega) = \frac{1}{4\pi^2} \int \frac{d^3 p}{\sqrt{\mathbf{p}^2 + m^2}} \int_0^{q_0} dq q \int_0^\infty dq \int_0^\infty \sqrt{\epsilon} \frac{d\epsilon}{\omega} \sum_{k_d} \left\{ f_q'(1 - f_{k_d}^i) \sum_{k_d} (f_{k_d}' - f_q^i) - (f_q - f_{k_d}^i) \delta(\epsilon_{k_d^i} - \epsilon - h\omega_q - h\omega) - \delta(\epsilon_{k_d^i} - \epsilon - h\omega_q - h\omega) \right\}.$$  

By using $f(x) = 1 - f(a)\delta(x-a) - f(b)\delta(x-b)$ we remove $\epsilon_k$ from the Fermi functions and integrate over $\epsilon'$ which we simply write $\epsilon'$

$$M''(\omega) = p_0 \int_0^{q_0} dq q \int_0^\infty \frac{d\epsilon}{\omega} \left[ \sqrt{\epsilon + h\omega_q - h\omega} \sum_{k_d} f'(\epsilon_k + h\omega_q - h\omega)(1 - f'(\epsilon_k)) \right.$$ 

$$\times \sum_{k_d} \left\{ f'(\epsilon_k + h\omega_q) - f'(\epsilon_{k_d^i}) \right\} - \left\{ f'(\epsilon_k + h\omega_q - h\omega) \right\} \sum_{k_d} f'(\epsilon_{k_d^i})(1 - f'(\epsilon_{k_d^i})) \right\} - \sqrt{\epsilon + h\omega_q + h\omega}$$

$$\times \left\{ f'(\epsilon_k + h\omega_q + h\omega)(1 - f'(\epsilon_k)) \sum_{k_d} (f'(\epsilon_{k_d^i}) - f'(\epsilon_{k_d^i})) - (f'(\epsilon_k) - f'(\epsilon_k + h\omega_q + h\omega)) \right\}$$

$$\times \sum_{k_d} f'(\epsilon_{k_d^i})(1 - f'(\epsilon_{k_d^i})) \right\},$$

where the prefactors $p_0 = \frac{1}{4\pi^2 \sqrt{\mathbf{p}^2 + m^2}}$. Define $\epsilon'_k = \epsilon$, $f'_1(q) = \sum_{k_d} (f'(\epsilon_{k_d^i}) - f'(\epsilon_{k_d^i}))$ and $f'_2(q) = \sum_{k_d} f'(\epsilon_{k_d^i})(1 - f'(\epsilon_{k_d^i}))$. With these definitions, we have

$$M''(\omega, T) = p_0 \int_0^{q_0} dq q \int_0^\infty \frac{d\epsilon}{\omega} \sqrt{\epsilon + h\omega_q - h\omega} f'(\epsilon + h\omega_q - h\omega)(1 - f'(\epsilon))$$

$$- \sqrt{\epsilon + h\omega_q + h\omega} f'(\epsilon + h\omega_q + h\omega)(1 - f'(\epsilon)) f'_2(q) + \int_0^\infty \frac{d\epsilon}{\omega} \sqrt{\epsilon + h\omega_q + h\omega} f'(\epsilon - f'(\epsilon + h\omega_q + h\omega))$$

$$- \sqrt{\epsilon + h\omega_q - h\omega} f'(\epsilon - f'(\epsilon + h\omega_q - h\omega)) f'_2(q)$$.

This is important general expression of imaginary part of the memory Function, which is valid for all frequencies and all temperature regimes. In what follows, we analyze the above expression in the DC limit and study the temperature dependence of the imaginary part of the memory function.

For performing the limit $\omega \rightarrow 0$, we rewrite the main result (equation (27)) in the following way:

$$M''(\omega) = p_0 \int_0^{q_0} dq q \int_0^\infty \frac{d\epsilon}{\omega} \sqrt{\epsilon + h\omega_q - h\omega} f'(\epsilon + h\omega_q - h\omega)$$

$$- \sqrt{\epsilon + h\omega_q + h\omega} f'(\epsilon + h\omega_q + h\omega) \left(1 - f'(\epsilon)\right) f'_2(q)$$

$$+ \int_0^\infty \frac{d\epsilon}{\omega} \sqrt{\epsilon + h\omega_q + h\omega} f'(\epsilon - f'(\epsilon + h\omega_q + h\omega)) f'_2(q) + \int_0^\infty \frac{d\epsilon}{\omega} \sqrt{\epsilon + h\omega_q - h\omega} f'(\epsilon + h\omega_q - h\omega)$$

$$- \sqrt{\epsilon + h\omega_q + h\omega} f'(\epsilon + h\omega_q + h\omega) \left(1 - f'(\epsilon)\right) f'_2(q).$$ (28)
On performing the limit $\omega \to 0$ for term \((\Sigma_1)\) we have

$$\frac{\partial \Sigma_1}{\partial \omega} \bigg|_{\omega = 0} = - \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0}} + \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0} - \omega_0}$$

\begin{align}
\times \left. \frac{\partial f'(e + \omega_0) - \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0}}}{\partial \omega} \left|_{\omega = 0} \right.ight.
\left. \frac{\partial f'(e + \omega_0 + \omega)}{\partial \omega} \right|_{\omega = 0}
\times \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0} - \omega_0}
\times \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0} - \omega_0}
\times \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0} - \omega_0}
\times \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0} - \omega_0}
\end{align}

and for term \((\Sigma_2)\), we have

$$\frac{\partial \Sigma_2}{\partial \omega} \bigg|_{\omega = 0} = \frac{e}{2\hbar^2} \mu \frac{e^{(s + \mu)}(e^{(s + \mu)} - 1)}{\sqrt{e + \omega_0} - \omega_0}$$

(30)

Substituting the above expressions into equation (28) we obtain the memory function in the DC limit

$$M'(T) = p_0 \hbar \int_0^{\beta T} dq q^3 \left[ \int_0^\infty dq q^3 \frac{e^{\beta\mu q}}{1 + e^{\beta\mu q}} \right]$$

(31)

There are a couple of reasonable assumptions which we would like to use to simplify the above expression: (1) the expression can be simplified as $k_BT \ll \mu_s$ (chemical potential for s-electrons) at temperature of interest ($\mu_s \approx 10 eV$ and room temperature is $\approx 300 K eV$). (2) $\omega_0 \ll \mu_s$, that is, the energy scale of magnetic excitation (which is in meV) is much less than $\mu_s (\approx 10 eV)$. On implementing the second assumption in the Fermi function $f'(e + \omega_0) = \frac{1}{e^{\beta\mu q} - 1}$ lead to $f'(e)$ and the above expression becomes

$$M''(T) = p_0 \hbar \left[ 2\beta \int_0^{\beta T} dq q^3 \int_0^\infty dq q^3 \frac{e^{\beta\mu q}}{1 + e^{\beta\mu q}} \right]$$

(32)

Next, on implementing the first assumption $k_BT \ll \mu_s$, we notice that factors of the form $f'(e)(1 - f'(e))$ are approximately like delta functions peaking at $\mu_s$. Thus the relevant range of the $e$ is around $\mu_s$ with width of order $k_BT$. Observing this fact we can write $\sqrt{e + \omega_0} \approx \sqrt{e}$ as $\omega_0 \ll \mu_s$:

$$M''(T) = p_0 \hbar \left[ 2\beta \int_0^\infty dq q^3 \frac{e^{\beta\mu q}}{1 + e^{\beta\mu q}} \right]$$

(33)

The above expression in more simplified form (see appendix E) and transformations of variables in all the integrands $x = \beta(\epsilon_{d} - \mu_s)$ reduced it to:

$$M'(T) = \frac{1}{12\pi^3 N^2 h^3 m\mu_s^3} \left[ \frac{\rho_0}{\beta^2} \int_{\beta \rho_0}^\infty \frac{dx}{x + \beta\mu_d e^x} + \frac{2}{3 \beta\mu_d} \int_{\beta \rho_0}^\infty \frac{dx}{x + \beta\mu_d e^x} \right]$$

(34)

We write $\sqrt{2m\mu_d} = h\tau_s$ and $\frac{\mu_s}{m} = \lambda$. The above expression attains the form

$$M'(T) = \frac{1}{12\pi^3 N^2 h^3 m\mu_s} \left[ \frac{\rho_0}{\beta^2} \int_{\beta \rho_0}^\infty \frac{dx}{x + \beta\mu_d e^x} + \frac{2}{3 \beta\mu_d} \int_{\beta \rho_0}^\infty \frac{dx}{x + \beta\mu_d e^x} \right]$$

(35)

This is our final simplified expression (after implementing the above mentioned assumptions (1) and (2)). Temperature dependence of the imaginary part of memory function gives the temperature dependence of resistivity $\rho(T) = \frac{\rho_0}{\beta^2} \int_{\beta \rho_0}^\infty \frac{dx}{x + \beta\mu_d e^x}$.
4. Analysis of the general expression in special cases

4.1. Low temperature limit ($k_B T \ll \mu_d$)

In this temperature limit we have $\beta \mu_d > 1$ thus the general expression (39) transforms to

$$M'(T) \approx \frac{1}{12 \pi^2} \frac{F^2 V^2 m^2}{N^2 \hbar^2 \mu_i} \left\{ \frac{1}{8 \pi^2} \left( \frac{q_0}{\mu_i} \right)^6 \frac{1}{q_i} \sqrt{\lambda} \right\}$$

$$\times \int_{-\mu_i}^{\mu_i} \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2} + \frac{2}{3} \beta \frac{\mu_i}{\sqrt{\mu_i}} \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2}$$

$$\times \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2}$$

$$+ \frac{1}{8 \pi^2} \left( \frac{q_0}{\mu_i} \right)^6 \frac{1}{q_i} \left( \frac{\lambda}{\mu_i} \right)^2 \left( \frac{\mu_i}{\beta} \right)^{1/2} \int_{-\mu_i}^{\mu_i} dx \, \frac{e^x}{(e^x + 1)^2}. \quad (36)$$

where we replaced $\sqrt{x + \beta \mu_d} \approx \sqrt{\beta \mu_d}$ as $\beta \mu_d \gg 1$ and $x \sim 1$ due to exponentially damped function of the form $e^{x + 1}/x^2$ in the integrands. With further rearrangements the above expression further simplifies to

$$M'(T) \approx \frac{1}{12 \pi^2} \frac{F^2 V^2 m^2}{N^2 \hbar^2 \mu_i} \left\{ \frac{1}{8 \pi^2} \left( \frac{q_0}{\mu_i} \right)^6 \frac{1}{q_i} \sqrt{\lambda} \right\}$$

$$\times \int_{-\mu_i}^{\mu_i} \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2} + \frac{2}{3} \beta \frac{\mu_i}{\sqrt{\mu_i}} \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2}$$

$$\times \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2}$$

$$\times \int_{-\mu_i}^{\mu_i} dx \, \left( \frac{e^x + 1}{e^x - 1} \right)^{2}$$

$$\times k_B T \sqrt{\mu_i} \int_{-\mu_i}^{\mu_i} dx \, \frac{e^x}{(e^x + 1)^2}. \quad (37)$$
In the low temperature limit, the dominating term is the middle one with prefactor proportional to $\frac{1}{T}$. Neglecting the subdominant terms the memory function in low temperature limit reduces to

$$M''(T \rightarrow 0) \sim \frac{1}{T} f_s(T),$$

$$f_s(T) = \int_{-\beta \mu_d}^{\infty} dx \left\{ \frac{e^x}{(e^x + 1)^2} - 2 \frac{e^{2x}}{(e^x + 1)^2} \right\},$$

where $f_s(T)$ is a slowly varying function$^7$ of temperature. So, in the low temperature limit resistivity displays an upturn, as seen in figure 1(a). An important point to be noted here is that the divergence in our case is of the form of power law instead of the logarithmic divergence in the original Kondo problem. The reason behind this difference is that we treated $d$ or $f$ electrons as quasi-localized (away from half-filling) instead of fully localized ones [1]. This is one of our important result.

4.2. High temperature limit ($k_B T \gg \mu_d$)

In high temperature limit we have $\beta \mu_d \ll 1$. In this limit expression from (39) changes to

$$M''(T) \simeq \frac{J^2 V^2 m^2}{12 \pi^2 N^2 h^2} \frac{1}{\mu_d} \left\{ \frac{q_D}{q_s} \right\}^6 q_s^2 \frac{\sqrt{\lambda}}{\beta \mu_d} \times \left( \int_{-\beta \mu_d}^{\infty} dx \frac{\sqrt{x} e^x}{(e^x + 1)^2} + \frac{2}{3} \int_{-\beta \mu_d}^{\infty} dx \frac{x^2 e^x}{(e^x + 1)^2} \right)$$

$$+ \frac{4}{3} \int_{-\beta \mu_d}^{\infty} dx \frac{x^3 e^x}{(e^x + 1)^3} + \frac{1}{8 \pi^2} \frac{q_D}{q_s} q_s^2 \left( \frac{\lambda}{\beta \mu_d} \right)^{\frac{1}{2}} \int_{-\beta \mu_d}^{\infty} dx \frac{\sqrt{x} e^x}{(e^x + 1)^{\frac{3}{2}}} \right\}.$$  

(39)

By direct computation we notice that the last term in the above expression is many order of magnitude larger than the first two terms. Thus,

$$M''(k_B T \gg \mu_d) \sim C T \int_{0}^{\infty} dx \frac{\sqrt{x} e^x}{(e^x + 1)^2} \simeq 0.536 C T^2 \times M''(k_B T \gg \mu_d) \sim T^2,$$

(40)

where prefactor $C = \frac{1}{96 \pi^2} \frac{J^2 V^2 m^2}{N^2 h^2} \frac{q_D}{q_s} q_s^2 \left( \frac{\lambda}{\mu_d} \right)^\frac{1}{2}$. Thus, in high temperature limit the memory function scales as $M''(k_B T \gg \mu_d) \sim T^2$. This is also observed in figure 1(c).

5. Comparison with experimental data

In this section we compare our theory with the experimental data. The Kondo-like behaviour was observed in the temperature dependence of resistivity in YbRhSn [24]. Resistivity shows low temperature upturn and a minimum around

$^7$ We have checked the relative variation of $f_s(T)$ as compared to $\frac{1}{T}$ and found that relative variation of $f_s(T)$ is very small.

It does show an up-turn at lower temperature, and as the temperature is raised it passes through a minima ($T_m \simeq 25$ K) and then it shows negative curvature at higher temperature ($T > T_m$). The experimental data in figure 2 of reference [24] is reproduced here in figure 2 (dashed line). The DC resistivity is computed using the present theory, and $\rho(T) = \frac{n e^2}{\tau} = \frac{n e^2}{\tau} M''(T)$ takes the form.

$$\rho(T) = \left( \frac{m}{ne^2} \right) \frac{1}{96 \pi^2} \frac{J^2 V^2 m^2}{N^2 h^2} \frac{q_D}{q_s} q_s^2 \frac{\sqrt{\lambda}}{\beta \mu_d} \times \left( \int_{-\beta \mu_d}^{\infty} dx \frac{\sqrt{x} e^x}{(e^x + 1)^2} + \frac{2}{3} \int_{-\beta \mu_d}^{\infty} dx (x + \beta \mu_d)^2 \right)$$

$$+ \left( \frac{4}{3} \int_{-\beta \mu_d}^{\infty} dx \frac{x e^x}{(e^x + 1)^3} \right)$$

(41)

By direct computation we notice that the last term in the above expression is many order of magnitude larger than the first two terms. Thus,

$$M''(k_B T \gg \mu_d) \sim C T \int_{0}^{\infty} dx \frac{\sqrt{x} e^x}{(e^x + 1)^2} \simeq 0.536 C T^2 \times M''(k_B T \gg \mu_d) \sim T^2,$$

(40)

where prefactor $C = \frac{1}{96 \pi^2} \frac{J^2 V^2 m^2}{N^2 h^2} \frac{q_D}{q_s} q_s^2 \left( \frac{\lambda}{\mu_d} \right)^\frac{1}{2}$. Thus, in high temperature limit the memory function scales as $M''(k_B T \gg \mu_d) \sim T^2$. This is also observed in figure 1(c).

6. Discussion

There are couple of comments that we would like to mention. The first one is that the parameter $\lambda$, $\mu_d$ and $q_D$ are phenomenological parameters. We obtain the values of these parameters by comparing the theory with experimental data. It would be great to independently measure these parameters for the considered system YbRhSn. For example, $\mu_d$ and $\lambda = \frac{m_d}{m}$ can be measured using quantum oscillation experiments [26].
The parameter $q_0$ can be measured using neutron scattering experiments (by measuring the dispersion of spin fluctuations) [27].

In the calculation of DC resistivity we have considered magnetic scattering only. However, quasi-localized $d$-electrons away from half filling will induce charge density (CD) fluctuations within $d$-band. These CD fluctuations will couple with $s$-electrons thereby inducing CD fluctuations in $s$-band also. So, one will have a coupled system CD fluctuations. These will constitute extra channel of momentum relaxation for $s$-electrons. And resistivity formula (41) will have extra term coming from this effect. Mathematical modeling of this effect from microscopic considerations, and then computing its effect on observable like DC resistivity is an important open issue.

7. Conclusion

The calculation of DC resistivity using the memory function formalism ($\rho(T) = \frac{ne}{m^2}M^\prime(T)$) for the Kondo lattice Hamiltonian (or $s-d$ Hamiltonian) is presented. We used the Wölfle–Götze approximation to compute the memory function. The scattering of conduction electrons via the quasi-localized $f$ or $d$ electrons is taken into account by treating the $H_{s-d}$ part of Hamiltonian as a perturbation. Dispersion of spin excitation is taken to be of the form $\hbar\omega_{k} = c_{df}q^{2}$. We find that the DC resistivity shows low temperature ($k_{B}T \ll \mu_{s}$) power law up-turn, and high temperature ($k_{B}T \gg \mu_{s}$) $T^{2}$ scaling. A qualitative agreement with experiment is found.

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Appendix A. Average of spin density operators of localized electrons

The commutator of spin density operators is written as:

$$\sum_{k'k}\langle[S^-(k'-k),S^+(k'-k)]\rangle = \langle[S^-(q),S^+(-q)]\rangle = \sum_{k}\langle[a_{k\uparrow}^{\dagger}a_{k\downarrow},a_{k\downarrow}^{\dagger}a_{k\uparrow}]\rangle \quad \text{(A.1)}$$

Here we set $k' - k = q$, and to treat $d$ electrons as quasi-localized we write $S^-$ and $S^+$ in terms of Fermi functions ($S^-(q) = \sum_{k}a_{k+q\uparrow}^{\dagger}a_{k\uparrow}$). The anticommutation property simplifies the equation (A.1) to

$$\sum_{k'k}\langle[S^-(k'-k),S^+(k'-k)]\rangle = \sum_{k,q}\langle[a_{k\uparrow}^{\dagger}a_{q\uparrow},a_{q\uparrow}^{\dagger}a_{k\uparrow}]\rangle
- \langle[a_{k\uparrow}^{\dagger}a_{q\downarrow},a_{q\downarrow}^{\dagger}a_{k\uparrow}]\rangle
= \sum_{k,q}(f_{k+q\uparrow}^{d} - f_{k\uparrow}^{d}) \quad \text{(A.2)}$$

We use $f_{k\uparrow}^{d} = \langle a_{k\uparrow}^{\dagger}a_{k\uparrow}\rangle$ notation to differentiate Fermi function of $d$-band electrons from that of $s$-band electrons. The other factor in equation (15) is:

$$\sum_{k'k}\langle[S^+(k'-k),S^-(k'-k)]\rangle = \langle[S^+(-q),S^-(-q)]\rangle
= \sum_{k,q}\langle[a_{k\uparrow}^{\dagger}a_{k+q\downarrow},a_{k+q\downarrow}^{\dagger}a_{k\uparrow}]\rangle
= \sum_{k,q}f_{k\uparrow}^{d}(1 - f_{k+q\downarrow}^{d}). \quad \text{(A.3)}$$

Appendix B. $\theta$ integral solution

In the presence of Fermi factors of the form $f_{k\uparrow}^{d}(1 - f_{k\downarrow}^{d})$ and at ordinary temperature $k_{B}T \ll \mu_{s}$ ($\sim$eV), one can replace $\epsilon$ and $\epsilon'$ inside the square root by $\mu_{s}$ for $s$ electrons ($\mu_{s} = \hbar k_{F}^{s}/2m$) where $q_{s}$ is Fermi wavevector for $s$-electrons:

$$\int_{0}^{\pi} \sin \theta d\theta d(q - \sqrt{2mq(1 - \cos \theta)}) \approx \int_{0}^{\pi} \sin \theta d\theta d(q - \sqrt{2q_{s}h(1 - \cos \theta)}). \quad \text{(B.1)}$$

Put $x = 1 - \cos \theta$ and define $\xi = hq_{s}/\sqrt{2x}$ and the limit of the integral changes to 0 and 2$q_{s}$ (note that 0 < $q$ < $q_{s}$). The integral becomes

$$\int_{0}^{\pi} \sin \theta d\theta d(q - \sqrt{2mq(1 - \cos \theta)}) \approx \int_{0}^{2q_{s}} \frac{\xi dq}{h^{2}q_{s}^{2}}.$$ \quad \text{(B.2)}$$

Appendix C. Expansion of $f_{k\uparrow}^{d}(q)$

$$f_{k\uparrow}^{d}(q) = \sum_{k_{d}}[f^{d}(\epsilon_{k_{d}}) - f^{d}(\epsilon_{k_{d}})] \quad \text{(C.1)}$$

The Taylor’s expansion for small ($q \rightarrow 0$) gives

$$f_{k\uparrow}^{d}(q) = \sum_{k_{d}}\left[f^{d}(\epsilon_{k_{d}}) - f^{d}(\epsilon_{k_{d}}) - q\frac{\partial f^{d}(\epsilon_{k_{d}})}{\partial q}\right]_{q=0} + \frac{q^{2}}{2!}\frac{\partial^{2} f^{d}(\epsilon_{k_{d}})}{\partial q^{2}}\bigg|_{q=0} + \frac{q^{3}}{3!}\frac{\partial^{3} f^{d}(\epsilon_{k_{d}})}{\partial q^{3}}\bigg|_{q=0} + \cdots. \quad \text{(C.2)}$$

on converting summation into integrals, we get
\[ f_d^{2}(q) = -\frac{V}{(2\pi)^2} \int_{0}^{\pi} k_d^2dk_d \int_{0}^{q} \sin \theta d\theta \left[ \partial f_d^{2}(\epsilon_d') \right] \bigg|_{\theta = q} \left( q - \frac{\partial f_d^{2}(\epsilon_d')}{\partial q} \right) \]

\[ + \frac{q^2}{2} \frac{\partial^2 f_d^{2}(\epsilon_d')}{\partial q^2} \bigg|_{\theta = q} + \frac{q^3}{3} \frac{\partial^3 f_d^{2}(\epsilon_d')}{\partial q^3} \bigg|_{\theta = q} \ldots \]  

(C.3)

We have Fermi function \( f_d(q, \alpha, \eta, \gamma, \theta) = \frac{1}{e^{\alpha + \beta q + \gamma q \cos \theta} + 1} \). For simplification, we put \( \alpha = \beta \frac{k^2_{2d}}{2md} - \mu_d \), \( \eta = \beta \frac{k^2_{2d}}{2md} \) and \( \gamma = \beta \frac{k^2_{2d}}{2md} \). The Fermi function set to

\[ f_d(q, \alpha, \eta, \gamma, \theta) = \frac{1}{e^{\alpha + \beta q + \gamma q \cos \theta} + 1}, \]

(C.4)

\[ \frac{\partial f_d^{2}(\alpha, \eta, \gamma, \theta)}{\partial q} \bigg|_{q = 0} = \frac{-e^{\beta q} \cos \theta}{(e^{\alpha + 1})^2}. \]

(C.5)

the third derivative becomes

\[ \frac{\partial^3 f_d^{2}(\alpha, \eta, \gamma, \theta)}{\partial q^3} \bigg|_{q = 0} = \frac{12\alpha e^{2\alpha} \cos \theta}{(e^{\alpha + 1})^3} - \frac{6\alpha e^{2\alpha} \cos \theta}{(e^{\alpha + 1})^2} - \frac{6e^{2\alpha} \gamma \cos \gamma}{(e^{\alpha + 1})^3} - \frac{e^{2\alpha} \gamma}{(e^{\alpha + 1})^2}. \]

(C.6)

We substitute derivative terms of \( f_d(q, \epsilon_d') \) from equations (C.4)-(C.6) in the expression (C.3) and perform \( \theta \) integration. Thus replacing \( \alpha, \eta \) and \( \gamma \) with their respective terms we obtain

\[ f_d^{2}(q) = V \frac{q^2}{(2\pi)^2} \frac{\sqrt{2md}}{h} \left[ \beta \int_{0}^{\infty} d\epsilon_d \sqrt{\epsilon_d} e^{\beta(\epsilon_d - \mu_d)} (e^{\beta(\epsilon_d - \mu_d) + 1})^2 \right] \]

\[ + \frac{2}{3} \int_{0}^{\infty} d\epsilon_d \epsilon_d^2 e^{\beta(\epsilon_d - \mu_d)} (e^{\beta(\epsilon_d - \mu_d) + 1})^2 \]

\[ - \frac{4}{3} \int_{0}^{\infty} d\epsilon_d \epsilon_d^2 e^{2\beta(\epsilon_d - \mu_d)} (e^{\beta(\epsilon_d - \mu_d) + 1})^3 \].

(C.7)

Appendix D. Term \( f_d^{2}(q) \) expansion

The Fermi function of d-band electrons \( f_d^{2}(q) \) is

\[ f_d^{2}(q) = \sum_{\epsilon_d} f_d^{2}(\epsilon_d) (1 - f_d^{2}(\epsilon_d)) \]

(D.1)

The Taylor’s expansion for small \( q \) expands the Fermi function in the form

\[ f_d^{2}(q) = \sum_{\epsilon_d} f_d^{2}(\epsilon_d) \left( 1 - f_d^{2}(\epsilon_d) - \frac{\partial f_d^{2}(\epsilon_d)}{\partial q} \right) \bigg|_{q = 0} \]

\[ - \frac{q^2}{2!} \frac{\partial^2 f_d^{2}(\epsilon_d)}{\partial q^2} \bigg|_{q = 0} - \ldots \]

(C.3)

\[ = \sum_{\epsilon_d} \left[ f_d^{2}(\epsilon_d) (1 - f_d^{2}(\epsilon_d)) - q f_d^{2}(\epsilon_d) \frac{\partial f_d^{2}(\epsilon_d)}{\partial q} \bigg|_{q = 0} \right] \]

(D.2)

On converting sum into integration

\[ f_d^{2}(q) = \int_{0}^{\pi} d\theta \int_{0}^{\infty} k_d^2dk_d f_d^{2}(\epsilon_d) (1 - f_d^{2}(\epsilon_d)) \int_{0}^{\pi} \sin \theta d\theta \]

\[ - \frac{q^2}{2!(2\pi)^2} \int_{0}^{\infty} k_d^2dk_d f_d^{2}(\epsilon_d) \int_{0}^{\pi} \sin \theta d\theta \frac{\partial f_d^{2}(\epsilon_d)}{\partial q} \bigg|_{q = 0} = \ldots \],

which can further be written in terms of energy

\[ \int_{0}^{\pi} d\theta \int_{0}^{\infty} k_d^2dk_d f_d^{2}(\epsilon_d) \int_{0}^{\infty} \sin \theta d\theta \frac{\partial f_d^{2}(\epsilon_d)}{\partial q} \bigg|_{q = 0} = \ldots \].

(D.3)

Appendix E. Mathematical details of \( M'(T) \)

The memory function expression from equation (33) can be rewritten as

\[ M'(T) = p_0 h \left[ 2\beta \int_{0}^{\infty} d\epsilon \ f'(\epsilon) (1 - f'(\epsilon)) \right] \]

\[ \times ((1 - f'(\epsilon))I_1(T) + I_2(T)) \]

\[ - \int_{0}^{\infty} d\epsilon \ f'(\epsilon) (1 - f'(\epsilon))I_1(T) \].

(E.1)

Integrals over \( \epsilon \) can be performed using the properties of delta functions \( f'(\epsilon) (1 - f'(\epsilon)) \approx \frac{\delta(\epsilon - \mu_1)}{\beta} \)

\[ M'(T) = \frac{p_0 h}{\beta} \left[ (\beta \mu_1 - 1)I_1(T) + 2\beta I_2(T) \right] \]

(E.2)

As \( \beta \mu_1 \gg 1 \), we get

\[ M'(T) = p_0 \mu_1 [I_1(T) + 2I_2(T)] \]

(E.3)

where

\[ I_1(T) = \int_{0}^{\mu_1} d\epsilon \ q^3 f_d^{2}(q) \].

(E.4)
and
\[ I_2(T) = \int_0^{\beta_0} dq \, q^2 f_2^2(q). \] (E.5)

The above simplified expression (equation (E.3)) is our main result in the DC limit. Our next aim is to reduce the expression for \( I_1(T) \) and \( I_2(T) \). For this we take the long wavelength approximation (small \( q \) expansion). It can be shown (refer to appendix C) that \( f_2^2(\epsilon_d) \) in long wavelength limit \( q \to 0 \) can be written as
\[
f_2^2(\epsilon_d) = \frac{V q^2 \sqrt{2m_d}}{4 \pi^2 \hbar} \left[ \beta \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{2\beta(\epsilon_d - \epsilon)} + 1)^2} \right],
\]
\[ + \frac{2}{3} \beta^2 \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{3\beta(\epsilon_d - \epsilon)} + 1)^2}, \]
\[ - \frac{4}{3} \beta^3 \int_0^\infty d\epsilon \epsilon^2 e^{3\beta(\epsilon_d - \epsilon)} \epsilon^2 (e^{3\beta(\epsilon_d - \epsilon)} + 1)^3, \] (E.6)
on substituting the above expression of \( f_2^2(\epsilon_d) \) into equation (E.4) we get
\[
I_1(T) = \frac{2 \beta}{6} V \frac{\sqrt{2m_d}}{4 \pi^2 \hbar} \left[ \beta \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{2\beta(\epsilon_d - \epsilon)} + 1)^2} \right],
\]
\[ + \frac{2}{3} \beta^2 \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{3\beta(\epsilon_d - \epsilon)} + 1)^2}, \]
\[ - \frac{4}{3} \beta^3 \int_0^\infty d\epsilon \epsilon^2 e^{3\beta(\epsilon_d - \epsilon)} \epsilon^2 (e^{3\beta(\epsilon_d - \epsilon)} + 1)^3 \] (E.7).

Similarly \( f_2^2 \) can be simplified (refer to appendix D) and the simplified expression of \( f_2^2 \) can be substituted into equation (E.5). The result is
\[
I_2(T) = \frac{V}{(2\pi)^2} \frac{(2m_d)^{3/2}}{h^3} \int_0^\infty dq \, q^3 \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{2\beta(\epsilon_d - \epsilon)} + 1)^2} + I_1(T), \] (E.8)
on substituting expressions of \( I_1(T) \) and \( I_2(T) \) into equation (E.3) we have
\[
M''(T) = \frac{1}{12\pi^2} \frac{J^2 V^2 m^2}{N^2 \hbar^4 n_d^2} \mu_b \left\{ \beta \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{2\beta(\epsilon_d - \epsilon)} + 1)^2} \right\},
\]
\[ \times \left[ \beta \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{3\beta(\epsilon_d - \epsilon)} + 1)^2} \right],
\]
\[ + \beta^2 \int_0^\infty \frac{d\epsilon d\epsilon \epsilon^2 e^{\beta(\epsilon_d - \epsilon)} \epsilon}{(e^{3\beta(\epsilon_d - \epsilon)} + 1)^2} \right]\] (E.9).

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