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AN EVALUATION OF OPTICAL CONDUCTIVITY OF PROTOTYPE NON-FERMI LIQUID KONDO ALLOYS

A. K. SINGH[*] and L. K. MISHRA[a]

Department of Physics, A.M. College, GAYA – 823001 (Bihar) INDIA
[a]Department of Physics, Magadh University, BODH GAYA – 824234 (Bihar) INDIA

ABSTRACT

An evaluation of real part of optical conductivity $\sigma_1 (\omega)$ as a function of ω for prototype non-Fermi Kondo alloys were performed at different temperature. Our evaluated results increases with frequency as per experimental observation but the magnitudes are smaller with the experimental data.

Key words: Prototype, Non-Fermi, Kondo alloys, Optical conductivity, Frequency, Real-Part.

INTRODUCTION

During the past 20 years there has been a great deal of interest in a narrow class of materials among the highly correlated metals, which exhibit non-Fermi liquid properties at low temperatures[1-6]. One of the central points of Fermi-liquid theory is the existence of a single scale, the Fermi energy E_F, and for energies $E \leq E_F$ and temperatures $K_\beta T \leq E_F$ the electronic properties display universal behavior[7]. Experimental works[8-13] have indicated that several heavy-electron compounds and related alloys (particularly f-electron alloys) display non-Fermi liquid behavior. Typically, the non-Fermi liquid behavior is observed as a diverging linear coefficient of specific-heat C for temperature T = 0. There is strong T dependence of the magnetic susceptibility χ as T = 0. The electrical resistivity ρ shows a peculiar T dependence ($\rho = A\ T^m$ having $A > 0$ and $m = 1$ instead of the Fermi-liquid behavior $m = 2$). In this paper, we have studied optical properties of some non-Fermi liquid alloys. Generally, optical investigations extending over a broad frequency range and at various temperatures are an efficient experimental tool for the simultaneous study of the energy and temperature of intrinsic parameter characterizing the systems. Of particular relevance in connection with the anomalous dc electrical resistivity, is the identification of energy and temperature dependence of the relaxation time τ.

[*]Author for correspondence; E-mail: muphysicslkm@gmail.com

In this paper, we have studied the optical properties of non-Fermi liquid Kondo alloys. The Kondo alloys of our investigation is the evaluation of real part of optical conductivity σ_1 (ω) as a function of ω at different temperatures for U_{02} $Y_{0.8}$ Pd_3, $U_{0.2}$ $Th_{0.8}$ Pd_2 Al_3 and U $Cu_{3.5}$ $Pd_{1.5}$. Our theoretically evaluated results are of good agreement with the other theoretical workers[14,15] and also from the experimental data[16,17].

Mathematical formula used in the evaluation

As we know that heavy electron compound exhibit both types of behavior, Fermi Liquid behavior and Non-Fermi liquid behavior (Kondo Liquid). In the Fermi liquid behavior the low temperature resistivity is written as –

$$\rho(T) \approx \rho_0 + AT^2 \qquad \ldots(1)$$

where ρ_o is the residual resistivity.

The specific heat coefficient γ is -

$$\gamma = \frac{\pi^2}{3} K^2{}_\beta N_F = \frac{k^3{}_F}{3\hbar^2} k_F m^* \qquad \ldots(2)$$

m* is the effective mass usually very high. Because of 4*f* and 5*f* electron heavy electron compounds behaves as non-Fermi liquid (Kondo liquid).

The energy per magnetic impurity is given by -

$$K_\beta T_K \sim E_F e \frac{-1}{N(E_F)J} \qquad \ldots(3)$$

Where J is the coupling between *f* and conduction electron and N (E_F) is the density of the conduction electron state at E_F. T_K is the Kondo temperature. The remarkable feature of the Kondo liquid is the formation of a sharp and narrow resonance in the density of state N (E_F) at E_F. The electrons sitting in the narrow resonance are the new "heavy" quasi particle with enhanced effective mass. These heavy electrons are responsible for the low temperature transport and thermodynamic properties.

For Kondo liquid there is an additional competing interaction of a magnetic nature, induced by the periodic array of magnetic impurities. This corresponds to (RKKY) (Runderman-Kittel-Kesuy-Yoshida) interaction, which defines an another relevant energy scale.

$$K_\beta T_{RKKY} \approx J^2 N(E_F) \qquad \ldots(4)$$

For small J, T_{RKKY} is larger than T_K and magnetic ordering is expected. Otherwise for large J, the formation of singlet Kondo will lead to a larger energy gain than by magnetic ordering. This shows that a heavy electron system balances Kondo fluctuation and correlation effect of the impurity magnetic moments. Such a behavior can also lead to the coexistence of various states, a heavy electron and magnetic order or even to a non-Fermi liquid state.

In such systems, there are two possible sources of scattering of electrons. One is the scattering of electrons off the impurities and other is the scattering from boson fluctuation.

If in the presence of impurities the conductivity is σ_i and in the presence of boson only the conductivity is σ_b then the total conductivity will be

$$\sigma^{-1} = \sigma_i^{-1} + \sigma_b^{-1} \qquad \ldots(5)$$

At sufficiently low temperature, only impurity scattering is relevant. If ε_f is the energy parameter analogous to Debye frequency in the electron phonon electron and w is the bare band width then for w $<< \varepsilon_f$, impurity scattering is written as -

$$\sigma_i(\omega) = \frac{ne^2}{m^*}\frac{\tau^*{}_i}{1+(\omega\tau^*{}_i)^2} \qquad \ldots(6)$$

Where

$\tau_i^* = \left(\frac{m^*}{m}\right)\tau_i$ k_F = Fermi wave vector

$n = \frac{Nk^3{}_F}{6\pi^2}$ n = Electron density

N is the orbital degeneracy of f-state. Generally conductivity is evaluated from the Kubo formula.

$$\sigma_{\mu\nu}(\omega,T) = \frac{1}{V}\int_0^\infty dte^{-i\omega t}\int_0^\beta dt \prec j_{e\mu}(-i\hbar\tau)j_{e\nu}(t) > \qquad \ldots(7)$$

Where $j_{e\mu}$ is the electrical current, V is the system volume and b the inverse temperature, with the simplifying assumption of isotropic dispersion we have[14] -

$$\sigma(\omega,T)=\frac{T_r\sigma_{\mu\nu}(\omega,T)}{3} \qquad \ldots(8)$$

One can obtain the result

$$\sigma(\omega,T)=\frac{i\omega^2{}_p}{4\pi\omega}\int_0^\infty d\varepsilon\frac{f(\varepsilon-\omega)-f(\varepsilon)}{\omega+\Sigma^A{}_c(\varepsilon-\omega,T)-\Sigma^R{}_c(\varepsilon,T)} \qquad \ldots(9)$$

Where Σ_c is the band electron self energy $\Sigma^A{}_c$ denotes the advanced and $\Sigma^R{}_c$ denotes the retarded. ω_p is the Drude plasma frequency and $f(\varepsilon)$ is the Fermi function. In the dc limit equation (9) reduces to the standard transport integral expansion for the resistivity ρ (T) is given by[15] -

$$\rho(T)=\frac{4\pi}{\omega^2{}_p<\tau>} \qquad \ldots(10)$$

Where τ is given by -

$$<\tau>=\frac{1}{12A_f}\left(\frac{T_K}{T_\beta T}\right)^2 \qquad \ldots(11)$$

Where A_f = 1/N (E_F)

N (E_F) is the density of state at the Fermi surface and T_K is the Kondo temperature. Now because of the low frequency ω^2 departure of the full Kondo lattice self energy is seen that -

$$\sigma^{-1}(\omega,T)\approx[\omega^2+(6K_\beta T)^2] \qquad \ldots(12)$$

Equation (12) is the well known result in the absence of inter-site interaction. Equation (12) also manifests the Fermi liquid nature of the Kondo like ground states -

$$\frac{1}{\tau}=a(\hbar\omega)^2+b(K_\beta T)^2 \qquad \ldots(13)$$

where a and b are temperature and frequency independent constants.

b/a = π^2 for quasi-particle scattering rate (seen in photoemission experiments)

b/a = 2 π^2 for transport scattering rate (seen in optical experiment)

Drude gives the free charge carrier contribution to the electrodynamics response[16]. The general formula for the complex dielectric function is -

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega^2{}_p}{\omega(\omega + i\Gamma)} - \Sigma_j \frac{\omega^2{}_{p,j}}{(\omega^2{}_j - \omega^2) - i\Gamma_j \omega} \qquad \ldots(14)$$

Where ω_p and $\Gamma = 1/\tau$ is the Drude term are the plasma frequency and the damping (i.e. scattering relaxation rate) of the free charge carriers ω_j, Γ_j and ω_{pj} are the resonance frequency, the damping and the mode strength of the harmonic oscillator, respectively. These high frequency absorptions above the ultraviolet spectral range are taken into account by ε_∞. Eqn. (14) is more general and can better reproduce the complex shape of the optical conductivity in heavy electron materials. Thompson et al.[10] have shown that the complex conductivity can be written in terms of frequency and temperature dependent m* and Γ.

$$\sigma(\omega) = \frac{\omega_p^2 / 4\pi}{\Gamma(\omega) - i\omega \frac{m^*(\omega)}{m_b}} \qquad \ldots(15)$$

m_b is the band mass -

$$\Gamma(\omega) = \left(\frac{\omega^2{}_p}{4\pi}\right) \frac{\sigma_1}{|\sigma|^2} \qquad \ldots(16)$$

$$m^*(\omega) = \left(\frac{\omega^2{}_p}{4\pi}\right) \frac{\sigma_2}{|\sigma|^2} \qquad \ldots(17)$$

Where

$$\sigma(\omega) = \sigma_1(\omega) + i\sigma_2|\omega) \qquad \ldots(18)$$

RESULTS AND DISCUSSION

In this paper, we have studied the optical properties of prototype non-Fermi Kondo alloys. The Kondo alloys of our studies are $U_{0.2}\,Y_{0.8}\,Pd_3$, $U_{0.2}\,Th_{0.8}\,Pd_2\,Al_3$ and $UCu_{3.5}\,Pd_{1.5}$ respectively. We have evaluated the frequency dependent real part of ac conductivity $\sigma_1(\omega)$ at different temperature. The evaluated results are shown in Table 1, 2 and 3 respectively.

Table 1: An evaluated result of real part of optical conductivity $\sigma_1(\omega)$ as a function of ω at different temperature for $U_{0.2}Y_{0.8}Pd_3$

Frequency cm^{-1}	$\sigma_1(\omega)$ $[\Omega\ cm]^{-1}$					
	T = 300 K		T = 100 K		T = 300 K	
	Theoretical	Experi-mental	Theoretical	Experi-mental	Theoretical	Experi-mental
10	5000	5892	2022	2146	1539	1665
50	4950	5746	2178	2257	1642	1788
100	4820	5036	2486	2533	1754	1944
150	4770	4855	2549	2745	1888	2053
500	4610	4776	2833	2930	2067	2186
1,000	4000	4532	3322	3416	3542	3692
1,500	3872	4217	3578	3710	3987	4007
2,000	3942	4008	4086	4182	4231	4352
3,000	4177	4032	3842	3956	4086	4122
5,000	3627	3854	3617	3733	3622	3788
7,000	3145	3329	3592	3644	3225	3353
10,000	2872	3058	3225	3357	3139	3224

Table 2: An evaluated result of real part of optical conductivity $\sigma_1(\omega)$ as a function of ω for Kondo liquid alloy $U_{0.2}$ $Th_{0.8}$ Pd_2Al_3 at different temperature

Frequency cm^{-1}	$\sigma_1(\omega)$ $[\Omega\ cm]^{-1}$					
	T = 300 K		T = 100 K		T = 30 K	
	Theoretical	Experi-mental	Theoretical	Experi-mental	Theoretical	Experi-mental
10	2.2×10^3	1.9×10^3	1.5×10^3	2.5×10^3	1.2×10^3	1.0×10^3
50	2.7×10^3	2.0×10^3	2.0×10^3	2.8×10^3	1.4×10^3	1.6×10^3
100	3.7×10^3	2.5×10^3	2.7×10^3	3.4×10^3	1.7×10^3	2.0×10^3
500	4.2×10^3	3.8×10^3	3.4×10^3	3.9×10^3	2.2×10^3	2.7×10^3

Cont…

Frequency cm^{-1}	$\sigma_1(\omega)$ $[\Omega\ cm]^{-1}$					
	T = 300 K		T = 100 K		T = 30 K	
	Theoretical	Experi-mental	Theoretical	Experi-mental	Theoretical	Experi-mental
1,000	4.6×10^3	4.5×10^3	4.1×10^3	4.5×10^3	3.5×10^3	3.8×10^3
1,500	5.2×10^3	4.9×10^3	5.2×10^3	5.0×10^3	4.2×10^3	4.7×10^3
2,000	5.7×10^3	5.5×10^3	5.8×10^3	6.2×10^3	5.7×10^3	6.2×10^3
5,000	4.3×10^3	4.0×10^3	5.0×10^3	5.4×10^3	5.2×10^3	5.4×10^3
8,000	4.0×10^3	3.5×10^3	4.2×10^3	5.0×10^3	4.0×10^3	4.3×10^3
10,000	3.2×10^3	3.0×10^3	3.7×10^3	4.2×10^3	3.2×10^3	3.7×10^3
15,000	2.5×10^3	2.5×10^3	2.5×10^3	3.2×10^3	2.8×10^3	2.9×10^3

Table 3: An evaluated result of real part of optical conductivity $\sigma_1(\omega)$ as a function of ω for Kondo liquid alloy $UCu_{3.5}\ Pd_{1.5}$ at different temperatures

Frequency cm^{-1}	$\sigma_1(\omega)$ $[\Omega\ cm]^{-1}$					
	T = 300K		T = 100K		T = 30K	
	Theoretical	Experi-mental	Theoretical	Experi-mental	Theoretical	Experi-mental
20	6.2×10^3	6.8×10^3	5.3×10^3	5.0×10^3	5.0×10^3	4.8×10^3
40	6.5×10^3	7.2×10^3	5.6×10^3	5.4×10^3	5.5×10^3	5.2×10^3
60	7.0×10^3	7.6×10^3	6.0×10^3	6.2×10^3	6.2×10^3	5.8×10^3
80	6.6×10^3	7.4×10^3	6.7×10^3	6.8×10^3	6.8×10^3	6.2×10^3
100	6.0×10^3	7.0×10^3	6.2×10^3	6.0×10^3	6.4×10^3	6.8×10^3
500	5.2×10^3	6.5×10^3	5.8×10^3	5.5×10^3	6.0×10^3	6.2×10^3
1,000	5.0×10^3	6.0×10^3	5.2×10^3	5.0×10^3	5.8×10^3	6.0×10^3
1,500	4.8×10^3	5.4×10^3	4.5×10^3	4.6×10^3	5.5×10^3	5.6×10^3
2,000	4.2×10^3	5.0×10^3	4.0×10^3	4.2×10^3	5.0×10^3	5.2×10^3
5,000	4.0×10^3	4.6×10^3	3.6×10^3	4.0×10^3	4.6×10^3	4.8×10^3
10,000	3.5×10^3	4.2×10^3	3.2×10^3	3.6×10^3	4.0×10^3	4.2×10^3
50,000	3.0×10^3	4.0×10^3	2.8×10^3	3.2×10^3	3.5×10^3	4.0×10^3

We have shown the evaluated result of $\sigma_1(\omega)$ as a function of frequency ω for Kondo alloys $U_{0.2}Y_{0.8}Pd_3$ at different temperature T = 30 K, 100 K and 300 K. We have compared our theoretically evaluated results with experimental data. Our theoretical results show that for T = 30 K and 100 K $\sigma_1(\omega)$ increases with ω but for T = 300 K it decreases with ω. Our evaluated results for all the above three temperature are smaller than the experimental values. In case of Kondo alloy $U_{0.2}Th_{0.8}Pd_2Al_3$, our evaluated results for $\sigma_1(\omega)$ for all the three temperatures increases with ω but values are smaller than the experimental data. In the case of third Kondo alloy $UCu_{3.5}Pd_{1.5}$ our evaluated results increases but results are smaller for T = 30 K and 100 K and larger for 300 K. Recent theoretical results also exhibit similar behavior[17-20].

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