

The Kondo Problem for very dilute ZnMn alloys under a Doorway State perturbation approach*

Rafael Martín Landrove

*Laboratorio de Física Estadística y Fenómenos Colectivos, Escuela de Física y Matemáticas,
Facultad de Ciencias. Universidad Central de Venezuela
Apartado 47586. Caracas 1041-A, Venezuela.
E-mail: landrove@neblina.reacciun.ve / rmartin@fisica.ciens.ucv.ve*

Recibido: 09-06-1999 Aceptado: 21-02-200

Abstract

An alternative perturbation treatment for the Kondo Problem is developed using a doorway state formalism for scattering process. Under this approach the behavior of resistivity is examined at the low temperature regime, below and above Kondo temperature, within the framework of the s-d model for very dilute ZnMn alloys, where the single impurity scattering assumption holds. The agreement with experiment is excellent in the entire low temperature regime.

Key words: Kondo problem, perturbation theory, low temperature resistivity, doorway state, moment methods.

El Problema Kondo para aleaciones de ZnMn muy diluidas en un acercamiento perturbativo de Estado Compuerta

Resumen

Se desarrolla un tratamiento perturbativo alternativo para el problema Kondo empleando un formalismo de estados compuesta para procesos de dispersión. Bajo este acercamiento al problema el comportamiento de la resistividad es examinado en el régimen de temperaturas bajas, por debajo y por encima de la temperatura Kondo, dentro del marco de referencia del modelo s-d para aleaciones de ZnMn muy diluida, donde la suposición de colisión con una impureza es válida. El acuerdo experimental es excelente en todo el régimen de baja temperatura.

Palabras clave: Formalismo de estado; métodos de momento; problema de Kondo, resistividad a baja temperatura, teoría de perturbación.

1. Introduction

So far there is no single theory that can describe the resistivity behavior for metallic alloys (even at very low impurity concentration) below and above Kondo temperature T_K in the entire low temperature regime (1).

Above T_K , standard perturbation theory works well and a major feature as the resistivity minimum (Kondo effect) can be appropriately reproduced in this way (2). In the standard s-d model (3) and for a single impurity (no interimpurity interactions) the perturbation \hat{V} is given by

* Trabajo presentado en el Primer Congreso Venezolano de Física, Facultad de Ciencias, Universidad de Los Andes. Mérida, del 7 al 12 de diciembre de 1997.

$$\hat{V} \equiv \hat{H}_{sd} = \sum_{\vec{k}, \vec{k}'} J_{\vec{k}, \vec{k}'} \left[S^+ \hat{c}_{\vec{k}, \downarrow}^+ \hat{c}_{\vec{k}, \uparrow} + S^- \hat{c}_{\vec{k}, \uparrow}^+ \hat{c}_{\vec{k}, \downarrow} + S_z \left(\hat{c}_{\vec{k}, \uparrow}^+ \hat{c}_{\vec{k}, \uparrow} - \hat{c}_{\vec{k}, \downarrow}^+ \hat{c}_{\vec{k}, \downarrow} \right) \right] \quad [1.1]$$

where S_z and $S^\pm \equiv S_x \pm iS_y$ are the impurity spin components and the coupling coefficient $J_{\vec{k}, \vec{k}'}$, can be written in a separable form given by (N atoms in volume V)

$$J_{\vec{k}, \vec{k}'} \equiv \frac{J}{N} \theta \left(D - \left| \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'} \right| \right) \theta \left(D - \left| \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'} \right| \right) \quad [1.2]$$

where ε_F is the Fermi energy and D is the metal band width. The unperturbed Hamiltonian \hat{H}_0 is simply taken as the one for free electrons and it is given by

$$\hat{H}_0 \equiv \sum_{\vec{k}, s} \varepsilon_{\vec{k}} \hat{c}_{\vec{k}, s}^+ \hat{c}_{\vec{k}, s} \quad [1.3]$$

where $s = \uparrow, \downarrow$ labels the spin projection. The calculated resistivity up to second order in standard perturbation theory can be written as

$$\rho(T) = \alpha T^5 + c_{imp} R_0 - c_{imp} R_1 \ln \left(k_B T / D \right) \quad [1.4]$$

where the first term is the phonon contribution and the second term is related to the residual resistivity. There is a minimum for this calculated resistivity located at

$$T_{\min} = \left(\frac{R_1}{5\alpha} \right)^{1/5} c_{imp}^{1/5} \quad [1.5]$$

In the limit $T \rightarrow 0$, Kondo approach under perturbation theory breaks down and several attempts using many-body techniques to include leading order logarithmically divergent terms proved to be inadequate. In the antiferromagnetic case, when $J > 0$, this summation leads to an unobserved divergence at T_K , which precisely defines Kondo temperature. When $T \ll T_K$ interimpurity interactions become important and careful experimental work to eliminate

these effects revealed that impurity contributions give T^2 terms, aside a constant term, when $T \rightarrow 0$. Renormalization group theory (4, 5) provides an exact description of this behavior. In this work perturbation theory is revisited under a doorway state approach for scattering processes and comparisons with experimental results for very dilute ZnMn alloys within the framework of a simple s-d model are going to be made.

2. The \hat{T} Operator, Doorway State formalism and moment methods

The relaxation collision rate can be written as (θ' angle between \vec{p} y \vec{p}')

$$\frac{1}{\tau(\vec{p})} = \frac{2\pi c_{imp}}{(2S+1)(2S+1)} \sum_{\eta, \eta'} \int \frac{d^3 p'}{(2\pi)^3} \delta(\varepsilon_{\vec{p}'} - \varepsilon_{\vec{p}}) (1 - \cos \theta') \left| \langle \vec{p}', \eta' | \hat{T} | \vec{p}, \eta \rangle \right|^2 \quad [2.1]$$

at impurity concentration c_{imp} and conductivity (or resistivity) can be estimated from

$$\sigma(T) = -\lambda_0 e^2 \int \frac{d^3 p}{(2\pi)^3} v_{\vec{p}}^2 \tau(\vec{p}) \frac{\partial f(\varepsilon_{\vec{p}})}{\partial \varepsilon_{\vec{p}}} = \frac{1}{\rho(T)} \quad [2.2]$$

where λ_0 is a constant related to the lattice symmetry for the particular metal, $\langle \vec{p}', \eta' | \hat{T} | \vec{p}, \eta \rangle$ can be taken as the on-shell matrix element for the \hat{T} operator, $\eta \equiv (s, S)$ denotes the spin degrees of freedom set (electron and impurity), $v_{\vec{p}}$ is the electron velocity and $f(\varepsilon_{\vec{p}})$ is the Fermi distribution given by ($\beta \equiv 1/k_B T$)

$$f(\varepsilon_{\vec{p}}) = \frac{1}{e^{\beta(\varepsilon_{\vec{p}} - \varepsilon_F)} + 1} \quad [2.3]$$

In what follows a doorway state formalism (6) for a scattering process is going to be applied to calculate the matrix element $\langle \vec{p}', \eta' | \hat{T} | \vec{p}, \eta \rangle$ required in Equation [2.1] under a perturbation scheme where the \hat{T} operator can be written as

$$\hat{T} = \hat{V} + \hat{V}\hat{G}\hat{V} = \hat{V} + \hat{V} \frac{1}{E - \hat{H}} \hat{V} \quad [2.4]$$

and where the Green's operator \hat{G}_0 for the unperturbed Hamiltonian \hat{H}_0 is explicitly omitted. The reason for this particular choice is related to the fact that in standard perturbation theory the integrals related to the matrix elements $\langle \bar{p}', \eta' | \hat{V}(\hat{G}_0 \hat{V})^n | \bar{p}, \eta \rangle$ should be avoided since they are singular when $T \rightarrow 0$ and in the application of the doorway state formalism very delicate limits should be taken. Due to the particular form given to the \hat{T} operator in Equation [2.4], it is convenient to combine the doorway state formalism (6) with moment methods (7) successfully applied to shell model calculations in nuclear physics in order to obtain $\langle \bar{p}', \eta' | \hat{V}\hat{G}\hat{V} | \bar{p}, \eta \rangle$, instead of $\langle \bar{p}', \eta' | \hat{T} | \bar{p}, \eta \rangle$. The initial states for the doorway basis can be taken as

$$|D_0\rangle = N_0 \hat{V} | \bar{p}, \eta \rangle \text{ and } |\bar{D}_0\rangle = \tilde{N}_0 \hat{V} | \bar{p}', \eta' \rangle \quad [2.5]$$

and the rest of the basis can be obtained recursively from

$$|D_n\rangle = N_n \left[\hat{H} |D_{n-1}\rangle - \sum_{j=0}^{n-1} \langle \bar{D}_j | \hat{H} |D_{n-1}\rangle |D_j\rangle \right] \quad [2.6a]$$

$$|\bar{D}_n\rangle = \tilde{N}_n \left[\hat{H} |\bar{D}_{n-1}\rangle - \sum_{j=0}^{n-1} \langle D_j | \hat{H} |\bar{D}_{n-1}\rangle |\bar{D}_j\rangle \right] \quad [2.6b]$$

The relevant matrix element is given as a continued fraction and at the first doorway truncation level it can be approximated by

$$\langle \bar{p}', \eta' | \hat{V}\hat{G}\hat{V} | \bar{p}, \eta \rangle = \frac{\langle \bar{p}', \eta' | \hat{V}^2 | \bar{p}, \eta \rangle}{E - \frac{\langle \bar{p}', \eta' | \hat{V}\hat{H}\hat{V} | \bar{p}, \eta \rangle}{\langle \bar{p}', \eta' | \hat{V}^2 | \bar{p}, \eta \rangle}} \quad [2.7]$$

provided that the following condition is fulfilled (which is going to be the case indeed)

$$\frac{\langle \bar{p}', \eta' | \hat{V}\hat{H}^2\hat{V} | \bar{p}, \eta \rangle}{\langle \bar{p}', \eta' | \hat{V}^2 | \bar{p}, \eta \rangle} - \left(\frac{\langle \bar{p}', \eta' | \hat{V}\hat{H}\hat{V} | \bar{p}, \eta \rangle}{\langle \bar{p}', \eta' | \hat{V}^2 | \bar{p}, \eta \rangle} \right)^2 \ll \left(\frac{\langle \bar{p}', \eta' | \hat{V}\hat{H}\hat{V} | \bar{p}, \eta \rangle}{\langle \bar{p}', \eta' | \hat{V}^2 | \bar{p}, \eta \rangle} \right)^2 \quad [2.8]$$

3. Resistivity at Low temperature regime for a dilute ZnMn Alloy

In order to compare with experimental results which are given in terms of relative resistivities and to keep the analysis as simple as possible, it is useful to introduce the Fermi energy as the energy scale and the relevant dimensionless quantities are defined as

$$\zeta \equiv P/k_F, \quad \xi \equiv D/\epsilon_F, \quad \gamma \equiv \epsilon_F/k_B T, \quad \alpha \equiv J/\epsilon_F \quad [3.1a]$$

$$\langle |T_\zeta|^2 \rangle \equiv \frac{1}{(2s+1)(2S+1)} \sum_{\substack{n, \eta' \\ |\zeta|=|\zeta'|=\zeta}} \frac{|\langle \bar{\zeta}', \eta' | \hat{T} | \zeta, \eta \rangle|^2}{\epsilon_F^2} \quad [3.1b]$$

The contribution from impurity scattering to the total relative resistivity can be obtained from Eqs. [2.1] and [2.2] and it can be added to the phonon contribution and residual resistivity to give

$$\frac{\rho(\gamma)}{\rho(\gamma_0)} = \frac{A_0}{\gamma^5} + B_0 + \frac{C_0}{\gamma \int_{\sqrt{1-\xi}}^{\sqrt{1+\xi}} \zeta^2 d\zeta \frac{e^{-\gamma(\zeta-1)}}{\langle |T_\zeta|^2 \rangle [e^{-\gamma(\zeta-1)} + 1]^2}} \quad [3.2]$$

where A_0, B_0 and C_0 are constants to be determined and $\rho(\gamma_0)$ is the reference resistivity value measured at a temperature of γ_0^{-1} . One interesting feature of the relative resistivity given by Equation [3.2] is that it reaches a finite value given by

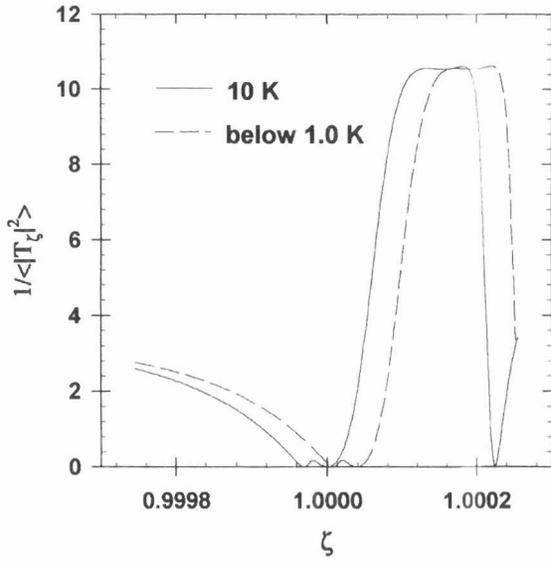


Figure 1. $\langle |T_\zeta|^2 \rangle^{-1}$ for different temperatures and within the range $\sqrt{1-\xi} \leq \zeta \leq \sqrt{1+\xi}$.

$$\frac{\rho(\infty)}{\rho(\gamma_0)} = B_0 + C_0 \langle |T_\zeta|^2 \rangle_{\zeta=1}^{-1} \quad [3.3]$$

when $\gamma \rightarrow \infty$ (or $T \rightarrow 0$) and where the on-shell scattering contribution from the Fermi level ($\zeta = 1$) is the only one that counts. The quantity $\langle |T_\zeta|^2 \rangle^{-1}$ is bound for all temperatures within the ζ range of interest, which includes $\zeta = 1$, and its zeroes are located at the effective poles for $\langle \tilde{\zeta}, \eta | \hat{T} | \tilde{\zeta}, \eta \rangle$ as it can be expected (Figure 1).

Comparison with experimental results for a ZnMn dilute alloy (0.00576%) is made in Figure 2 where the phonon contribution and residual resistivity are included. Assuming a Fermi energy of 9.47 eV (almost pure Zn), the parameters defined by Equation [3.1a] give $\alpha = 0.4$ ($J = 3.79$ eV) and $\xi = 0.00051$ (very narrow band, $D = 4.83$ meV) and it can be seen that provide an excellent agreement with measurements. The minimum around $T \approx 10$ K can be reproduced as well as the behavior in the $T \rightarrow 0$ limit. In Figure 3 the calculated curve in the absence of a phonon

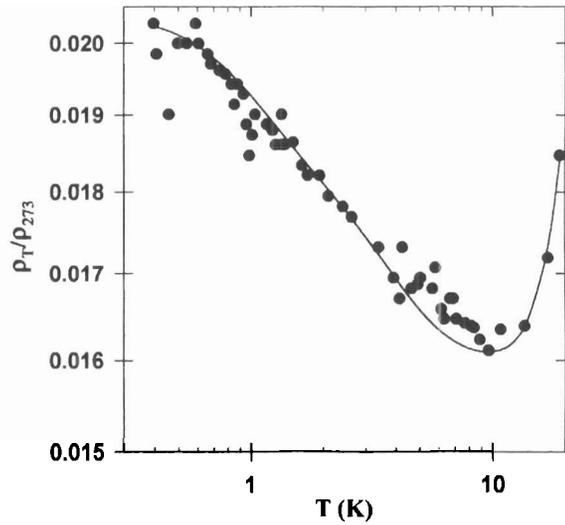


Figure 2. Comparison with experimental results for a dilute ZnMn alloy (0.00576%). The solid line represents the relative resistivity (resistivity at $T = 273$ K is the reference value) calculated from Equation [3.2] and data were taken from ref. (8).

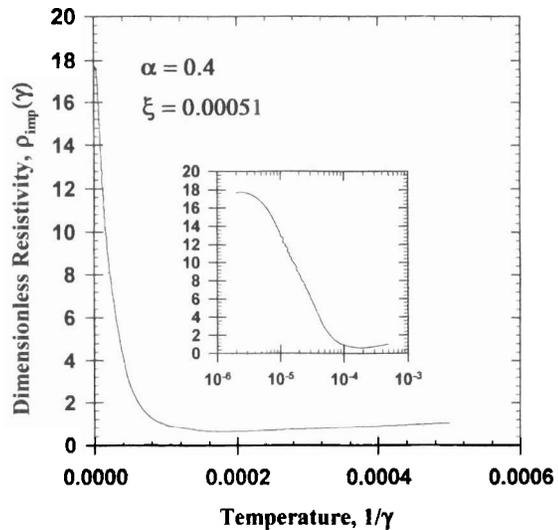


Figure 3. Calculated dimensionless relative resistivity in the absence of phonon contribution and residual resistivity, for the same dilute ZnMn alloy (0.00576%) depicted in Figure 1 ($A_0 = B_0 = 0$, $C_0 = 1$). The expected round top behavior as $\gamma^{-1} \rightarrow 0$ is clearly observed.

term and residual resistivity is depicted to show in more detail the expected low temperature behavior.

4. Conclusion

A modified doorway state perturbation scheme at the first truncation level can be applied successfully to a simple s-d model to describe the resistivity behavior in the entire low temperature range for ZnMn very dilute alloys, where the single impurity assumption clearly holds. In a forthcoming article all the available experimental data is going to be analyzed within the framework of this formalism and the effects of interimpurity interactions are going to be weighed for low concentration problems.

References

1. HEWSON A.C. *The Kondo problem to Heavy Fermions*, Cambridge University Press, Cambridge (UK), 1993.
2. KONDO, J. *Solid State Physics* (Eds. Seitz F., Turnbull D. & Ehrenreich H.), Academic Press, New York (USA), 23:183-281, 1964.
3. ZENER, C. *Phys Rev* 81:440-444, 1951.
4. WILSON, K.G. *Rev Mod Phys* 47:773-840, 1975.
5. NOZIERES, P. *J Low Temp Phys* 17:31-42, 1974.
6. LENZ F., MONIZ E.J., YAZAKI K. *Annals of Physics* 129:84-109, 1980.
7. WHITEHEAD R.R., WATT A., COLE B.J., MORRISON I. *Advances in Nuclear Physics* (Eds. Baranger M. & Vogt E.), 9:123-176, 1977.
8. HEDGCOCK F.T., RIZZUTO C. *Phys Rev* 163:517-522, 1967.