

ON THE INTERACTION BETWEEN ELECTRONS AND  
TUNNELING LEVELS IN METALLIC GLASSES\*

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**MASTER**

ABSTRACT: We consider a simple model in which the conduction electrons of a metallic glass experience a local time-dependent potential due to two-level tunneling states. We show that the model exhibits interesting divergent behavior which is, nevertheless, quite different from that predicted by the "s-d Kondo" model of a Cochrane et al. [9].

RÉSUMÉ: Nous considérons un modèle simple dans lequel les électrons d'un verre métallique sont soumis à un potentiel local dépendant du temps, du à des double puits à deux niveaux. Nous montrons que ce modèle possède des divergences intéressantes qui sont toutefois très différentes des prédictions du modèle "s-d Kondo" de Cochrane et al. [9].

Recently there has been considerable experimental evidence for the existence of tunneling levels in metallic glasses [1-5]. Such tunneling states, presumably arising from local atomic rearrangements as proposed by Anderson et al. [6] and Phillips [7], explain a variety of low-temperature anomalies in insulating glasses [8]. In the case of metallic glasses, an interesting new question arises: How do they interact with the degenerate Fermi system of the conduction electrons? Here we report on a preliminary study of a simple model which treats the tunneling states as localized scattering centers with an internal degree of freedom. We show that the instability of the electron gas to such perturbations leads to interesting behavior which nevertheless differs from that encountered in the Kondo and x-ray problems.

Considering the same problem, Cochrane, et al. [9] have proposed a model which is in one-to-one correspondence with the s-d Kondo Hamiltonian [10]

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and have consequently predicted a logarithmic contribution to the resistivity. However, this analogy relies upon the questionable assumption that the current-carrying conduction electrons can be labeled by an index which corresponds to the spin of the electron in the s-d model. As an alternative we consider a model in which an electron undergoes ordinary potential scattering dependent upon the state of the tunneling level but not upon an internal electronic degree of freedom corresponding to the spin.

Describing the tunneling level by an  $s = \frac{1}{2}$  pseudospin, the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \Delta S_z + \Delta_0 S_x + K_{\parallel} S_z \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}'}, \quad (1)$$

where  $\epsilon_{\mathbf{k}}$  is the single-particle electron energy,  $\Delta$  is the tunneling-level asymmetry [8,11], and  $\Delta_0$  is the quantum-mechanical tunneling frequency [8,11]. The coupling constant  $K_{\parallel}$  accounts for the change in potential seen by the electrons when the tunneling system changes states. This Hamiltonian is similar to a model for crystal-field-split levels considered by Fulde and Peschel [12] and is essentially the same as one recently studied by Kondo [13]. Clearly Eq. (1) neglects many important scattering mechanisms as well as all  $\mathbf{k}$ -dependence of  $K_{\parallel}$ . Furthermore Eq. (1) may not accurately reflect the situation when the electronic mean free path is smaller than the extent of the tunneling system (which is not known). Nevertheless, we feel that this model is useful for a qualitative understanding of the electron-tunneling-level interactions.

Rotating the pseudospin basis states in Eq. (1) diagonalizes the non-interacting part of the Hamiltonian:

$$\mathcal{H}' = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + 2\delta_0 S_z + (V_{\parallel} S_z + V_{\perp} S_x) \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}'}, \quad (2)$$

where  $(2\delta_0)^2 = \Delta^2 + \Delta_0^2$ ,  $V_{\parallel} = K_{\parallel} (\Delta/2\delta_0)$  and  $V_{\perp} = -K_{\parallel} (\Delta_0/2\delta_0)$ .

Using Abrikosov's pseudofermion representation for  $S_x$  and  $S_z$  [14] and finite-temperature perturbation theory, the electronic self-energy  $\sum^{(E_n)}$  is given by

$$\sum^{(E_n)} = \sum_{\alpha\alpha'} \sum_{\lambda\lambda'} V_{\alpha\alpha'} \mathcal{D}_{\alpha\alpha'}(\varepsilon_\lambda) \mathcal{D}_{\alpha'\alpha'}(\varepsilon_{\lambda'}) \mathcal{G}(E_n + \varepsilon_\lambda - \varepsilon_{\lambda'}) \times \gamma_{\alpha'\alpha}(\varepsilon_\lambda, \varepsilon_{\lambda'}; \varepsilon_\lambda + E_n), \quad (3)$$

where  $\mathcal{D}_{\alpha\alpha'}(\varepsilon_\lambda) = (i\varepsilon_\lambda - \delta_\alpha)^{-1}$ ,  $\mathcal{G}(E_n) = \rho \int_{-D}^D d\xi (iE_n - \xi)^{-1}$ ,  $\delta_\alpha = \pm \delta_0$ ,  $\rho$  is the density of states at  $E_F$ , and  $D$  is the bandwidth. The vertex part  $\gamma_{\alpha\alpha'}$  is given by a perturbation expansion in terms of the bare coupling constant matrix

$$2V_{\alpha\alpha'} = V_{||} (\text{sgn} \delta_\alpha) \delta_{\alpha\alpha'} + V_{\perp} (1 - \delta_{\alpha\alpha'}). \quad (4)$$

The first corrections,  $\gamma_{\alpha\alpha'}^{(2)}$ , to Eq. (4) are the particle-particle and particle-hole bubble diagrams, which are separately logarithmically divergent. As in the Kondo [14] and x-ray edge [15] problems, these divergences arise from the instability of the electron gas to a sudden localized change in the external potential. However, the algebra of the  $\alpha$  summation results in qualitatively different behavior of the vertex part.

For example, all logarithmic corrections cancel if the "magnetic field"  $\delta_0$  is zero [13]. Furthermore, even when  $\delta_0 \neq 0$ , there is no divergent contribution to  $\sum^{(3)}(E=0)$ , as would be the case in the Kondo problem [10]. In fourth order, however, we find to leading logarithmic accuracy.

$$\text{Im} \sum^{(4)}(0) = 4\pi \rho^3 \tanh^2 \frac{\beta\delta_0}{2} V_{||}^2 V_{\perp}^2 \ell n^2 \frac{D}{2k_B T}. \quad (5)$$

In order to gain further insight into the nature of this divergence we have studied the lowest order "parquet" equations [14] for the vertex part  $\gamma_{\alpha\alpha'}$  within this approximation. We find that the diagonal component  $\gamma_{\alpha\alpha}$  is not renormalized but the off-diagonal part diverges as a power law at the energies  $\varepsilon_\lambda + E_n = \pm i\delta_0$ . Namely, for electron energies

$E < |\delta_0|$  at  $T = 0$

$$\gamma_{\perp} (+i\delta_0, -i\delta_0, \pm i\delta_0 + E) = v_{\perp} e^{\pm 2\rho(0)V_{11}} \left| \frac{D}{E} \right|. \quad (6)$$

While reminiscent of both the Kondo and the x-ray edge singularity behavior, the above result differs from both.

This conclusion is further supported by a separate analysis of Eq. (1) in which we rely on the work of Schotte [16] and Blume et al. [17] and use  $\Delta_0 S_x$  as a perturbation. This procedure is entirely analogous to the reformulation of the Kondo problem as a sequence of x-ray edge problems [15] by Anderson, et al. [18]. In their language, our model differs from the Kondo problem because "x-ray edge" is replaced by "x-ray photoemission" [19], in which the creation of a deep core hole (i.e., spin flip) is not accompanied by the injection of an electron at the Fermi surface.

Thus the relationship between our model and the usual Kondo problem, in terms of the respective free energies  $F_{MG}$  and  $F_K$  is

$$F_{MG} = F_K(\epsilon = 2 - (\rho K_{\parallel})^2, J_{\perp} = \Delta_0, H = \Delta) + \text{constant}. \quad (7)$$

The Kondo free energy,  $F_K$ , is defined in the presence of a magnetic field,  $H$ , and depends upon the usual coupling constants [18]  $\rho J_{\perp}$  and  $\rho J_{\parallel} \equiv \frac{1}{2}\epsilon$ . Thus the weak-coupling ( $\rho K_{\parallel} \ll 1$ ) version of the metallic glass free energy corresponds to a particular anisotropic strong-coupling Kondo problem ( $1 < \rho J_{\parallel} \gg \rho J_{\perp}$ ). This relationship does not, of course, imply that the response functions in our model are simply related to those in the Kondo problem. Nevertheless, it does suggest that the metallic glass divergences can be studied by renormalization group methods [18]. Work is in progress on this approach and on the question of response functions.

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