Microscopic Theory of Tunneling Anomalies

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In this paper we shall develop[5] a microscopic theory of the zero-bias magnetic anomalies which is valid for both the weak-coupling limit discussed by Appelbaum and Anderson and the strong-coupling (low-temperature) limit, starting from the model Hamiltonian proposed by Appelbaum. Our approach is based on a generalization of a method employed by Ambegaokar and Baratoff for superconducting tunneling and employs the self-consistent solution to the Kondo effect given by Nagaoka for bulk samples.

I. INTRODUCTION

DYNAMIC anomalies centered at zero bias have been observed in both p-n semiconductor and metal–metal-oxide–metal tunnel junctions.[1]

Recently Appelbaum[2,3] and Anderson[4] (AA) explained the weak zero-bias anomalies by attributing the anomalies to the exchange scattering of conduction electrons by localized paramagnetic states (lms) assumed to be present near the metal-oxide interface. Their calculations were based on perturbation theory and were consequently limited to the regime where the anomalous tunneling current is small. In this limit Appelbaum obtained for ΔG, the anomalous conductance

$$\Delta G \alpha - |T_J|^2 J(\rho^a)^2 \rho^b \ln\left(\frac{|eV|+kT}{E_0}\right),$$

where all the symbols have the same meaning as those which were used by Appelbaum.[3] For $J>0$, corresponding to antiferromagnetic coupling, ΔG enhances the conductance.

Clearly, at sufficiently low temperature the perturbation approach breaks down, and it becomes necessary to resort to more powerful nonperturbational methods.

This strong-coupling regime may be realized experimentally either by studying tunneling junctions which exhibit weak anomalies at much lower temperatures than have been previously used, or by constructing tunneling junctions which have a larger effective J and, consequently, a much higher Kondo transition temperature. The strong-coupling calculation of this paper suggests the possibility that the giant anomalies recently observed by Rowell and Shen[5] in Cr–chromium-oxide–Ag tunnel junctions may fall into the second category.

In this paper we shall develop a microscopic theory of the zero-bias magnetic anomalies which is valid for both the weak-coupling limit discussed by AA and the strong-coupling (low-temperature) limit starting from the model Hamiltonian proposed by Appelbaum. Our approach is based on a generalization of a method employed by Ambegaokar and Baratoff[6] for superconducting tunneling and employes the self-consistent solution to the Kondo effect given by Nagaoka[7] (N) for bulk samples.

In Sec. II we discuss the terms which enter our model-tunneling Hamiltonian. In addition, we discuss the connection between the tunneling-Hamiltonian method we use to calculate the current and a method recently proposed by Zawadowski.[8] We find that the tunneling-Hamiltonian approach is quite capable of including all contributions to the current obtained from Zawadowski's approach (Z) as well as important nonlocal dynamic terms which are not contained in the Z theory.

In Sec. III an expression is derived for the tunneling current in terms of Green's functions from the left and right sides of the tunneling junction.

These Green's functions are examined in Sec. IV. It is found that some of them may be obtained directly from the work of Nagaoka while for others new equations must be derived different from those already obtained by (N). The tunneling current is examined in Sec. V in both the low- and high-temperature limits.

In Sec. VI we extend the work of the previous sections, which have been restricted to a single lms to the case where one has a distribution of lms.

In Sec. VII a discussion of the results of this paper is given.

II. TUNNELING HAMILTONIAN

We assume we are dealing with an idealized (metal A)–(metal-A oxide)–(metal B) tunneling junction. It is further assumed that lms are present in the vicinity of the (metal A)–(metal-A oxide) interface.

The various terms that may appear in the model

[1] A. F. G. Wyatt, Phys. Rev. Letters **13**, 401 (1964); R. A. Logan and J. M. Rowell, *ibid.* **13**, 404 (1964); J. M. Rowell and L. Y. L. Shen, *ibid.* **17**, 15 (1966).
[2] J. Appelbaum, Phys. Rev. Letters **17**, 91 (1966).
[3] Joel A. Appelbaum, Phys. Rev. **154**, 633 (1967).
[4] P. W. Anderson, Phys. Rev. Letters **17**, 95 (1966).
[5] J. M. Rowell and L. Y. L. Shen, see Ref. 1.
[6] V. Ambegaokar and A. Baratoff, Phys. Rev. Letters **10**, 486 (1963).
[7] Y. Nagaoka, Phys. Rev. **138**, A1112 (1965).
[8] A. Zawadowski (unpublished).

Hamiltonian have been discussed by Appelbaum.[3] Here we shall use the phenomenological form in which the spins of the paramagnetic states are treated as operators external to the electron system. The Hamiltonian, assuming the presence of a single lms, then has the form (in the absence of a magnetic field)

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1+\mathcal{H}_2+\mathcal{H}_3+\mathcal{H}_4\,, \tag{2.1}$$

$$\mathcal{H}_0=\sum_{1\sigma}\tilde{\xi}_{1\sigma}a_{1\sigma}{}^\dagger a_{1\sigma}+\sum_{r\sigma}\xi_{r\sigma}b_{r\sigma}{}^\dagger b_{r\sigma}\,, \tag{2.2}$$

where

$$\tilde{\xi}_{1\sigma}=\xi_{1\sigma}+eV \tag{2.3}$$

and $a_{1\sigma}(b_{r\sigma})$ refer to the destruction operator for an electron with momentum state $\mathbf{l}(\mathbf{r})$, spin state σ, and energy $\tilde{\xi}_1(\xi_r)$ on the left-(right-) hand side of the junction. V is the applied voltage.

$$\mathcal{H}_1=\sum_{1,r,\sigma}\tilde{T}_{1r}a_{1\sigma}{}^\dagger b_{r\sigma}+\tilde{T}_{1r}{}^*b_{r\sigma}{}^\dagger a_{1\sigma}\,, \tag{2.4}$$

represents the usual tunneling through the barrier without spin flip. This type of tunneling conserves the transverse component of momentum of the tunneling electrons, so that

$$\tilde{T}_{1r}=T_{1r}\delta_{1_\perp,r_\perp}\,, \tag{2.5}$$

where $\mathbf{k}_\perp$ is the transverse component of momentum for an electron with momentum $\mathbf{k}$. We ignore for simplicity the dependence of T_{1r} on $\mathbf{l}$ and $\mathbf{r}$, writing it as T.

$$\mathcal{H}_2=T_a\sum_{1,r,\sigma}a_{1\sigma}{}^\dagger b_{r\sigma}+b_{r\sigma}{}^\dagger a_{1\sigma} \tag{2.6}$$

corresponds to impurity-assisted nonmagnetic tunneling. The fact that the tunneling electron scatters off, the localized state breaks down momentum conservation, hence T_a does not have the delta function conserving transverse momentum that T contains. This distinction between T_a and T will be of importance as we proceed.

$$\mathcal{H}_3=T_J\sum_{11',\sigma\sigma'}\mathbf{S}\cdot\boldsymbol{\tau}_{\sigma\sigma'}(a_{1\sigma}{}^\dagger b_{r\sigma'}+b_{r\sigma'}{}^\dagger a_{1\sigma})\,, \tag{2.7}$$

where $\boldsymbol{\tau}$ is the Pauli spin operator, and $\mathbf{S}$, the spin of the localized magnetic state, describes tunneling with spin-flip. The same comments about momentum nonconservation applying to T_a are valid in the same way for T_J.

$$\mathcal{H}_4=-J\sum_{1,1',\sigma,\sigma'}\mathbf{S}\cdot\boldsymbol{\tau}_{\sigma\sigma'}a_{1\sigma}{}^\dagger a_{1'\sigma'}\,, \tag{2.8}$$

describes the scattering of conduction electrons on the a side of the junction back into the a side.

In concluding this section we would like to comment on the difference between the tunneling-Hamiltonian method for calculating the current employed in this paper and the method recently proposed by Zawadowski (Z). Z divides the tunneling junction problem into two parts, which he calls the left- and right-hand problems. The only effect of the magnetic states in Zawadowski's approach (Z) is to introduce a self-energy into the Green's function for the left-hand side problem (lhp). The magnetic states are assumed by (Z) to lie on the left-hand side of the oxide barrier. This is justified by the argument that the exchange interaction is local in nature and therefore only affects the lhp through the self-energy of the lhp Green's function. This assumption corresponds to retaining in the tunneling Hamiltonian only the terms $\mathcal{H}_0$, $\mathcal{H}_1$, $\mathcal{H}_2$, $\mathcal{H}_4$, and dropping $\mathcal{H}_3$.

Now $\mathcal{H}_3$ contains the nonlocal part of the exchange interaction. This nonlocal behavior arises from two sources. The first is the fact that the exchange interaction is generally nonlocal in the bulk. Second, and even more important, the distinction between an electron from the left- and right-hand side of the junction necessarily breaks down in the junction, which has the effect of breaking down the local nature of exchange interaction further. Hence we feel that the tunneling-Hamiltonian method is more general than Zawadowski's approach.

III. TUNNELING CURRENT

We shall calculate the tunneling current on the assumption that the contribution to the current from each localized state is additive. This assumption is valid if one can neglect spin-spin interactions among the localized spins. The presence of a short mean free path at the junction interface should have the effect of weakening the long-range spin-spin interaction, therefore making the independent impurity assumption valid at even relatively high concentrations.

We shall further neglect $\mathcal{H}_1$ in calculating the current, thereby including only tunneling which proceeds through the localized states. The necessary modifications of the current resulting from the inclusion of $\mathcal{H}_1$ will be considered when we turn to the many-lms problem in Sec. VI.

We calculate the tunneling current by a generalization of a method employed for superconducting tunneling by Ambegaokar and Baratoff.[6]

We divide $\mathcal{H}$ into

$$\mathcal{H}=\mathcal{H}_B+\mathcal{H}_T\,, \tag{3.1}$$

where

$$\mathcal{H}_B=\mathcal{H}_0+\mathcal{H}_4 \tag{3.2}$$

and

$$\mathcal{H}_T=\mathcal{H}_2+\mathcal{H}_3\,. \tag{3.3}$$

Now, the current is given by

$$j=-e\left\langle\frac{dN^a}{dt}\right\rangle_{\text{th.av.}}\,, \tag{3.4}$$

where th.av. refers to the appropriate thermal average.

$$N^a=\sum_{1,\sigma}n_{1\sigma}{}^a\,. \tag{3.5}$$

Setting $\hbar=1$,

$$i\frac{d}{dt}N^a=[N^a,\mathcal{H}] \tag{3.6}$$

from which we obtain

$$j=-4eT\sum_{1r}\mathrm{Im}\langle a_{1+}^\dagger(t)b_{r+}(t)\rangle -6eT_J\sum_{1,r}\mathrm{Im}\langle a_{1+}^\dagger(t)b_{r-}(t)S_-(t)\rangle. \tag{3.7}$$

We have used the fact that our system is invariant under spin rotations to simplify Eq. (3.7). (We assume $S=\frac{1}{2}$.)

Treating $\mathcal{H}_T$ as a perturbation, we evaluate

$$\langle a_{1+}^\dagger(t)b_{r+}(t)\rangle \quad\text{and}\quad \langle a_{1+}^\dagger(t)b_{r-}(t)S_-(t)\rangle$$

to lowest order in $\mathcal{H}_T$. When this is done and inserted into (3.7) we have for

$$\begin{aligned}j=&+4eT^2\,\mathrm{Re}\sum_{1,r}\int_{-\infty}^{t}d\tau\,[G_1^<(\tau-t)G_r^>(t-\tau)-G_1^>(\tau-t)G_r^<(t-\tau)]\\&+6eT_J^2\,\mathrm{Re}\sum_{1,r}\int_{-\infty}^{t}d\tau\,[L_1^<(\tau-t)G_r^>(t-\tau)-L_1^>(\tau-t)G_r^<(t-\tau)]\\&+4eTT_J\,\mathrm{Re}\sum_{1,r}\int_{-\infty}^{t}d\tau\,[\Gamma_1^<(\tau-t)G_r^>(t-\tau)-\Gamma_1^>(\tau-t)G_r^<(t-\tau)]\\&+6eT_JT\,\mathrm{Re}\sum_{1,r}\int_{-\infty}^{t}d\tau\,[\theta_1^<(\tau-t)G_r^>(t-\tau)-\theta_1^>(\tau-t)G_r^<(t-\tau)],\end{aligned} \tag{3.8}$$

where

$$G_1^<(\tau-t)=\sum_{1'}\langle a_{1+}^\dagger(t)a_{1'+}(\tau)\rangle, \tag{3.9}$$

$$G_r^<(\tau-t)=\sum_{r'}\langle b_{r+}^\dagger(t)b_{r'+}(\tau)\rangle, \tag{3.10}$$

$$L_1^<(\tau-t)=\sum_{1'}\langle a_{1+}^\dagger(t)S_-(t)\{a_{1'+}(\tau)S_+(\tau)-a_{1'-}(\tau)S_z(\tau)\}\rangle, \tag{3.11}$$

$$\Gamma_1^<(\tau-t)=\sum_{1'}\langle a_{1+}^\dagger(t)\{a_{1'+}(\tau)S_z(\tau)+a_{1'-}(\tau)S_-(\tau)\}\rangle, \tag{3.12}$$

$$\theta_1^<(\tau-t)=\sum_{1'}\langle a_{1+}^\dagger(t)S_-(t)a_{1'-}(\tau)\rangle. \tag{3.13}$$

The corresponding expressions with $<$ replaced by $>$ are identical to those above except that the operators at time t are interchanged with those at time τ.

The above correlation functions can be expressed in terms of the imaginary parts of the corresponding retarded double time Green's[9] functions employing the usual spectral theorems. The integrals over τ may then be performed quite trivially and one obtains for j

$$\begin{aligned}j=&16\pi eT_a^2\sum_{1,r}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)][\mathrm{Im}G_1(\omega)][\mathrm{Im}G_r(\omega+eV)]\\&+24\pi eT_J^2\sum_{1,r}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)][\mathrm{Im}L_1(\omega)][\mathrm{Im}G_r(\omega+eV)]\\&+16\pi eT_aT_J\sum_{1,r}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)][\mathrm{Im}\Gamma_1(\omega)][\mathrm{Im}G_r(\omega+eV)]\\&+24\pi eT_JT_a\sum_{1,r}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)][\mathrm{Im}\theta_1(\omega)][\mathrm{Im}G_r(\omega+eV)],\end{aligned} \tag{3.14}$$

where

$$G_1=\sum_{1'}G_{11'}^a, \tag{3.15}$$

$$G_r=\sum_{r'}G_{rr'}^a, \tag{3.16}$$

$$L_1=\sum_{1'}L_{11'}^a, \tag{3.17}$$

$$\theta_1=\sum_{1'}\theta_{11'}^a, \tag{3.18}$$

$$\Gamma_1=\sum_{1'}\Gamma_{11'}^a. \tag{3.19}$$

[9] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Physics—Uspekhi **3**, 320 (1960)].

[The subscripts l, r refer to quantities on the a (left) and b (right) sides, respectively.]

$$G_{ll'}{}^a=\langle\langle a_{l'+}\,|\,a_{l+}{}^\dagger\rangle\rangle_\omega\,, \tag{3.20}$$

$$G_{rr'}{}^b=\langle\langle b_{r'+}\,|\,b_{r+}{}^\dagger\rangle\rangle_\omega\,, \tag{3.21}$$

$$\Gamma_{ll'}{}^a=\langle\langle a_{l'+}S_z+a_{l'-}S_-\,|\,a_{l+}{}^\dagger\rangle\rangle_\omega\,, \tag{3.22}$$

$$L_{ll'}{}^a=\langle\langle a_{l'+}S_+-a_{l'-}S_z\,|\,a_{l+}{}^\dagger S_-\rangle\rangle_\omega\,, \tag{3.23}$$

$$\theta_{ll'}{}^a=\langle\langle a_{l'-}\,|\,a_{l+}{}^\dagger S_-\rangle\rangle_\omega\,. \tag{3.24}$$

$$f(\omega)=\frac{1}{e^{\omega\beta}+1}\,,\quad \beta=1/kT \tag{3.25}$$

$\langle\langle\ |\ \rangle\rangle_\omega$ denotes the Fourier transform of the retarded double-time Green's function, which, for completeness, we define below:

$$\langle\langle A\,|\,B\rangle\rangle_\omega=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\theta(t)[\langle A(t)B(0)+B(0)A(t)\rangle]e^{i\omega t}dt \tag{3.26}$$

and

$$\theta(t)=0\,,\quad t<0$$
$$=1\,,\quad t>0\,. \tag{3.27}$$

Our problem is essentially reduced to calculating the Green's function (3.20) to (3.24).

IV. GREEN'S FUNCTIONS

In calculating the Green's functions (3.20) to (3.24) we shall utilize the self-consistent solution to the bulk Kondo effect given by N. In what follows we shall adhere as closely as possible to his notation.

Now $G_{ll'}{}^a(\omega)$ and $\Gamma_{ll'}{}^a(\omega)$ have already been calculated by N. Unfortunately this is not the case for $L_{ll'}{}^a$ and $\theta_{ll'}{}^a$, and it becomes necessary to solve for these quantities using standard equation of motion techniques. Setting

$$L_{ll'}=\Phi_{ll'}-\Lambda_{ll'}\,, \tag{4.1}$$

(we drop the superscript a and b from now on), where

$$\Phi_{ll'}=\langle a_{l'+}S_+\,|\,a_{l+}{}^\dagger S_-\rangle\,, \tag{4.2}$$

$$\Lambda_{ll'}=\langle a_{l'-}S_z\,|\,a_{l+}{}^\dagger S_-\rangle\,, \tag{4.3}$$

we obtain equations for $\Phi_{ll'}$, $\Lambda_{ll'}$, and $\theta_{ll'}$

$$(\omega-\xi_{l'})\Phi_{ll'}=\frac{1}{2\pi}(\tfrac{1}{2}\delta_{ll'}-\langle S_-a_{l+}{}^\dagger a_{l'-}\rangle)+J(n_{l'}-\tfrac{1}{2})\sum_{\mathbf{k}'}\Phi_{l\mathbf{k}'}+\tfrac{2}{3}J(m_{l'}-\tfrac{3}{4})\sum_{\mathbf{k}'}\theta_{l\mathbf{k}'}{}^a+2J(n_{l'}-\tfrac{1}{2})\sum_{\mathbf{k}'}\Lambda_{l\mathbf{k}'}{}^a\,, \tag{4.4}$$

$$(\omega-\xi_{l'})\Lambda_{ll'}(\omega)=\frac{1}{2\pi}\langle a_{l+}{}^\dagger a_{l'-}S_-\rangle-\tfrac{1}{3}J(m_{l'}-\tfrac{3}{4})\sum_{\mathbf{k}'}\theta_{l\mathbf{k}'}+J(n_{l'}-\tfrac{1}{2})\sum_{\mathbf{k}}\Phi_{l\mathbf{k}'}(\omega)\,, \tag{4.5}$$

and

$$(\omega-\xi_{l'})\theta_{ll'}(\omega)=-J\sum_{\mathbf{k}'}L_{l\mathbf{k}'}\,. \tag{4.6}$$

To obtain the above equations, it was necessary to factorize higher-order Green's functions generated by the equation-of-motion technique in order to close the hierarchy of equations. The required factorizations, listed below, are entirely consistent with those employed by N:

$$\langle a_{l'-}a_{\mathbf{k}+}{}^\dagger a_{\mathbf{k}'-}S_-\,|\,a_{l+}{}^\dagger S_-\rangle=\langle a_{l'-}a_{\mathbf{k}+}{}^\dagger S_-\rangle\langle a_{\mathbf{k}'-}\,|\,a_{l+}{}^\dagger S_-\rangle+\langle a_{\mathbf{k}+}{}^\dagger a_{\mathbf{k}'-}S_-\rangle\langle a_{l'-}\,|\,a_{l+}{}^\dagger S_-\rangle\,, \tag{4.7}$$

$$\langle S_+a_{\mathbf{k}-}{}^\dagger a_{l'-}a_{\mathbf{k}'+}\,|\,a_{l+}{}^\dagger S_-\rangle=-\langle S_+a_{\mathbf{k}-}{}^\dagger a_{\mathbf{k}'+}\rangle\langle a_{l'-}\,|\,a_{l'+}{}^\dagger S_-\rangle+\langle a_{\mathbf{k}-}{}^\dagger a_{l'-}\rangle\langle S_+a_{\mathbf{k}'+}\,|\,a_{l+}{}^\dagger S_-\rangle\,, \tag{4.8}$$

$$\langle a_{\mathbf{k}+}{}^\dagger a_{\mathbf{k}'+}a_{l'+}S_+\,|\,a_{l+}{}^\dagger S_-\rangle=\langle a_{\mathbf{k}+}{}^\dagger a_{\mathbf{k}'+}\rangle\langle a_{l'+}S_+\,|\,a_{l+}{}^\dagger S_-\rangle-\langle a_{\mathbf{k}+}{}^\dagger a_{l'+}\rangle\langle a_{\mathbf{k}'+}S_+\,|\,a_{l+}{}^\dagger S_-\rangle\,, \tag{4.9}$$

$$\langle a_{\mathbf{k}-}{}^\dagger a_{\mathbf{k}'-}a_{l'+}S_+\,|\,a_{l+}{}^\dagger S_-\rangle=\langle a_{\mathbf{k}-}{}^\dagger a_{\mathbf{k}'-}\rangle\langle a_{l'+}S_+\,|\,a_{l+}{}^\dagger S_-\rangle-\langle a_{\mathbf{k}-}{}^\dagger a_{l'+}S_+\rangle\langle a_{\mathbf{k}'-}\,|\,a_{l+}{}^\dagger S_-\rangle\,, \tag{4.10}$$

$$\langle S_za_{\mathbf{k}+}{}^\dagger a_{l'+}a_{\mathbf{k}-}\,|\,a_{l+}{}^\dagger S_-\rangle=\langle a_{\mathbf{k}+}{}^\dagger a_{l'+}\rangle\langle S_za_{\mathbf{k}-}\,|\,a_{l+}{}^\dagger S_-\rangle+\langle S_za_{\mathbf{k}+}{}^\dagger a_{l'+}\rangle\langle a_{\mathbf{k}-}\,|\,a_{l+}{}^\dagger S_-\rangle\,. \tag{4.11}$$

Subtracting Eq. (4.4) from (4.5) we obtain

$$(\omega-\xi_{l'})L_{ll'}(\omega)=\frac{1}{2\pi}\{\tfrac{1}{2}\delta_{ll'}-2\langle a_{l+}{}^\dagger a_{l'-}S_-\rangle\}-2J(n_{l'}-\tfrac{1}{2})\sum_{\mathbf{k}'}L_{l\mathbf{k}'}(\omega)+J(m_{l'}-\tfrac{3}{4})\sum_{\mathbf{k}'}\theta_{l\mathbf{k}'}(\omega)\,, \tag{4.12}$$

where

$$n_l=\sum_{\mathbf{k}}\langle a_{\mathbf{k}-}{}^\dagger a_{l-}\rangle\,, \tag{4.13}$$

$$m_{l'}=3\sum_{\mathbf{k}}\langle a_{\mathbf{k}+}{}^\dagger a_{l'-}S_-\rangle\,. \tag{4.14}$$

From (4.12) and (4.6) one obtains

$$\theta_l(\omega)=-JF^a(\omega)L_l(\omega) \tag{4.15}$$

and

$$L_l(\omega)=\frac{1}{2\pi d(\omega)}\left\{\frac{1}{2}\frac{1}{\omega-\xi_l}-g_l(\omega)\right\}\,, \tag{4.16}$$

where

$$d(\omega)=1+2JG(\omega)+J^2F^a(\omega)\Gamma(\omega)\,, \tag{4.17}$$

$$g_l(\omega)=2\sum_{l'}\frac{\langle a_{l+}{}^\dagger a_{l'-}S_-\rangle}{\omega-\xi_{l'}}\,, \tag{4.18}$$

and

$$F^{(a,b)}(\omega)=\sum_{(1',r')}\frac{1}{\omega-\xi_{(1',r')}}\,, \tag{4.19}$$

$$\Gamma(\omega)=\sum_{1'}\frac{m_{1'}-\frac{3}{4}}{\omega-\xi_{1'}}\,, \tag{4.20}$$

$$G(\omega)=\sum_{1'}\frac{n_{1'}-\frac{1}{2}}{\omega-\xi_{1'}}\,. \tag{4.21}$$

The remaining Green's functions may be obtained directly from N. We conclude this section by listing them below for convenience.

$$G_1(\omega)=\frac{1}{2\pi}\frac{1}{\omega-\xi_1}\frac{1}{d(\omega)}\{1+2JG(\omega)\}\,, \tag{4.22}$$

$$\Gamma_1(\omega)=\frac{1}{2\pi}\frac{1}{\omega-\xi_1}\frac{1}{d(\omega)}\{J\Gamma(\omega)\}\,, \tag{4.23}$$

$$G_r(\omega)=\frac{1}{2\pi}\frac{1}{\omega-\xi_r}\,. \tag{4.24}$$

V. TUNNELING CURRENT

A. Weak Coupling (High Temperature)

We consider the tunneling current in the weak-coupling regime.

Summing over the remaining indices in Eqs. (4.15), (4.16), and (4.22)–(4.24), we obtain

$$\theta^a(\omega)=\sum_1\theta_1(\omega)=\frac{J}{3\pi}\frac{F^a(\omega)\Gamma(\omega)}{d(\omega)}\,, \tag{5.1}$$

$$L^a(\omega)\equiv\sum_1 L_1(\omega)=\frac{1}{2\pi d(\omega)}[-\tfrac{2}{3}\Gamma(\omega)]\,, \tag{5.2}$$

$$G^a(\omega)\equiv\sum_1 G_1(\omega)=\frac{1}{2\pi}\frac{F^a(\omega)[1+2JG(\omega)]}{d(\omega)}\,, \tag{5.3}$$

$$\Gamma^a(\omega)\equiv\sum_1\Gamma_1(\omega)=\frac{1}{2\pi}\frac{JF^a(\omega)}{d(\omega)}\Gamma(\omega)\,, \tag{5.4}$$

$$G^b(\omega)=\sum_r G_r(\omega)=\frac{1}{2\pi}F^b(\omega)\,. \tag{5.5}$$

We now evaluate (5.1)–(5.5) to lowest order in which anomalous (log) terms appear.

$$\mathrm{Im}G^a(\omega)\cong-\tfrac{1}{2}\rho^a(\omega)\times\left[1-\tfrac{3}{4}\pi^2(J\rho^a)^2\left(1+2J\rho^a\ln\left|\frac{\omega}{D}\right|\right)\right], \tag{5.6}$$

$$\mathrm{Im}L^a(\omega)\cong-\tfrac{1}{4}\rho^a(\omega)\left(1+4J\rho^a\ln\left|\frac{\omega}{D}\right|\right), \tag{5.7}$$

$$\mathrm{Im}\theta^a(\omega)\cong-\rho^a(\omega)(J\rho^a)^2\left(\frac{\pi^2}{4}\right)\times\tanh\frac{\omega}{2k_BT}\left(1+6J\rho^a\ln\left|\frac{\omega}{D}\right|\right), \tag{5.8}$$

$$\mathrm{Im}\Gamma^a(\omega)=\tfrac{3}{2}\,\mathrm{Im}\theta^a(\omega)\,, \tag{5.9}$$

$$\mathrm{Im}G^b(\omega)=-\tfrac{1}{2}\rho^b(\omega)\,. \tag{5.10}$$

When these expressions are substituted into (3.14), we obtain for the total tunneling current

$$j_{\text{weak coupling}}=4\pi eT_a{}^2\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)]\rho^b(\omega+eV)\rho^a(\omega)\left[1-\tfrac{3}{4}\pi^2(J\rho^a)^2-\tfrac{3}{2}\pi^2(J\rho^a)^3\ln\left|\frac{\omega}{D}\right|\right] \tag{5.11a}$$

$$+3\pi eT_J{}^2\int_{-\infty}^{\infty}d\omega\,\{[f(\omega)-f(\omega+eV)]\rho^b(\omega+eV)\rho^a(\omega)\}\left(1+4J\rho^a\ln\left|\frac{\omega}{D}\right|\right) \tag{5.11b}$$

$$+6\pi eT_aT_J\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)]\rho^b(\omega+eV)\rho^a(\omega)\tanh\frac{\omega}{2k_BT}\left(1+6J\rho^a\ln\left|\frac{\omega}{D}\right|\right)\pi^2(J\rho^a)^2. \tag{5.11c}$$

B. Strong Coupling (Low Temperature)

In the low-temperature limit it becomes necessary to adopt a self-consistent procedure for evaluating our Green's functions in the case where $J<0$.

The self-consistent solution we adopt, due to Nagaoka, is equivalent to assuming

$$G(\omega)=\frac{\omega}{\alpha}\Gamma(\omega)-\frac{1}{2J}\,, \tag{5.12}$$

where

$$\alpha=2\Delta/\pi|J|\rho^a \tag{5.13}$$

and Δ is determined by

$$1=2|J|\rho^a\int_0^D\frac{\xi}{\xi^2+\Delta^2}\tanh\frac{\xi}{2k_BT}d\xi\,, \tag{5.14}$$

at $T=0$ (where T here denotes temperature),

$$\Delta=De^{-1/2|J|\rho^a}\,. \tag{5.15}$$

D, the energy cutoff introduced by N, is identical to E_0. Using (5.12) to evaluate (5.6) to (5.10) one obtains

$$\theta^a(\omega)=-\frac{i\rho^a\alpha}{6}\frac{1}{\omega+i\Delta}, \quad (5.16)$$

$$L^a(\omega)=-\frac{\alpha}{6\pi J}\frac{1}{\omega+i\Delta}, \quad (5.17)$$

$$G^a(\omega)=-\frac{i}{2}\rho^a\frac{\omega}{\omega+i\Delta}, \quad (5.18)$$

$$\Gamma^a(\omega)=-\frac{i\rho^a\alpha}{4}\frac{1}{\omega+i\Delta}, \quad (5.19)$$

$$G^b(\omega)=-\frac{i\rho^b}{2}, \quad (5.20)$$

where we have assumed $F^{(a,b)}(\omega)=-i\pi\rho^{(a,b)}(\omega)$. Inserting the above into (3.14), the total current in the low-temperature regime now becomes

$$j_{\text{strong coupling}}=4\pi eT_a^2\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)]\times\rho^b(\omega+eV)\rho^a(\omega)\frac{\omega^2}{\omega^2+\Delta^2} \quad (5.21)$$

$$+\frac{4e}{\pi}\frac{T_J^2}{(J\rho^a)^2}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)]\times\rho^b(\omega+eV)\rho^a(\omega)\frac{\Delta^2}{\Delta^2+\omega^2} \quad (5.22)$$

$$+8e\frac{T_aT_J}{|J\rho^a|}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)]\times\rho^b(\omega+eV)\rho^a(\omega)\frac{\Delta\omega}{\omega^2+\Delta^2}. \quad (5.23)$$

The relative importance of the various terms which contribute to the current depend on the relative size of T_a, T_J, and J, quantities which *a priori* are difficult to determine. It is to be expected that T_a, representing direct tunneling, would be greater than its exchange counterpart. However, whereas the anomalous behavior (in the weak-coupling regime) in the terms proportional to T_a^2 appear first in order J^3, those proportional to T_J^2 appear first in order J. The interference terms proportional to T_aT_J first exhibit anomalous behavior in order J^3 and consequently are smaller than either the T_a^2 or the T_J^2 terms. Furthermore the interference term (T_JT_a) leads to a conductance which is odd in the voltage. In addition, if we assume the presence of localized paramagnetic states on both sides of the tunneling junction, this term would be zero. A combination of these facts probably accounts for the fact that these odd anomalous terms have not yet been observed experimentally. For simplicity, therefore, we restrict our attention to the T_a^2 and T_J^2 terms below.

Focusing on the conductance

$$\mathcal{G}=\frac{\partial j}{\partial V}, \quad (5.24)$$

one finds that $\mathcal{G}^{\text{wc}}$ (wc≡weak coupling) can be written as

$$\mathcal{G}^{\text{wc}}=\mathcal{G}_{\text{const}}{}^{\text{wc}}+\mathcal{G}_{\text{anomalous}}{}^{\text{wc}}, \quad (5.25)$$

where

$$\mathcal{G}_{\text{const}}{}^{\text{wc}}=\rho^a\rho^b\left\{3\pi e^2T_J^2+4\pi e^2T_a^2\left[1-\frac{3\pi^2}{4}(J\rho^a)^2\right]\right\} \quad (5.26)$$

and

$$\mathcal{G}_{an}{}^{\text{wc}}=\mathcal{G}_{an_1}{}^{\text{wc}}+\mathcal{G}_{an_2}{}^{\text{wc}}, \quad (5.27)$$

$$\mathcal{G}_{an_1}{}^{\text{wc}}=12\pi e^2T_J^2\rho^a\rho^bJ\rho^a\mathfrak{F}(eV), \quad (5.28)$$

$$\mathcal{G}_{an_2}{}^{\text{wc}}=-6\pi^3T_a^2\rho^a\rho^b(J\rho^a)^3\mathfrak{F}(eV), \quad (5.29)$$

where

$$\mathfrak{F}(eV)=\int_{-\infty}^{\infty}\frac{\partial f}{\partial\omega}(\omega+eV)\frac{\partial f}{\partial\omega'}(\omega')\ln\left|\frac{\omega-\omega'}{D}\right|d\omega d\omega'. \quad (5.30)$$

$G_{an_1}{}^{\text{wc}}$ was first derived by Appelbaum while $G_{an_2}{}^{\text{wc}}$ was obtained by Sólyom and Zawadowski[10] by another method. They have identical voltage and temperature dependence, but while $G_{an_2}{}^{\text{wc}}$ yields a conductance peak for ferromagnetic coupling ($J>0$), $G_{an_1}{}^{\text{wc}}$ yields a conductance peak for antiferromagnetic coupling ($J<0$). These terms would be expected to behave differently in a magnetic field.

In the low-temperature regime (we shall assume $T=0$) one obtains (sc = strong coupling)

$$G^{\text{sc}}=G_1{}^{\text{sc}}+G_2{}^{\text{sc}}, \quad (5.31)$$

where

$$G_1{}^{\text{sc}}(eV)=\frac{4e^2}{\pi}\frac{T_J^2}{(J\rho^a)^2}\rho^b\rho^a\frac{\Delta^2}{(eV)^2+\Delta^2}, \quad (5.32)$$

$$G_2{}^{\text{sc}}(eV)=4\pi e^2T_a^2\rho^a\rho^b\frac{(eV)^2}{(eV)^2+\Delta^2}. \quad (5.33)$$

These results are valid for antiferromagnetic coupling ($J<0$). In a tunneling junction in which T_J terms are important one expects a peak in the conductance varying initially as $\ln|D/(eV+k_BT)|$, but saturating at low temperatures and voltages to the value given by $G_1{}^{\text{sc}}(0)$. For a junction in which the Ta terms are dominant one expects a dip in the conductance varying as $\ln[(|eV|+k_BT)/D]$ and eventually going to zero as T and $V\to 0$. It should be emphasized that the asymptotic behavior of $\mathcal{G}_1{}^{\text{sc}}$ and $\mathcal{G}_2{}^{\text{sc}}$ as given by (5.32) and (5.33) only sets in for k_BT, $eV\lesssim\Delta$ which may correspond to very low temperatures and applied voltage ($\Delta\sim 2.5\times10^{-4}$ eV for $J\rho\sim0.05$ and $D\sim5$ eV). These results will be somewhat modified by the presence

[10] J. Sólyom and A. Zawadowski (unpublished).

of many impurities, even in the independent-impurity model, because the Δ corresponding to a single impurity at a fixed distance from the (metal A)–(metal-A oxide) would be replaced by a range of Δ's which would have to be averaged over. This is considered in the next section.

VI. THE MANY-LOCALIZED-MAGNETIC-STATES PROBLEM

Up until now, we have pictured the localized magnetic states as confined to a plane parallel and close to the (metal A)–(metal-A oxide) interface. It will be our intention in this section to relax this restriction by admitting a distribution of lms in the direction perpendicular to the junction interface. This introduces a range of values for the exchange interaction J over which it will become necessary to average.

Before considering this problem it would be appropriate to consider in some detail the lms-averaging problem when the lms are confined to a single plane. In Secs. III–V we bypassed this averaging by assuming that only a single lms was present.

In order to focus on the essential aspects of the problem we consider as our Hamiltonian

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_2+\mathcal{H}_4, \tag{6.1}$$

where now

$$\mathcal{H}_2=T_a\sum_{\mathbf{k},\mathbf{k}'}\sum_n(e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n}a_{\mathbf{k}}^\dagger b_{\mathbf{k}'}+e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n}b_{\mathbf{k}'}^\dagger a_{\mathbf{k}}), \tag{6.2}$$

where $\mathbf{R}_n$ is the position of the nth lms and

$$\mathcal{H}_4=-J\sum_{\mathbf{k}\mathbf{k}',\sigma\sigma'}\sum_n e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n}a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}'\sigma'}\mathbf{S}\cdot\boldsymbol{\tau}_{\sigma\sigma'}. \tag{6.3}$$

The expression for the tunneling current now becomes

$$j=4eT_a^2\,\mathrm{Re}\sum_{\mathbf{l},\mathbf{l}',\mathbf{r}}\int_{-\infty}^{\infty}d\omega\,[f(\omega)-f(\omega+eV)]\times[-2\,\mathrm{Im}G_{\mathbf{l}\mathbf{l}'}(\omega)][-2\,\mathrm{Im}G_{\mathbf{r}}(\omega)]\times\sum_{n,n'}e^{i(\mathbf{r}-\mathbf{l}')\cdot\mathbf{R}_{n'}-i(\mathbf{r}-\mathbf{l})\cdot\mathbf{R}_n}, \tag{6.4}$$

where we have used the fact that the right-hand side of the junction has no lms, so that

$$G_{\mathbf{r}\mathbf{r}'}(\omega)=G_{\mathbf{r}}(\omega)\delta_{\mathbf{r}\mathbf{r}'}. \tag{6.5}$$

The current averaged over the position of the localized states is what one is after, so one needs to know

$$\sum_{\mathbf{l},\mathbf{l}'}\langle[-2\,\mathrm{Im}G_{\mathbf{l}\mathbf{l}'}(\omega)]\sum_{n,n'}e^{i(\mathbf{r}-\mathbf{l}')\cdot\mathbf{R}_{n'}-i(\mathbf{r}-\mathbf{l})\cdot\mathbf{R}_n}\rangle_{\mathrm{av}}. \tag{6.6}$$

One cannot break this average up into

$$\langle-2\,\mathrm{Im}G_{\mathbf{l}\mathbf{l}'}(\omega)\rangle\langle\sum_{n,n'}e^{i(\mathbf{r}-\mathbf{l}')\cdot\mathbf{R}_{n'}-i(\mathbf{r}-\mathbf{l})\cdot\mathbf{R}_n}\rangle_{\mathrm{av}} \tag{6.7}$$

without losing completely the dependence of $G_{\mathbf{l}\mathbf{l}'}$ on J. This is essentially because a surface density of lms could not affect the bulk spectral function $\mathrm{Im}G_{\mathbf{l}\mathbf{l}'}(\omega)$. To perform the average it is necessary to express $G_{\mathbf{l}\mathbf{l}'}(\omega)$ in terms of

$$\rho(\mathbf{k}-\mathbf{k}')=\sum_n e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n}. \tag{6.8}$$

This is difficult to do in the s-d exchange problem but one can see how it comes out by considering the case where $\mathcal{H}_4$ is replaced by

$$v\sum_{\mathbf{k},\mathbf{k}',\sigma}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n}a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}'\sigma}. \tag{6.9}$$

Then one finds that (6.6) becomes

$$M_a\{\sum_{\mathbf{l},\mathbf{l}'}-2\,\mathrm{Im}G_{\mathbf{l}\mathbf{l}'}(\omega)\}, \tag{6.10}$$

where $G_{\mathbf{l}\mathbf{l}'}(\omega)$ is the Green's function for a single lms, and where M_a is the number of lms in the plane. We choose units where $M_a=1$. These results are modified if we replace $\mathcal{H}_2$ by $\mathcal{H}_1$. Then one has to consider

$$\langle\sum_{\mathbf{l},\mathbf{l}'}-2\,\mathrm{Im}G_{\mathbf{l}\mathbf{l}'}(\omega)\delta_{\mathbf{l}_\perp,\mathbf{l}'_\perp}\rangle \tag{6.11}$$

which yields no terms dependent upon J. This is for the same reason we could not write (6.6) as (6.7): A surface density of states cannot affect a bulk spectral function.

An analysis of what modifications result from the inclusion of $\mathcal{H}_1$ in our tunneling current leads to the following conclusions.

1. Interference terms proportional to TT_J and TT_a appear with the same dependence on voltage and temperature as the $T_aT_J+T^2$ terms.

2. There are no anomalous T^2 terms except for a constant conductance term.

Since we are primarily interested in the functional dependence of the conductance upon voltage and temperature and we expect $T\ll T_a$,[4,3] we shall not concern ourselves with these terms.

We return now to the question of averaging over the distribution of impurities in the direction perpendicular to the tunnel junction. We assume that we may perform this averaging by first calculating the tunneling current for a given value of J and then averaging over this value.

This assumes again that we may ignore the interference effects among various localized spins. This assumption, which appears valid for the weak-coupling limit, would become less so as we enter the strong-coupling regime because of the long-range nature of Nagaoka's solutions below T_c. In order to make any progress, however, we will continue to assume an independent-spin model even below $T_c(k_BT_c\sim\Delta)$.

In order to bring out the relevant features of this averaging we assume that the lms are uniformly distributed in the perpendicular direction from the (metal A)–(metal-oxide A) interface to a distance d.

We expect J to be a function of x, the distance from the A interface to the lms, as shown below

$$J(x)\approx J_0e^{-2kx}, \tag{6.12}$$

where k is the wave number of the tunneling electron.

Furthermore

$$\Delta = De^{-1/(2J\rho^a)}. \qquad (6.13)$$

We shall be primarily interested in the effect of averaging on the functional dependence of the conductance on voltage and temperature.

In the high-temperature regime the conductance varies as

$$\mathcal{G}(V,T) \sim a(J) + b(J) \ln \frac{|eV| + k_B T}{D}, \qquad (6.14)$$

where $a(J)$ and $b(J)$ are functions of J. It is clear that averaging over a distribution of impurities will lead to no change in the functional dependence of $\mathcal{G}(V,T)$. In the strong-coupling regime this will not be the case. In averaging over $\mathcal{G}_1^{sc}(eV)$ and $\mathcal{G}_2^{sc}(eV)$ we observe from (6.13) Δ is a very much more quickly varying function of x than J, so we shall average only over Δ.

From our assumption of a uniform distribution of impurities we obtain for $P(\Delta)$, the probability of an impurity having a Δ between Δ and $\Delta + d\Delta$,

$$P(\Delta) \propto \frac{d\Delta}{\Delta}. \qquad (6.15)$$

In deriving (6.15) we have assumed that J is essentially a constant in comparison with Δ.

If we average (5.32) and (5.33) we obtain

$$\langle \mathcal{G}_1^{sc}(eV) \rangle_{av} = \frac{4e^2}{\pi} \left\langle \left(\frac{T_J}{\rho^a J} \right)^2 \right\rangle_{av} \times \rho^b \rho^a \ln\left(\frac{\Delta_0}{|eV|} \right) \Big/ \ln \frac{\Delta_0}{\Delta_1} \qquad (6.16)$$

and

$$\langle \mathcal{G}_2^{sc}(eV) \rangle_{av} = 4\pi e^2 T_a{}^2 \rho^a \rho^b \ln \frac{|eV|}{\Delta_1} \Big/ \ln \frac{\Delta_0}{\Delta_1}. \qquad (6.17)$$

The above expressions are valid in the limit $\Delta_1 \lesssim |eV| \lesssim \Delta_0$.

$$\Delta_0 = De^{-1/2|J_0|\rho}, \qquad (6.18)$$

$$\Delta_1 = De^{-1/2|J_1|\rho}, \qquad (6.19)$$

where

$$J_1 = J_0 e^{-2dk}. \qquad (6.20)$$

VII. CONCLUSIONS

It has been our intention to examine in as much detail as possible the tunneling current which results from the model Hamiltonian proposed by Appelbaum. The results we have obtained in the weak-coupling limit, based as they are on the well-understood solution to the Kondo problem in the perturbation-theory limit, are fairly certain.

Our strong-coupling solution, on the other hand, must be viewed with considerable reserve. The first difficulty is that, while a number of theories have been advanced to describe the strong-coupling Kondo problem,[11] there appears at present to be no clear and conclusive description of the low-temperature Kondo "bound state." However, in order to investigate the implication of such a bound state on the tunneling characteristics, we have chosen the solution advanced by Nagaoka.

The implications of N solution are rather striking. For those functions in which the T_a terms are predominant, the conductance goes to zero as $(T,V) \to 0$. This behavior is similar to what has been observed in Cr-(chromium oxide)-Ag tunneling junction, where one finds a large rise in the resistance of the junction centered on zero-voltage bias. In those junctions in which the $T_J{}^2$ terms are predominant, one has the conductance saturating as $(T,V) \to 0$, as described by (5.33) or (6.16).

There is no doubt that a better solution to the lower-temperature Kondo problem will modify our conclusions, especially so because tunneling measures the spectral function quite directly and therefore would be sensitive to different solutions to the Kondo problem. While this makes the present work more tentative, it also points out the inherent advantages of the tunneling measurements in exploring the Kondo problem.

Note added in manuscript. A more careful solution of N's self-consistent equations has recently been performed by Hamann.[12] The new solutions do not change the basic conclusion that $\mathcal{G}_1^{sc}(\text{eV}) \to \mathcal{G}_1^{sc}(0)$ [as given in (5.32)] or that $\mathcal{G}_2^{sc}(eV) \to 0$ as $eV \to 0$. However, $\mathcal{G}_1^{sc}(eV)$ approaches $G_1^{sc}(0)$ as $\ln^{-2}|eV/\Delta|$ and $G_2^{sc} \times (eV) \to 0$ as $\ln^2|eV/\Delta|$.

Note that because Δ now appears in a logarithm this result will not be substantially changed in averaging over the lms. Averaging over this quantity leads qualitatively to $\ln^{-2}|eV/\Delta'|$, where $\Delta' = De^{-1/2\rho^a \langle J \rangle_{av}}$.

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[11] A. A. Abrikosov, Physics **2**, 61 (1965); H. Suhl, Phys. Rev. **138**, A515 (1965).
[12] D. R. Hamann (unpublished).