# The theory of zero-bias tunnelling anomalies



1994 J. Phys.: Condens. Matter 6 223

(http://iopscience.iop.org/0953-8984/6/1/021)

J. Phys.: Condens. Matter 6 (1994) 223–236. Printed in the UK

# The theory of zero-bias tunnelling anomalies

F Wright
Department of Physics, San Diego State University, San Diego, CA 92182, USA

Received 11 January 1993, in final form 8 September 1993

**Abstract.** In this paper the current–voltage characteristics and dynamic conductance are computed for a tunnel junction with an embedded magnetic impurity which is subjected to a steady magnetic field. Using a theory that does not employ the transfer Hamiltonian technique, the approach is based on a dynamical method described by Cini, and employs the Keldysh formalism.

## 1. Introduction

Recent experimental work (Gregory 1992, Manassen *et al* 1989) has generated a renewed interest in the zero-bias conductance peak of tunnel junctions with imbedded magnetic impurities. This zero-bias anomaly is believed to be caused by exchange scattering of the tunnelling electrons by local magnetic moments within the tunnel barrier, and various theories have been proposed to explain these anomalies (Appelbaum 1967, Gupta 1973). These theories, however, are generally phenomenological in nature, and rely on decoupling procedures of questionable validity. They employ transfer Hamiltonian techniques (Appelbaum and Brinkman 1970), which introduce *ad hoc* coupling terms in the Hamiltonian, and which, as pointed out by several authors (Duke *et al* 1972, Feuchtwang 1974), neglect the possibility of some important scattering processes.

An alternative formulation of the theoretical problem is to employ a rigorous microscopic approach, and to consider the quantum statistical system as being driven to a steady state by the potential applied to the tunnel junction. This is the approach taken by Feuchtwang (1974) and Caroli *et al* (1971). Cini has also proposed a technique along these lines (Cini 1980), but differing in that his approach is time dependent. This dynamic formulation of the problem proves to be simple to apply, and has the benefit that no 'pseudo Hamiltonian' need be introduced in an unperturbed partitioned system. It is, therefore, closer to the actual experimental situation than static models. The problem can be treated with perturbation theory by applying the Keldysh formalism (Keldysh 1965). The results are correct to all orders in the applied potential, which is already contained in the unperturbed Hamiltonian. The solution of the problem is found within the framework of the Keldysh formalism by an equation of motion approach, and the magnetic impurity interaction can be introduced in the same manner as Feuchtwang has done in the case of the electron–photon interaction (Feuchtwang 1979).

In order to discuss the current–voltage characteristics of the tunnel junction in rigorous quantum mechanical terms, a simple model will be developed in the following section. The time-dependent problem of a tunnel junction of infinitesimal width, and with a single embedded paramagnetic impurity in a steady magnetic field, will be formulated. The current will be seen to be an expression in terms of a retarded Green's function and the

Keldysh retarded s-electron self-energy. This current will be compared with the results of Appelbaum–Brinkman theory in the light of the shortcomings of the transfer Hamiltonian approach.

The Keldysh retarded Green's function and the retarded self-energy will be analysed by summing, in the same way that Abrikosov has done (Abrikosov 1965), the leading logarithmic terms ('parquet' diagrams), using a s–d scattering perturbation. The Appelbaum–Brinkman transfer Hamiltonian technique rests heavily on the decoupling procedure that Nagaoka (1965) used to evaluate the low-temperature Kondo anomalies of the s–d exchange interaction. Since any decoupling of the Green's function equation of motion is equivalent to a partial sum in the perturbation series (Cheung and Mattuck 1970), one could conclude that the Nagaoka solution corresponds to Abrikosov's sum over parquet diagrams, and that there should be a correspondence between Appelbaum–Brinkman results, In their transfer Hamiltonian treatment, and the results of a microscopic calculation using sum over ladder diagrams. As Abrikosov points out (Abrikosov 1968) there is serious doubt of the validity of the Nagaoka decoupling scheme with impurity spins other than $s = 1/2$. Therefore, we confine the comparison to systems with impurity spins of $1/2$.

The sum over diagram is a bare ladder approximation, and the Keldysh s–d vertex part and the s-electron retarded self-energy diverge at the Kondo temperature (Kondo 1964). Of course, this divergence is implicit in the decoupling scheme. It can, however, be pushed to zero temperature, in the ladder approximation, by dressing the s-electron Green's function and evaluating the vertex part, self-energy, and d spin–s electron pair bubble in a self-consistent fashion (Cheung and Mattuck 1970). This renormalization is not available to the decoupling scheme, and it is reasonable to expect that one could, in principle, remove the limitations of the present theory presented by the Kondo divergence. We see some advantage, therefore, in avoiding the transfer Hamiltonian altogether, and employing, instead, a self-consistent sum over all orders of perturbation.

The tunnel current will be evaluated, by using the procedure of Cini, to obtain the system Green's functions from singularities of their Fourier transforms. Finally, the current–voltage characteristics of the system will be discussed, and compared with the results of the transfer Hamiltonian approach.

## 2. Formulation

We are looking for a theoretical description of an experiment in which the current response of a junction device is measured. It is assumed that the system consists of an infinitesimally thin device, located at $x = 0$, and connected with two wires extending to plus and minus infinity. For times $t < 0$, the system is assumed to be in thermal equilibrium, and described by a one-electron Hamiltonian, $H_0$. At time $t = 0$, a perturbation Hamiltonian $H(t)$ is switched on. This time-dependent perturbation describes the potential which causes current to flow. We assume that the potential goes to zero far to the left of the junction, and tends to a positive constant $V$, far to the right of the junction. That is, we take $H(t) = \theta(t)V(x)$, with $V(x)$ tending to a constant $V$, for $x$ tending to infinity, and $V(x) = 0$, for $x$ tending to minus infinity. Following Cini (1980), we are concerned with the calculation of the time-ordered finite-temperature Green's function. Defined in the standard way it is

$$G^{\mathrm{T}}(x, t; x', t') = -\mathrm{i}\langle T[\psi(x, t)\psi^{\dagger}(x', t')]\rangle \tag{1}$$

where $T$ represents the time ordering, and $\psi$ are Heisenberg electron field operators. The angular brackets denote a thermal average taken with an unperturbed density matrix

$$\langle A\rangle = \mathrm{Tr}(\rho_0 A) \qquad \rho_0 = \mathrm{e}^{-\beta H_0}/\mathrm{Tr}(\mathrm{e}^{-\beta H_0}). \tag{2}$$

The number density is given by

$$\rho(x,t) = -\mathrm{i} \lim_{t'\to t+0} \lim_{x'\to x} G^{\mathrm{T}}(x,t;x',t') \tag{3}$$

and the current density is

$$j(x,t) = -(1/2m) \lim_{t'\to t+0} \lim_{x'\to x} (\nabla_x - \nabla_{x'}) G^{\mathrm{T}}(x,t;x',t'). \tag{4}$$

In the Keldysh formalism the Green's function becomes a matrix quantity satisfying Dyson's equation

$$\mathbf{G} = \mathbf{g} + \mathbf{g}\cdot\Sigma\cdot\mathbf{G} \tag{5}$$

where matrix multiplication implies integration over internal variables, and the matrix quantities are

$$\mathbf{G} = \begin{Bmatrix} G^{\mathrm{c}} & G^{-} \\ G^{+} & \tilde{G}^{\mathrm{c}} \end{Bmatrix} \qquad \mathbf{g} = \begin{Bmatrix} g^{\mathrm{c}} & g^{-} \\ g^{+} & \tilde{g}^{\mathrm{c}} \end{Bmatrix} \qquad \Sigma = \begin{Bmatrix} \Sigma^{\mathrm{c}} & \Sigma^{+} \\ \Sigma^{-} & \tilde{\Sigma}^{\mathrm{c}} \end{Bmatrix}. \tag{6}$$

The matrix elements are defined by a time-ordering contour integration. Since such quantities are not linearly independent a Keldysh transformation (Keldysh 1965) reduces the system of Dyson equations

$$\mathbf{G} \Rightarrow \begin{Bmatrix} 0 & G^{\mathrm{a}} \\ G^{\mathrm{r}} & F \end{Bmatrix} \qquad \mathbf{g} \Rightarrow \begin{Bmatrix} 0 & g^{\mathrm{a}} \\ g^{\mathrm{r}} & f \end{Bmatrix} \qquad \Sigma \Rightarrow \begin{Bmatrix} \Omega & \Sigma^{\mathrm{r}} \\ \Sigma^{\mathrm{a}} & 0 \end{Bmatrix} \tag{7}$$

where $G^{\mathrm{r}}$ and $G^{\mathrm{a}}$ are the standard retarded and advanced Green's functions, and $F$ is a single-particle density matrix. Using the Keldysh formalism, we write an equation of motion for the retarded Green's function

$$G^{\mathrm{r}} = g^{\mathrm{r}} + g^{\mathrm{r}}\Sigma^{\mathrm{r}}G^{\mathrm{r}} \tag{8}$$

whose Fourier time transform is

$$G^{\mathrm{r}}(x,x';\omega) = g^{\mathrm{r}}(x,x';\omega) + \int\int g^{\mathrm{r}}(x,x_1;\omega)\Sigma^{\mathrm{r}}(x_1,x_2;\omega)G^{\mathrm{r}}(x_2,x';\omega)\,\mathrm{d}x_1\,\mathrm{d}x_2. \tag{9}$$

We write

$$g^{-1}(x,t) = \mathrm{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - V\theta(x)\theta(t). \tag{10}$$

Using the fact that

$$g^{-1}(x;\omega)g^{\mathrm{r}}(x,x';\omega) = \delta(x-x') \tag{11}$$

we write the equation of motion in the following form

$$\left(\omega - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) G^{\mathrm{r}}(x,x';\omega) = \delta(x-x') + V\theta(x')G^{\mathrm{r}}(x,x';\omega) + \int \Sigma^{\mathrm{r}}(x,x_1;\omega)G^{\mathrm{r}}(x_1,x';\omega)\,\mathrm{d}x_1 \tag{12}$$

where $V(x) = V\theta(x)$.

We assume that the system Hamiltonian evolves to a constant final value, $H^{\mathrm{f}}$, as $t$ goes to infinity. As Cini points out, a thermal average over the exact single-particle eigenstates of $H_{\mathrm{f}}$ yields the result

$$G^{\mathrm{r}}(k, k'; t, 0) = G^{\mathrm{r,f}}(k, k'; t) \tag{13}$$

where $G^{\mathrm{r,f}}$ is a single-electron Green's function, calculated with the constant final-state Hamiltonian. The system number density and current density at $x$, and at time $t$, are

$$\rho(x, t) = \sum_q |G^{\mathrm{r,f}}(x, q; t)|^2 \tag{14}$$

$$j(x, t) = \frac{e\hbar}{m} \operatorname{Im} \sum_q f_q G^{\mathrm{r,f}}(x, q; t)^* \frac{\partial}{\partial x} G^{\mathrm{r,f}}(x, q; t). \tag{15}$$

$f_q$ is the Fermi function, and the summation sign in equation (15) implies an integration over the momenta which participate in the tunnelling process.

Our task becomes the determination of $G^{\mathrm{r,f}}(x, x', \omega)$ from the equation of motion (12), and the computation of its spatial Fourier transform. In order to solve equation (15) for the current density, the assumption is made that the system Hamiltonian evolves to a constant final value after a long period of time, and thus the asymptotic form of the Fourier frequency transform of the retarded Green's function is considered. Before such a program can be completed, however, the retarded self-energy, appearing in the equation of motion, must be determined. This is done in the following section.

## 3. The self-energy

The interaction Hamiltonian we will use is the same as that of Abrikosov (1965). The total time-independent Hamiltonian for a single-spin impurity is given by

$$H = \sum_{k\alpha} \epsilon_k c_{k\alpha}^+ c_{k\alpha} + \sum_\beta \epsilon_d c_{d\beta}^+ c_{d\beta} - \frac{J}{2N} \sum_{\alpha\alpha'\beta\beta'kk'} (\sigma_{\alpha'\alpha} \cdot S_{\beta'\beta}) c_{d\beta'}^+ c_{k'\alpha}^+ c_{k\alpha'} c_{d\beta} \tag{16}$$

where $N$ is the number of atoms, $J$ is the s–d coupling constant, $\epsilon_k$, $\epsilon_d$, are the bare s–d electron energies relative to the Fermi level, $c_{k\alpha}^+$, $c_{k\alpha}$, $c_{d\beta}^+$, $c_{d\beta}$ are creation and destruction operators for s, d electrons and $\sigma_{\alpha'\alpha}$ and $2S_{\beta'\beta}$ are the Pauli matrices for s, d electrons.

As Abrikosov points out (Abrikosov 1968), the representation of the spin operator in terms of second quantized operators yields, for spin other than 1/2, extra 'unphysical states'. If, however, we take $\epsilon_d$ to be zero (Cheung and Mattuck 1970), then the average number of d electrons is equal to one, and the only effect of the unphysical states is to introduce a normalization factor of two.

It should be noted that equation (16) is the same as that used by Nagaoka (1965) and by Appelbaum and Brinkman (1970). So a connection with the theory of these authors requires that we multiply our results by $cN$, where $c$ is the concentration of impurity atoms.

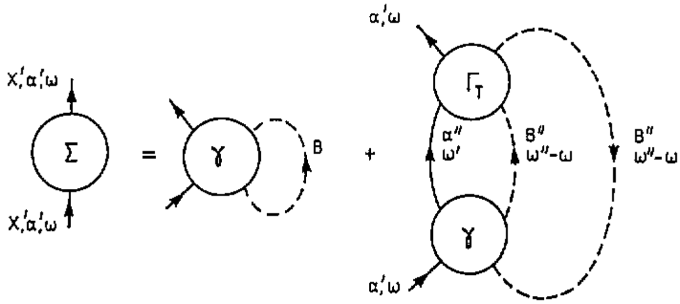


**Figure 1.** The s-electron self-energy $\Sigma$ in terms of the total proper Keldysh vertex part $\Gamma_T$ and the Keldysh vertex $\gamma$. The full curves are bare s-electron propagators and the dotted curves are bare d-spin propagators. The Keldysh indices are not shown.

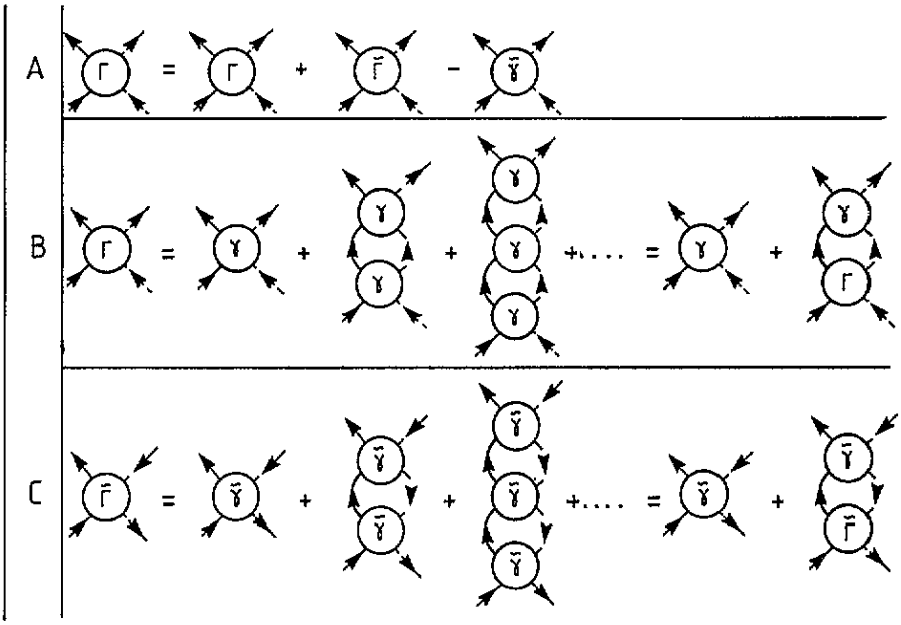


**Figure 2.** The s–d Keldysh vertex part in the ladder approximation. (A) Shows the total proper vertex part $\Gamma_T$ in terms of the proper particle–particle part, $\Gamma$, the proper time reversed particle–hole part $\tilde{\Gamma}$, and the Keldysh vertex $\gamma$. (B) and (C) show the ladder sum and integral equation for $\Gamma$ and $\tilde{\Gamma}$, respectively, in terms of $\gamma$ and the time-reversed Keldysh vertex $\tilde{\gamma}$.

The self-energy is evaluated by performing the sum and integrations represented by figure 1. The vertex part can be computed from figure 2, and used to evaluate the self-energy in a self-consistent manner.

The perturbation expansion for the s–d vertex part, in the parquet series, is the sum of an electron–electron part, $\Gamma$, and an electron–hole part, $\gamma$, as shown in figure 2 (roman superscripts will denote the Keldysh indices). The diagrams in figure 2 represent integral equations, which may be translated into functions by associating with each full curve one of three Keldysh s-electron propagators

$$g^{\mathrm{r}}(x,x';\omega) = \lim_{\delta\to 0^+} \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\rho(x,x';\omega')\,\mathrm{d}\omega'}{\omega-\omega'+\mathrm{i}\delta} \tag{17}$$

$$g^{\mathrm{a}}(x,x';\omega) = \lim_{\delta\to 0^-} \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\rho(x,x';\omega)\,\mathrm{d}\omega'}{\omega-\omega'-\mathrm{i}\delta} \tag{18}$$

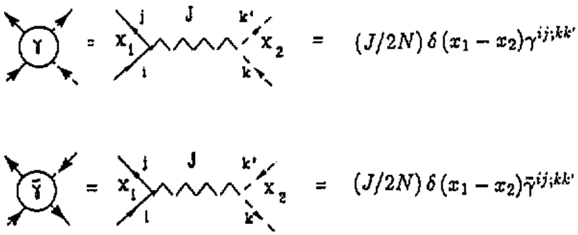


**Figure 3.** The upper bubble is an abbreviated form of the s–d interaction at the Keldysh vertex, with the long form of the interaction (represented by the wavy line) shown immediately to its right-hand side. To the right of the long form of the interaction is the mathematical representation of the bubble as the product of the Keldysh tensor with the Dirac delta function and the interaction strength. The lower bubble is the interaction at the time-reversed Keldysh vertex.

$$g^{\mathrm{F}}(x, x'; \omega) = 2g^{\pm} \mp (g^{\mathrm{r}} - g^{\mathrm{a}}) = -\mathrm{i}\tan(\beta\omega/2)\rho(x, x'; \omega) \tag{19}$$

where

$$g^{\pm}(x, x'; \omega) - \pm\mathrm{i} f(\pm\omega)\rho(x, x'; \omega) \tag{20}$$

and where $\rho(x, x'; \omega)$ is the s-electron spectral density, $f(\omega)$ is the Fermi function, and $\beta$ is $1/KT$. In likewise fashion, each dotted curve is associated with one of three d-spin propagators:

$$d^{\mathrm{r}}(x, x'; \omega) = \lim_{\delta\to 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sigma(x, x'; \omega')\,\mathrm{d}\omega'}{\omega - \omega' + \mathrm{i}\delta} \tag{21}$$

$$d^{\mathrm{a}}(x, x'; \omega) = \lim_{\delta\to 0^-} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sigma(x, x'; \omega')\,\mathrm{d}\omega'}{\omega - \omega' - \mathrm{i}\delta} \tag{22}$$

$$d^{\mathrm{F}}(x, x'; \omega) = -\mathrm{i}\tan(\beta\omega/2)\sigma(x, x'; \omega) \tag{23}$$

where $\sigma(x, x'; \omega)$ is the spectral density of the impurity d spin.

The Keldysh $\gamma$ bubble is an abbreviated form of the s–d interaction and the Keldysh vertex as shown in figure 3. The value $(J/2N)(\sigma_{\alpha'\alpha} \cdot S_{\beta'\beta})\gamma^{ijkl}$ is associated with each bubble, with $\gamma^{ijkl}$ being a bare Keldysh vertex matrix, where the Greek subscripts are associated with a Pauli matrix spin index. The Keldysh vertex matrix is given by

$$\gamma^{ijkk'} - \delta_{ij}\delta_{jk}\sigma^{z}_{kk'} \tag{24}$$

where $\sigma_z$ is the third Pauli spin matrix. The vertex is a unit tensor in the $i, j$ indices, reflecting that the electron, at the vertex, enters and leaves the same space–time point. A change in $\{k, k'\}$ will change the sign of the tensor, reflecting that the point at the other end of the d-spin propagator can reside on either the upper or the lower branch of the Keldysh time contour (Rammer and Smith 1986). The $k$–$j$ indices of the unit tensor reflect the assumption that we are dealing with a delta function contact interaction between the s conduction electron and the d spin impurity. On performing a transformation in the Keldysh space, like the one described in the previous section, the Keldysh vertex function is written as

$$\gamma^{11}_{mn} = \gamma^{22}_{mn} = \sigma^{x}_{mn} = \tilde{\gamma}^{12}_{mn} = \tilde{\gamma}^{21}_{mn} \tag{25}$$

$$\gamma^{12}_{mn} = \gamma^{21}_{mn} = \delta_{mn} = \tilde{\gamma}^{11}_{mn} = \tilde{\gamma}^{22}_{mn} \tag{26}$$

where the tilde indicates a time-reversed impurity spin matrix.

Let us examine the electron–electron vertex part first. Figure 2(B) yields

$$\Gamma^{ij;kl}_{\alpha\beta\alpha''\beta''}(x,x';\omega',\omega'',\omega''') = \frac{J}{2N}(\sigma_{\alpha\alpha''}\cdot S_{\beta\beta''})\gamma^{ij;kl} + \frac{J}{2N}\sum_{mnop,\alpha'\beta'}\iiint \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}\omega\,\gamma^{im;ko} g_{mn}(x_1,x_2;\omega)d_{op}(x_1,x_2;\omega''-\omega) \times \Gamma^{nj;pl}_{\alpha'\beta'\alpha''\beta''}(x_1,x';\omega,\omega',\omega''). \tag{27}$$

The spin impurity is assumed to be located at $x = 0$.

Writing $\Gamma$ as the sum of a scalar and vector part in the spin indices (Abrikosov 1965)

$$\Gamma^{ij;kl}_{\alpha\beta\alpha''\beta''} = {}^0\Gamma^{ij;kl}\delta_{\alpha\alpha''}\delta_{\beta\beta''} + {}^1\Gamma^{ij;kl}\sigma_{\alpha\alpha''}\cdot S_{\beta\beta''} \tag{28}$$

and utilizing the fact that

$$\sum_{\alpha'\beta'}(\sigma_{\alpha\alpha'}\cdot S_{\beta\beta'})(\sigma_{\alpha'\alpha''}\cdot S_{\beta'\beta''}) = \frac{3}{4}\delta_{\alpha\alpha''}\delta_{\beta\beta''} - \sigma_{\alpha\alpha''}\cdot S_{\beta\beta''} \tag{29}$$

yields the coupled equations

$${}^0\Gamma^{ij;kl}(x,x',\omega',\omega'',\omega''') = \frac{3}{8N}\iiint \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}\omega\,\gamma^{im;ko}J(x_1) \times g_{mn}(x_1,x_2;\omega)d_{op}(x_1,x_2;\omega'''-\omega)\,{}^1\Gamma^{nj;pl}(x_2,x';\omega,\omega'',\omega''') \tag{30}$$

and

$${}^1\Gamma^{ij;kl}(x,x';\omega',\omega'',\omega''') = \frac{J(x')}{2N}\gamma^{ij;kl} + \frac{1}{2N}\iiint \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}\omega\,\gamma^{im;ko}J(x_1) \times g_{mn}(x_1,x_2;\omega)d_{op}(x_1,x_2;\omega'''-\omega) \times [{}^0\Gamma^{nj;pl}(x_2,x';\omega,\omega',\omega'') - {}^1\Gamma^{nj;pl}(x_2,x';\omega,\omega'',\omega''')] \tag{31}$$

where a sum is implied over repeated Keldysh indices. Substituting (31) into (30), and noting that the ${}^1\Gamma$ is independent of $x$ and $\omega'$ so that it can be factored out of the integral, we write ${}^1\Gamma$ as a column vector

$$({}^1\Gamma) = \frac{J\delta(x)}{2N}(\gamma) + \frac{1}{2N}\mathbf{A}({}^0\Gamma) - \frac{1}{2N}\mathbf{A}({}^1\Gamma) \tag{32}$$

$$({}^0\Gamma) = \frac{3}{8N}\mathbf{A}({}^1\Gamma) \tag{33}$$

where $\mathbf{A}$ is a $16\times16$ matrix, and where the first entry in the $\Gamma$ column is $\Gamma^{11;11}$, the second entry is $\Gamma^{12;11}$, etc.

Before computing the elements of $\mathbf{A}$, we note that they are sums of terms of the form

$$\iiint \mathrm{d}x\,\mathrm{d}x'\,\mathrm{d}\omega\,J(x)g_{ij}(x,x';\omega)d_{kl}(x,x';\omega'-\omega) \tag{34}$$

where the spectral density of the s conduction electron, $\rho(x, x'; \omega)$, is assumed to be confined to band of width $2D$. Evaluating $g^{r}$ with this density we find

$$g^{r} = g^{a*} = \lim_{\delta \to 0^{+}} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{[\theta(\omega' + D) - \theta(\omega' - D)]\, d\omega'}{\omega - \omega' + i\delta} = i \frac{e^{\eta\omega}}{\pi} \sinh(\eta D). \tag{35}$$

$\eta$ is infinitesimal and so $g^{r,a}$ is infinitesimal. Since $g_{11} = 0$, only terms involving $g_{22} = g^{F} = -i\rho(x, x') \tanh(\beta\omega/2)$ are considered when evaluating the elements of **A**.

The spectral density of the impurity is a delta function, and on evaluating the frequency integration in equation (34), we see that the number of terms needed to evaluate each element of **A** is reduced from sixteen to two. These terms are

$$z_1(\omega') = \frac{1}{2N} \iiint J(x) g_{22}(x, x'; \omega) d_{12}(x, x'; \omega' - \omega)\, dx\, dx'\, d\omega \tag{36}$$

and

$$z_2(\omega') = \frac{1}{2N} \iiint J(x) g_{22}(x, x'; \omega) d_{21}(x, x'; \omega' - \omega)\, dx\, dx'\, d\omega. \tag{37}$$

We introduce a local impurity density of states and assume that

$$\sigma(x, x'; \omega) = \sigma(x', x'; \omega) = \sigma(x'; \omega)$$

which obey the sum rule

$$\int_{-\infty}^{\infty} \sigma(x'; \omega) dx' = \sigma(\omega) = \delta(\omega - \epsilon_d) = \delta(\omega). \tag{38}$$

Evaluating equation (36) using equations (38) and (19), we find

$$\begin{aligned} z_1(\omega) &= \frac{1}{2N} \iiint dx\, dx'\, d\omega\, J(x) g_{22}(x, x'; \omega) d_{21}(x, x'; \omega' - \omega) \\ &= -i \frac{\rho J}{2N} \int_{-D}^{D} \frac{d\omega' \tanh(\beta\omega'/2)}{2\pi(\omega' - \omega)} - \frac{\rho J}{4N} \tanh\left(\frac{\beta\omega}{2}\right) \\ &\simeq \frac{\rho J}{4N} \tanh\left(\frac{\beta\omega}{2}\right) - i \frac{\rho J}{4\pi N} \ln\left(\frac{D^2}{\omega^2 + (2KT)^2}\right) = z(\omega) \end{aligned} \tag{39}$$

where we have used the assumption that $\rho(x, x') = \rho$, a constant. The remaining term needed to evaluate the elements of **A** is computed in a similar fashion, and found to be

$$\begin{aligned} z_2(\omega) &= \frac{1}{2N} \iiint dx\, dx'\, d\omega\, J(x) g_{22}(x, x'; \omega) d_{12}(x, x'; \omega' - \omega) \\ &\simeq -\frac{\rho J}{4N} \tanh\left(\frac{\beta\omega}{2}\right) + i \frac{\rho J}{4\pi N} \ln\left(\frac{D^2}{\omega^2 + (2KT)^2}\right) = -z^{*}(\omega). \end{aligned} \tag{40}$$

We now evaluate the elements of **A**. Substituting equation (32) into equation (33), and solving for the column vector ${}^{1}\Gamma$, we find in particular that

$$\begin{aligned} {}^{1}\Gamma^{12;11}(x, \omega) &= {}^{1}\Gamma^{22;21}(x, \omega) = (J/2N)\delta(x)/[1 + A(\omega)] \\ {}^{1}\Gamma^{12;22}(x, \omega) &= {}^{1}\Gamma^{22;12}(x, \omega) = (J/2N)\delta(x)/[1 + A^{*}(\omega)] \end{aligned} \tag{41}$$

where

$$A(\omega) = z(\omega)[1 - \tfrac{3}{4}z(\omega)]. \tag{42}$$

Similarly, we evaluate ${}^1\tilde{\Gamma}$ using figure 2(B), and find that

$$\begin{aligned}{}^1\tilde{\Gamma}^{12;11}(x,\omega) &= {}^1\tilde{\Gamma}^{22;21}(x,\omega) = (-J/2N)\delta(x)A^*(\omega)/[1-|A(\omega)|^2] \\ {}^1\tilde{\Gamma}^{12;22}(x,\omega) &= {}^1\tilde{\Gamma}^{22;12}(x,\omega) = (-J/2N)\delta(x)A(\omega)/[1-|A(\omega)|^2].\end{aligned} \tag{43}$$

The conduction electron retarded self-energy may be obtained from the vertex part, as shown in figure 1. From the figure, we see that the outgoing spin must always be the same as the incoming spin, and hence, following the analysis of Cheung and Mattuck, the spin sum for figure 1 is

$$\sum_{\beta\beta''\alpha''}[{}^0\Gamma_{\mathrm{T}}^{ij;kl}\delta_{\alpha'\alpha''} + {}^1\Gamma_{\mathrm{T}}^{ij;kl}(\boldsymbol{\sigma}_{\alpha'\alpha''}\cdot \boldsymbol{S}_{\beta\beta''})](\boldsymbol{\sigma}_{\alpha''\alpha}\cdot \boldsymbol{S}_{\beta''\beta}) = \tfrac{3}{2}\,{}^1\Gamma_{\mathrm{T}}^{ij;kl}\delta_{\alpha'\alpha} \tag{44}$$

where

$${}^1\Gamma_{\mathrm{T}}^{ij;kl}(x,\omega) = {}^1\Gamma^{ij;kl}(x,\omega) + {}^1\tilde{\Gamma}^{ij;kl}(x,\omega) - (J\delta(x)/2N)\gamma^{ij;kl}. \tag{45}$$

Expanding figure 1 in the Keldysh indices gives

$$\begin{aligned}\Sigma_{ij}(0,x;\omega) = \frac{3}{2}\frac{J\delta(x)}{2N}&\iiiint \mathrm{d}x'\,\mathrm{d}x''\,\mathrm{d}\omega'\,\mathrm{d}\omega''\,\delta(x') \\ &\times\Bigg(\sum_{nn'oo'lm}\gamma^{il;nn'}g_{lm}(x',x'',\omega')d_{n'o}(x',x'';\omega''-\omega')d_{no'}(x',x'';\omega''-\omega) \\ &\times[{}^1\Gamma^{oo';mj}(\omega'') + {}^1\tilde{\Gamma}^{oo';mj}(\omega'') - (J/2N)\gamma^{oo';mj}]\Bigg).\end{aligned} \tag{46}$$

Noting that terms in the sum involving $d_{22}$ integrate to zero, we find that

$$\begin{aligned}\Sigma_{12}(0,x;\omega) &= \Sigma^{\mathrm{r}}(0,x;\omega) \\ &= \frac{3}{2}\frac{J\delta(x)}{2N}\iiiint \mathrm{d}x'\,\mathrm{d}x''\,\mathrm{d}\omega'\,\mathrm{d}\omega''\,\delta(x') \\ &\times\{g_{22}(x',x'',\omega')d_{12}(x',x'';\omega''-\omega')d_{12}(x',x'';\omega''-\omega) \\ &\times[{}^1\Gamma^{12;11}(\omega'') + {}^1\tilde{\Gamma}^{12;11}(\omega'')] \\ &+ g_{22}(x',x'',\omega')d_{21}(x',x'';\omega''-\omega')d_{21}(x',x'';\omega''-\omega) \\ &\times[{}^1\Gamma^{12;22}(\omega'') + {}^1\tilde{\Gamma}^{12;22}(\omega'')]\}.\end{aligned} \tag{47}$$

Also

$$\begin{aligned}\Sigma_{22}(0,x;\omega) = 0 = \frac{3}{2}\frac{J\delta(x)}{2N}&\iiiint \mathrm{d}x'\,\mathrm{d}x''\,\mathrm{d}\omega'\,\mathrm{d}\omega''\,\delta(x') \\ &\times\{g_{22}(x',x'',\omega')d_{12}(x',x'';\omega''-\omega')d_{21}(x',x'';\omega''-\omega) \\ &\times[{}^1\Gamma^{22;21}(\omega'') + {}^1\tilde{\Gamma}^{22;21}(\omega'') - (J/2N)] \\ &+ g_{22}(x',x'',\omega')d_{21}(x',x'';\omega''-\omega')d_{12}(x',x'';\omega''-\omega) \\ &\times[{}^1\Gamma^{22;12}(\omega'') + {}^1\tilde{\Gamma}^{22;12}(\omega'') - (J/2M)]\}.\end{aligned} \tag{48}$$

We subtract equation (45) from equation (46), and perform the spatial integration to find

$$\Sigma^{\mathrm{r}}(0,x;\omega)=\frac{3}{2}\frac{\rho J^2\delta(x)}{2\pi(2N)^2}\bigg(\frac{\mathrm{i}}{2\pi}\int_{-D}^{D}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\mathrm{d}\omega''\frac{\tanh(\beta\omega'/2)}{(\omega''-\omega')(\omega''-\omega)}$$
$$+2\int_{-D}^{D}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\mathrm{d}\omega''\frac{\delta(\omega''-\omega)\tanh(\beta\omega'/2)}{(\omega''-\omega')}$$
$$\times[{}^1\Gamma^{12;11}(\omega'')+{}^1\tilde{\Gamma}^{12;11}(\omega'')-{}^1\Gamma^{12;22}(\omega'')-{}^1\tilde{\Gamma}^{12;22}(\omega'')]$$
$$+\frac{2\mathrm{i}}{\pi}\int_{-D}^{D}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\mathrm{d}\omega''\,\delta(\omega''-\omega')\delta(\omega''-\omega)\tanh(\beta\omega'/2)$$
$$\times[{}^1\Gamma^{12;11}(\omega'')+{}^1\tilde{\Gamma}^{12;11}(\omega'')+{}^1\Gamma^{12;22}(\omega'')+{}^1\tilde{\Gamma}^{12;22}(\omega'')-1]\bigg). \tag{49}$$

These integrations are elementary, and on dividing $\Sigma^{\mathrm{r}}$ into its real and imaginary parts:

$$\Sigma^{\mathrm{r}}(0,x;\omega)=\mathrm{Re}\,\Sigma^{\mathrm{r}}(0,x;\omega)+\mathrm{i}\,\mathrm{Im}\,\Sigma^{\mathrm{r}}(0,x;\omega) \tag{50}$$

we find

$$\mathrm{Re}\,\Sigma^{\mathrm{r}}(0,x;\omega)=\tfrac{3}{2}(\rho J^2\delta(x)/8\pi N^2)[\![\log\{D^2/[\omega^2+(2KT)^2]\}]\!] \tag{51}$$

and

$$\mathrm{Im}\,\Sigma^{\mathrm{r}}(0,x;\omega)=-\frac{3}{2}\frac{\rho J^2\delta(x)}{8\pi N^2}\bigg\{\frac{1}{2}\log\left(\frac{D^2}{\omega^2+(2KT)^2}\right)$$
$$\times\frac{(A(\omega)-A^*(\omega))}{\mathrm{i}}\frac{2|A(\omega)|^2+A(\omega)+A^*(\omega)}{(1+A(\omega))(1+A^*(\omega))(1-|A(\omega)|^2)}+\frac{\pi}{2}\tanh(\beta\omega/2)$$
$$\times(A(\omega)+A^*(\omega)+2)(1-|A(\omega)|^2)-(A(\omega)+A^*(\omega))$$
$$\times(A(\omega)+1)(A^*(\omega)+1)[(A(\omega)+1)(A^*(\omega)+1)(1-|A(\omega)|^2)]^{-1}\bigg\}. \tag{52}$$

In the next section we shall use this retarded self-energy to evaluate the retarded Green's function and its first spatial derivative. Having obtained these, we shall be able to express the current density of the junction, a function of the applied potential, in terms of an integral equation.

## 4. The current

On performing the $x_1$ integration in equation (12), and taking the spatial Fourier transform with respect to $x'$, we find

$$G(0,q;\omega)=\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)-V}+a}\frac{1}{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)}-a} \tag{53}$$

where

$$\Sigma^{\mathrm{r}}(\omega)=\int_{-\infty}^{\infty}\mathrm{d}x_1\,\Sigma^{\mathrm{r}}(0,x_1,\omega)\qquad\text{and}\qquad a=q\sqrt{\frac{\hbar^2}{2m}}.$$

Also

$$\left.\frac{\mathrm{d}G(x,q;\omega)}{\mathrm{d}x}\right|_{x=0} = \mathrm{i}\sqrt{\frac{m}{\pi\hbar^2}}\frac{1}{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)}+\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)-V}}$$
$$\times\left\{\frac{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)}}{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)-V}+a}-\frac{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)-V}}{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)}-a}\right\}. \tag{54}$$

The superscript on $G$ has been dropped, and it is understood that we are dealing with the retarded Green's function.

We shall consider the current of electrons with positive momenta, and seek the Fourier frequency transform of equations (53) and (54) in an asymptotic form. This is accomplished by the method of generalized functions, where the Fourier transform is approximated in the vicinity of its poles (Lighthill 1959). A direct approach is to recognize that $G(0,q,\omega)$ can be approximated by

$$G(0,q;\omega)\simeq g(q,\omega)/(\omega-\omega_0) \tag{55}$$

where $\omega$ is a complex constant, and $g(q,\omega)$ has no poles for the momenta being considered. The Fourier transform of this equation (55) is, asymptotically

$$\mathrm{i}\theta(-\operatorname{Im}\omega_0)\operatorname{sgn}(\operatorname{Im}\omega_0)\mathrm{e}^{-\mathrm{i}\omega_0 t}g(\omega_0).$$

For $q>0$, the only pole of $G(0,q,\omega)$ is such that

$$q=\sqrt{2m}\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)}. \tag{56}$$

We expand $G(0,q;\omega)$ about $a^2$:

$$\frac{1}{\sqrt{\omega-\Sigma^{\mathrm{r}}(\omega)}}\simeq\left[\sqrt{a^2-\Sigma^{\mathrm{r}}(a^2)}+\frac{(\omega-a^2)(1-\partial\Sigma^{\mathrm{r}}(\omega)/\partial\omega|_{\omega=a^2})}{2\sqrt{a^2-\Sigma^{\mathrm{r}}(a^2)}}\right]^{-1}. \tag{57}$$

We get

$$G(0,q;t)\simeq\frac{\theta(-\operatorname{Im}\omega_0(\epsilon_q))\operatorname{sgn}(\operatorname{Im}\omega_0(\epsilon_q))(\zeta(\epsilon_q)/\lambda(\epsilon_q))\mathrm{e}^{-\mathrm{i}\omega_0(\epsilon_q)t}}{\sqrt{\omega_0(\epsilon_q)-\Sigma^{\mathrm{r}}(\omega_0(\epsilon_q))}+\sqrt{\epsilon_q}} \tag{58}$$

and

$$\left.\frac{\mathrm{d}G(x,q;t)}{\mathrm{d}x}\right|_{x=0}\simeq\sqrt{\frac{m}{\pi}}\theta(-\operatorname{Im}\omega_0(\epsilon_q))\operatorname{sgn}(\operatorname{Im}\omega_0(\epsilon_q))$$
$$\times\frac{\sqrt{\omega_0(\epsilon_q)-\Sigma^{\mathrm{r}}(\omega_0(\epsilon_q))-V}[\zeta(\omega_0(\epsilon_q))/\lambda(\omega_0(\epsilon_q))]\mathrm{e}^{-\mathrm{i}\omega_0(\epsilon_q)t}}{\sqrt{\omega_0(\epsilon_q)-\Sigma^{\mathrm{r}}(\omega_0(\epsilon_q))}+\sqrt{\omega_0(\epsilon_q)-\Sigma^{\mathrm{r}}(\omega_0(\epsilon_q))-V}} \tag{59}$$

where

$$\omega_0(\epsilon_q)=\epsilon_q+\sqrt{\epsilon_q}\zeta(\epsilon_q)/\lambda(\epsilon_q)-\zeta(\epsilon_q)^2/\lambda(\epsilon_q) \tag{60}$$

$$\zeta(\epsilon_q)=\sqrt{\epsilon_q-\Sigma^{\mathrm{r}}(\epsilon_q)} \tag{61}$$

$$\lambda(\epsilon_q)=\frac{1}{2}\left(1-\left.\frac{\partial\Sigma^{\mathrm{r}}(\omega)}{\partial\omega}\right|_{\omega=\epsilon_q}\right) \tag{62}$$

and $\omega$ is a complex variable:

$$\omega = \omega_1 + \mathrm{i}\omega_2. \tag{63}$$

The current is, from equation (15),

$$j(x,t) = \frac{2e\hbar}{\pi m} \sum_q f_q \frac{|\zeta(\epsilon_q)|^2}{|\lambda(\epsilon_q)|^2} \{[(\sqrt{\epsilon_q} + \sqrt{R_1}\cos(\theta_1))$$
$$\times (R_2 + \sqrt{R_1 R_2}\cos((\theta_2 - \theta_1)/2)) - R_1\sqrt{R_2}\sin(\theta_1/2)\sin((\theta_2 - \theta_1)/2)]\}$$
$$\times \{[(\sqrt{\epsilon_q} + \sqrt{R_1}\cos(\theta_1/2))^2 + R_1 \sin^2(\theta_1/2)]$$
$$\times [R_1 + R_2 + 2\sqrt{R_1 R_2}\cos((\theta_2 - \theta_1)/2)]\}^{-1} \tag{64}$$

with

$$R_1 = \sqrt{(\mathrm{Re}\,\omega_0 - \mathrm{Re}\,\Sigma^{\mathrm{r}}(\omega_0))^2 + (\mathrm{Im}\,\omega_0 - \mathrm{Im}\,\Sigma^{\mathrm{r}}(\omega_0))^2} \tag{65}$$

$$R_2 = \sqrt{(\mathrm{Re}\,\omega^0 - \mathrm{Re}\,\Sigma^{\mathrm{r}}(\omega_0) - V)^2 + (\mathrm{Im}\,\omega_0 - \mathrm{Im}\,\Sigma^{\mathrm{r}}(\omega_0))^2} \tag{66}$$

$$\theta_1 = \tan^{-1}[(\mathrm{Im}\,\omega_0 - \mathrm{Im}\,\Sigma^{\mathrm{r}}(\omega_0))/(\mathrm{Re}\,\omega_0 - \mathrm{Re}\,\Sigma^{\mathrm{r}}(\omega_0))] \tag{67}$$

$$\theta_2 = \tan^{-1}[(\mathrm{Im}\,\omega_0 - \mathrm{Im}\,\Sigma^{\mathrm{r}}(\omega_0))/(\mathrm{Re}\,\omega_0 - \mathrm{Re}\,\Sigma^{\mathrm{r}}(\omega_0) - V)]. \tag{68}$$

As a steady magnetic field is applied perpendicularly to the direction of the electron current the energy spectrum $\epsilon$ of motion (neglecting spin splitting) coincides with the spectrum of the linear oscillator and consists of discrete levels

$$\epsilon = (n + \tfrac{1}{2})\hbar\omega_{\mathrm{c}} \qquad n = 0, 1, 2\ldots \qquad \omega_{\mathrm{c}} = \frac{eH}{mc} \tag{69}$$

where $e$ and $m$ are the electronic charge and mass, $c$ is the speed of light, and $H$ is the magnetic field. At $H = 0$, the allowed tunnelling states are uniformly distributed in the Fermi sphere and the sum in equation (64) is over these momenta, with corresponding states of energy between $\epsilon_{\mathrm{F}}$ and $\epsilon_{\mathrm{F}} + V$.

With an applied steady magnetic field the discrete levels $(n + \frac{1}{2})\hbar\omega_{\mathrm{c}}$ then become the allowed values of energy $\epsilon$ related to the electronic motion. The momentum $q$ relating to a level with a quantum number $n$ is found by the correspondence principle, which can be written as

$$(\hbar q)^2/2m = (n + \tfrac{1}{2})\hbar\omega_{\mathrm{c}} \tag{70}$$

whence

$$q_n = \sqrt{(2m\omega_{\mathrm{c}}/\hbar)(n + \tfrac{1}{2})}. \tag{71}$$

The sum in equation (64) is now over $q_n$ with the first $n$ determined from

$$\epsilon_{\mathrm{F}} = (n_{\mathrm{first}} + \tfrac{1}{2})\hbar\omega_{\mathrm{c}} \tag{72}$$

and the last $n$ determined from

$$\epsilon_{\mathrm{F}} + V = (n_{\mathrm{last}} + \tfrac{1}{2})\hbar\omega_{\mathrm{c}}. \tag{73}$$

Hence, $n_{\mathrm{first}}$ is interpreted to be the closest integer to the value $\epsilon_{\mathrm{F}}/(\hbar\omega_{\mathrm{c}}) - \frac{1}{2}$, and $n_{\mathrm{last}}$ the closest integer to the value $(\epsilon_{\mathrm{F}} + V)/(\hbar\omega_{\mathrm{c}}) - \frac{1}{2}$.

## 5. Discussion

$I$–$V$ curves were computed numerically using expression (64). In figure 4 we present a current curve and the dynamic conductance, $dI/dV$, derived from it with $KT = 0.06$ meV, and no applied magnetic field. An antiferromagnetic coupling constant with the value $J\rho/N = -0.10$ was used for computing these curves in order to come into touch with the Nagaoka decoupling procedure; this is the value for $J\rho/N$ which Nagaoka used in his paper (Nagaoka 1965), and from that paper the critical temperature at which instabilities in the decoupling procedure set in is determined from

$$KT_c = (1.14D)e^{-N/|J|\rho}.$$

A value for $D$ of 1.4 eV was used for computing our current curves and we find that the temperature below which the Appelbaum approach is expected to break down is 0.07 meV. We infer therefore that figure 4 shows the current and conductance below the Nagaoka critical temperature. This corresponds to the so called 'tight binding' region referred to in Gregory's paper (Gregory 1992).

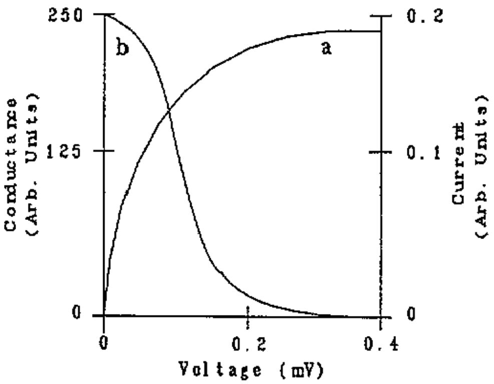


**Figure 4.** The current, curve a, and the variation of the conductance, curve b, with applied bias voltage, computed for the case where conduction electrons and impurity electrons are interacting antiferromagnetically with no applied magnetic field, with the parameters: $KT = 0.06$ meV, $J\rho/N = -0.1$, and $D = 1.4$ eV.

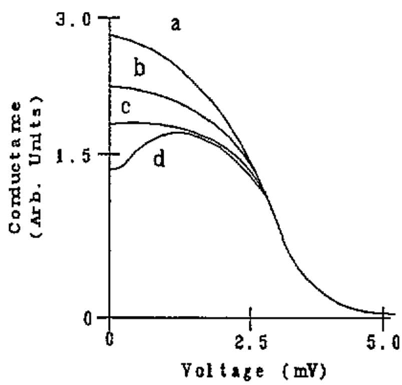


**Figure 5.** Variation of dynamic conductance with applied bias voltage with different applied magnetic fields. Curves a, b, c and d correspond to Zeeman energies with $g = 2$ and magnetic fields of $H = 0$ T, 3 T, 5 T, and 10 T, respectively, and with the parameters: $KT = 0.11$ meV, $J\rho/N = -0.1$, and $D = 1.4$ eV.

In figure 5 we present conductance curves computed with various applied magnetic field intensities, and with $KT = 1.14$. In this case we are well above the Nagaoka critical temperature in a region where the transfer Hamiltonian technique is expected to be valid. The characteristic evolution of the line shape with increasing field strength is clear from this figure, and compares favorably (at least qualitatively) with Gregory's experimental results (Gregory 1992). It is not apparent from these plots as to whether or not a central peak develops, but it is quite clear that there is the characteristic splitting of the anomalous conductance peak. The bias voltage of the peak maximum is $g\mu_B H$ (assuming $g = 2$), and the height of the peak decreases with increasing magnetic field. These features are similar to the results of a transfer Hamiltonian calculation (Shen and Rowell 1967).

The band width we have used is 1.4 eV, and this parameter corresponds roughly to the cut-off parameter in the Appelbaum theory, which requires a much smaller value than one would expect from an estimated variation of the density of states of transition metals near the Fermi surface (Appelbaum 1967). In the present formulation $D$ is not a phenomenological fitting parameter in the following sense: $D$ obtains a finite value reflecting the fact that the localized d-spin impurity orbital has a limited spatial extent of non-negligible amplitude. We note that equation (12) holds when the motion in both wires is free; in which case $D = \infty$.

For the sake of simplicity, we have restricted our discussion to a one-dimensional junction. The amount of algebra required to secure a closed expression for the spatial Fourier transform of equation (12) increases considerably when extending the analysis to three dimensions. The junction width has been assumed to be infinitesimally small, but the effect of junction width can be introduced by making an appropriate modification to the perturbing potential, $V(x)$. Also, we have not considered the electron–phonon interaction; it may be introduced, in a simple manner, by adding a retarded self-energy term to the Hamiltonian, corresponding to the Migdal approximation, and using the Einstein phonon density of states to evaluate phonon propagators.

Finally, we have not estimated the effects of impurity concentration. A correct procedure would be to average the Hamiltonian over a random distribution of impurity positions.

In conclusion, I have found that the $I$–$V$ characteristics of a tunnel junction, with imbedded magnetic impurities, can be computed from a first-principles analysis using the Keldysh formalism. The results are qualitatively similar to phenomenological theories, but the analysis provides a flexibility, not found in transfer Hamiltonian schemes, for modelling conduction electron interactions with bound spins. The time-dependent technique of Cini provides a broad approach to tunnel junction behaviour, which is free of arbitrary fitting parameters.

## References


Abrikosov A A 1965 *Physics* **2** 5–20

—— 1968 *Sov. Phys.–JETP* **26** 641–6

Appelbaum J A 1967 *Phys. Rev.* **154** 633–43

Appelbaum J A and Brinkman W F 1970 *Phys. Rev.* B **2** 907–15

Caroli C, Combescot R, Nozieres P and Saint-James D 1971 *J. Phys. C: Solid State Phys.* **4** 916–29

Cheung C Y and Mattuck R D 1970 *Phys. Rev.* B **2** 2735–45

Cini M 1980 *Phys. Rev.* B **22** 5887–99

Duke C B, Kleiman G G and Stakelon T E 1972 *Phys. Rev.* B **6** 2389-409

Feuchtwang T E 1974 *Phys. Rev.* B **10** 4121–34

—— 1979 *Phys. Rev.* B **20** 430–45

Gregory S 1992 *Phys. Rev. Lett.* **68** 2070–3

Gupta H M 1973 *J. Phys. C: Solid State Phys.* **6** 686–98

Keldysh L V 1965 *Sov. Phys.–JETP* **20** 1018–26

Kondo J 1964 *Prog. Theor. Phys.* **32** 37–49

Lighthill M J 1959 *Introduction to Fourier Analysis and Generalized Functions* (Cambridge: Cambridge University Press) pp 44–75

Manassen Y, Hamers R J, Demuth J E and Castellano A J Jr 1989 *Phys. Rev. Lett.* **62** 2531–4

Nagaoka Y 1965 *Phys. Rev.* **138** A1112–20

Rammer J and Smith H 1986 *Rev. Mod. Phys.* **58** 323–59

Shen L Y L and Rowell J M 1967 *Phys. Rev.* **165** 566–77