ON THE THEORY OF TUNNELING ANOMALIES

O. D. CHEĬSHVILI

Institute of Physics, Georgian Academy of Sciences

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Tunneling through a normal metal—dielectric—normal metal system is investigated using the Abrikosov graph technique, assuming paramagnetic impurities near the barrier. It is shown that in the case of ferromagnetic coupling between the electron and the paramagnetic impurity the resistance of the system decreases with decreasing applied potential. In the case of antiferromagnetic coupling the effect is reversed and more pronounced. In both cases the effect increases with increasing surface density of the paramagnetic impurities near the barrier.

ANOMALIES in the tunneling current have been observed experimentally in many recent works.[1-4] Theoretically, these questions have been studied in[5-8], starting from the idea that the anomalies in the tunneling current are due to the interaction of the conduction electrons with paramagnetic impurities. The calculations of Anderson[5] and Appelbaum[6] use perturbation theory and, of course, describe a situation where the anomalies in the tunneling current are small. Appelbaum et al.[7] used Green's functions[9] for massive homogeneous specimens in their calculation of the tunneling current. In the work of Solyom and Zawadowski[8] the solutions of Abrikosov[10] and Nagaoka[9] for massive homogeneous specimens are somewhat modified (the spatial dependence of the density of states due to the presence of the barrier is taken into account). In contrast to these works, we determine, in the present paper, the corrections to the Green's functions which are proportional to the transmission amplitude. They are very important for the calculation of the conductivity which is known to be proportional to the transmission coefficient.

We consider a system (normal metal—dielectric—normal metal) which contains paramagnetic impurities in a certain layer of thickness z_0 on both sides of the barrier (the impurities on different sides can be of a different kind). It is assumed that this effective thickness z_0 is much larger than the interatomic distance $1/p_0$ and much smaller than the length $\xi = \min(v_0/eV, v_0/T)$, where V is the applied potential difference and p_0 and v_0 are the Fermi momentum and velocity.

We represent the dielectric layer by a δ function-like potential barrier with the parameter $a = mU/\hbar^2$ (U is the intensity height of the barrier; $\hbar = 1$ in the following). The electrons tunneling through the barrier have momenta close to the Fermi momentum; therefore the transmission coefficient will be $\sim p_0^2/a^2$ (we consider a system with small transmissivity so that the quantity p_0/a will serve as a small parameter in the following).

The operator of the electron field for the system NIN, where the potential difference 2V is applied to the barrier, can be written in the form

$$\hat{\psi}(\mathbf{r}, t)=\sum_{p\eta}\psi_{p\eta}(\mathbf{r})\exp\{-i(\varepsilon_p-\varepsilon_F-\eta eV)t\}\hat{a}_{p\eta}. \quad (1)$$

In the case of a δ-function potential we have in the free electron approximation

$$\psi_{p\eta}(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}\left\{\left(\exp\{-ip_z\eta z\}-\frac{a}{a-ip_z}\exp\{ip_z\eta z\}\right)\theta(\eta z)-\frac{ip_z}{a-ip_z}\exp\{-ip_z\eta z\}\theta(-\eta z)\right\}\exp\{ip_x x+ip_y y\}; \quad (2)$$

here $p_z > 0$, and $\theta(x)$ is the step function. The index η takes the two values ± 1 corresponding to the twofold degeneracy of the states of the electron,[11] because of the infiniteness of the motion of the electron in both directions of z (z is perpendicular to the plane of the dielectric).

After introduction of the operator (1) it is easy to write down the zero order Green's function:

$$\hat{G}_0(\mathbf{r},\mathbf{r}';\omega)=\sum_\eta\int d\mathbf{p}\,\psi_{p\eta}(\mathbf{r})\psi_{p\eta}^*(\mathbf{r}')\hat{G}_0(\mathbf{p},\omega+\eta eV). \quad (3)$$

For the calculation of the current through the potential barrier it is convenient to use the Green's functions introduced by Keldysh.[12] Thus the Green's function (3) will correspond to the two-by-two matrix (cf.[12])

$$\hat{G}_0=\begin{pmatrix}G_0^c & G_0^-\\ G_0^+ & \tilde{G}_0^c\end{pmatrix}=G_{0ij}. \quad (4)$$

With the help of the Green's function, the tunneling current through the barrier can be written in the following form;

$$I=\frac{e}{m}\lim_{zz'\to+0,\mathbf{r}_\perp\to\mathbf{r}_\perp'}\left(\frac{\partial}{\partial z'}-\frac{\partial}{\partial z}\right)\int\frac{d\omega}{2\pi}G^+(\mathbf{r},\mathbf{r}';\omega), \quad (5)$$

where $\mathbf{r}_\perp = (x, y)$,

$$G^+(\mathbf{r},\mathbf{r}';\omega)=\sum_{\eta\eta'}\int d\mathbf{p}\,d\mathbf{p}'\,\psi_{p\eta}(\mathbf{r})\psi^*_{p'\eta'}(\mathbf{r}')G^+(\mathbf{p}\eta,\mathbf{p}'\eta';\omega). \quad (6)$$

Using (2), we find

$$\lim_{z,z'\to+0,\mathbf{r}_\perp\to\mathbf{r}_\perp'}\left(\frac{\partial}{\partial z'}-\frac{\partial}{\partial z}\right)\psi_{p\eta}(\mathbf{r})\psi^*_{p'\eta'}(\mathbf{r}')$$

$$=\frac{p_z p_z'}{(2\pi)^3}\{i(p_z\eta+p_z'\eta')+2a[\eta'\theta(\eta')-\eta\theta(\eta)]\}\frac{\exp\{i(\mathbf{p}_\perp-\mathbf{p}_\perp')\mathbf{r}_\perp\}}{(a-ip_z)(a+ip_z')} \quad (7)$$

Since this expression is proportional to the transmission amplitude p_0/a, we need determine the Green's function only with an accuracy up to p_0/a.

The expression for the current can be simplified by assuming that the electrons for which p_z is close to p_0 give the main contribution to the tunneling. We therefore replace p_z and p'_z in (7) by p_0 and take them outside the integral in (6). With this procedure we will make an error which can be absorbed in a certain numerical factor; however, this is not essential, since we are interested in a ratio of currents (the currents with and without the presence of impurities). It follows from the symmetry of the problem that

$$G^{+}(\mathbf{p}\eta, \mathbf{p}'\eta'; \omega) = \delta(p_x - p_x')\delta(p_y - p_y')G^{+}(\mathbf{p}\eta, \tilde{\mathbf{p}}'\eta'; \omega).$$

It will be seen in the following that the Green's function in zeroth order in the transmission amplitude is $\sim\delta_{\eta\eta'}$. The Green's function in first order is $\sim\delta_{\eta,-\eta'}$. Taking all this into account, we can rewrite the expression for the current in the form

$$I = \frac{2e}{m}\frac{p_0^2}{a}\int\frac{d\tilde{\omega}}{2\pi}\int\frac{d\mathbf{p}\,dp_z'}{(2\pi)^3}\sum_\eta \eta\left[i\frac{p_0}{a}G^{(0)+}(\mathbf{p}\eta, \tilde{\mathbf{p}}'\eta; \omega) - G^{(1)+}(\mathbf{p}\eta, \tilde{\mathbf{p}}' - \eta; \omega)\right]. \tag{8}$$

Here $\tilde{\mathbf{p}}' = (p_x, p_y, p_z')$.

For the calculations we shall use the graph technique of Abrikosov.[10] Here we must take into account that the density of electron states and the density of the impurities are not constant over the whole specimen. We now compute the vertex function with due regard to this point.

As is known, we are dealing, in the Keldysh method,[12] with elementary vertices of two types: + and −. It is easy to verify that a vertex with different elementary vertices,

(9)

is equal to zero with logarithmic accuracy. Here the dashed line going from the point + to the point −, corresponds to the impurity Green's function

$$g^{-}(\omega) = -2\pi i(1 - n_\lambda)\delta(\omega), \quad n_\lambda = [e^{\lambda/T} + 1]^{-1},$$

where λ is a parameter introduced by Abrikosov.[10] The solid electron line corresponds to

$$G_0^{-}(\mathbf{p}, \omega) = -2\pi i(1 - n_\mathbf{p})\delta(\omega - \xi),$$

where $\xi = \epsilon_\mathbf{p} - \epsilon_F$ and $n_\mathbf{p}$ is the Fermi distribution. The lines going from − to + correspond to the Green's functions

$$g^{+}(\omega) = 2\pi i n_\lambda\delta(\omega), \quad G_0^{+}(\mathbf{p}, \omega) = 2\pi i n_\mathbf{p}\delta(\omega - \xi).$$

The lines going from + to + and, correspondingly, from − to − correspond to the Green's functions

$$g^{c}(\omega) = \frac{1 - n_\lambda}{\omega + i\delta} + \frac{n_\lambda}{\omega - i\delta}, \quad G_0^{c}(\mathbf{p}, \omega) = \frac{1 - n_\mathbf{p}}{\omega - \xi + i\delta} + \frac{n_\mathbf{p}}{\omega - \xi - i\delta}$$

$$\bar{g}^{c}(\omega) = -\frac{1 - n_\lambda}{\omega - i\delta} - \frac{n_\lambda}{\omega + i\delta}, \quad \bar{G}_0^{c}(\mathbf{p}, \omega) = -\frac{1 - n_\mathbf{p}}{\omega - \xi - i\delta} - \frac{n_\mathbf{p}}{\omega - \xi + i\delta}.$$

It is easy to see that the nonvanishing (with logarithmic accuracy) vertices correspond to graphs with identical points. Summing over the "parquet floor" graphs we can find an equation for the total vertex function when all points in the graph correspond to +.

If we write the vertex function in the form

$$\Gamma(z_n, \omega) = \Gamma^{+}(z_n, \omega)\sigma\mathbf{S}, \tag{10}$$

we find for Γ^+ the following equation:

$$\Gamma^{+}(z_n, \omega) = \frac{f}{N} + i\int\frac{d\omega_1}{2\pi}g^{c}(\omega_1)G_0^{c}(\mathbf{r}_n, \mathbf{r}_n; \omega - \omega_1)[\Gamma^{+}(z_n, \omega_1)]^2 \tag{10'}$$

$$- i\int\frac{d\omega_1}{2\pi}g^{c}(\omega_1)G_0^{c}(\mathbf{r}_n, \mathbf{r}_n; \omega + \omega_1)[\Gamma^{+}(z_n, \omega_1)]^2;$$

z_n is the position of the impurity. It is easy to show that the solution of this equation yields with an accuracy up to p_0/a

$$\Gamma(z_n, \tilde{\omega}) = \frac{j}{N}\left[1 + \frac{j}{N}\frac{p_0 m}{\pi^2}\left(1 - \frac{\sin\zeta}{\zeta}\right)\ln\frac{\varepsilon_F}{\tilde{\omega}}\right]^{-1}\sigma\mathbf{S}$$
$$+ \frac{p_0}{a}\left(\frac{\cos\zeta}{\zeta} - \frac{\sin\zeta}{\zeta^2}\right)\frac{p_0 m}{\pi^2}\left(\frac{j}{N}\right)^2$$
$$\times\ln\frac{\varepsilon_F}{\tilde{\omega}}\left[1 + \frac{j}{N}\frac{p_0 m}{\pi^2}\left(1 - \frac{\sin\zeta}{\zeta}\right)\ln\frac{\varepsilon_F}{\tilde{\omega}}\right]^{-2}\sigma\mathbf{S}, \tag{11}$$

where $\xi = 2p_0 z_n$ and $\tilde{\omega} = \max(|\omega|, eV)$.

It is easy to see that the "minus" vertex function differs from (11) only by a sign. Finally, we can write the total vertex in the form

$$\Gamma_{ij}^{mn}(z_n, \tilde{\omega}) = \Gamma(z_n, \tilde{\omega})\delta_{ij}\delta_{mn}(\sigma_z)_{im}. \tag{12}$$

In this way of writing we have taken account of the fact that in each vertex two electron and two impurity lines converge, and in order to connect these, one must write the vertex function in the form of fourth-rank tensor. The lower indices in (12) are electron indices, the upper ones are impurity indices.

Now we can write down the equation for the Green's function:

$$G_{ij}(\mathbf{r}, \mathbf{r}'; \omega) = G_{0ij}(\mathbf{r}, \mathbf{r}'; \omega) + \lim_{\lambda\to\infty}\frac{e^{\lambda/T}}{2S + 1}\mathrm{Sp}\int d\mathbf{r}_n f(\mathbf{r}_n)G_{0ii'}(\mathbf{r}, \mathbf{r}_n; \omega)$$

$$\times\int\frac{d\omega_1\,d\omega_2}{(2\pi)^2}\Gamma_{i'l}^{mn}g_{m'm}(\omega_1)g_{nn'}(\omega_2)G_{0ll'}(\mathbf{r}_n, \mathbf{r}_n; \omega + \omega_1 - \omega_2)\Gamma_{l'j'}^{n'm'}G_{j'j}(\mathbf{r}_n, \mathbf{r}'; \omega). \tag{13}$$

In this equation, all Green's functions (the impurity as well as the electron ones) are second-rank matrices, and $f(\mathbf{r}_n)$ is the distribution function of the impurity centers in the specimen, which is taken in the form[1)]

$$f(\mathbf{r}_n) = \sum_\eta n_\eta\frac{z_\eta^2}{z_n^2 + z_\eta^2}\theta(\eta z_n); \tag{14}$$

η takes two values: n_+ and n_-, the volume densities of the impurities on the right and left-hand sides of the barrier, respectively. The final results will be functions of the effective surface density of the impurities $N_\eta = \pi n_\eta z_\eta/2$.

After integration over the frequencies and summation over the spin states of the impurities in (13), we obtain

$$\hat{G}(\mathbf{r}, \mathbf{r}'; \omega) = \hat{G}_0(\mathbf{r}, \mathbf{r}'; \omega) + S(S + 1)\int d\mathbf{r}_n f(\mathbf{r}_n)\hat{G}_0(\mathbf{r}, \mathbf{r}_n; \omega)$$
$$\times[\Gamma^{+}(z_n, \tilde{\omega})]^2\sigma_z\hat{G}_0(\mathbf{r}_n, \mathbf{r}_n; \omega)\sigma_z\hat{G}(\mathbf{r}_n, \mathbf{r}'; \omega). \tag{15}$$

Taking the average, introducing the surface density N_η and going to the limit $p_0 z_\eta \to \infty$ and $(p_z - p_z')z_\eta \to 0$, we find[2)]

$$\hat{G}(\mathbf{p}\eta, \mathbf{p}'\eta'; \omega) = \hat{G}_0(\mathbf{p}, \omega + \eta eV)\delta(\mathbf{p} - \mathbf{p}')\delta_{\eta\eta'} + \Sigma(\eta)\hat{G}_0(\mathbf{p}, \omega + \eta eV)$$
$$\times\sigma_z\int\hat{G}_0(\mathbf{p}, \omega + \eta eV)\frac{d\xi}{\pi}\sigma_z\int dp_{1z}\hat{G}(\tilde{\mathbf{p}}_1\eta, \mathbf{p}'\eta'; \omega) + \frac{ip_0}{2a}\hat{G}_0(\mathbf{p}, \omega + \eta eV)$$

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1)We note that the final results do not depend on the specific form of the function $f(\mathbf{r}_n)$ if that function falls off so rapidly away from the barrier that it is meaningful to introduce an effective surface density.

2)We take into account that those electrons are important for the tunneling which have energies close to the Fermi energy and momentum components p_x and p_y close to zero (since the probability for finding electrons inside the barrier with nonvanishing momentum components p_x and p_y is strongly suppressed); therefore $p_z - p_z' \sim \max(eV, T)/v_0$.

$$\times \sigma_z \left\{ \Sigma(\eta) \int \hat{G}_0(\mathbf{p}, \omega + \eta eV) \frac{d\xi}{\pi} - \Sigma(-\eta) \int \hat{G}_0(\mathbf{p}, \omega - \eta eV) \frac{d\xi}{\pi} \right\}$$

$$\times \sigma_z \int dp_{1z} \hat{G}(\tilde{\mathbf{p}}_1, -\eta; \mathbf{p}'\eta'; \omega), \quad (16)$$

where the vector $\tilde{\mathbf{p}}_1 = (p_x, p_y, p_{1z})$,

$$\Sigma(\eta) = \frac{p_0 m}{2\pi^2} S(S+1) N_\eta \left(\frac{j_\eta}{N}\right)^2 \left[1 + \frac{p_0 m}{\pi^2} \frac{j_\eta}{N} \ln \frac{\varepsilon_F}{\bar{\omega}}\right]^{-2} \quad (17)$$

and j_η is the constant for the interaction of the electron with the paramagnetic impurity; it is understood that impurities of different kinds can exist on different sides of the barrier; therefore, in general $j_+ \neq j_-$. The solution of this integral equation is not very difficult.[3)] However, it is easier to find the integrals of the Green's functions in terms of which the tunneling current (8) is expressed.

Finally, we obtain for the transmission amplitude in zeroth order

$$\int G^{(0)+}(\mathbf{p}\eta, \tilde{\mathbf{p}}'\eta; \omega)\, d\mathbf{p}\, dp_z' = \frac{i\pi}{v_0}\left(1 - \mathrm{th}\frac{\omega + \eta eV}{2T}\right)$$

$$\times \left(1 + \frac{\pi\Sigma(\eta)}{v_0}\right)^{-1} \int dp_x \int dp_y; \quad (18)$$

in first order, we have

$$\int G^{(1)+}(\mathbf{p}\eta, \tilde{\mathbf{p}}' - \eta, \omega)\, d\mathbf{p}\, dp_z' = \frac{p_0}{2a}\left(\frac{\pi}{v_0}\right)^2$$

$$\times \left\{ \Sigma(\eta)\left(1 - \mathrm{th}\frac{\omega - \eta eV}{2T}\right) - \Sigma(-\eta)\left(1 - \mathrm{th}\frac{\omega + \eta eV}{2T}\right) \right\}$$

$$\times \left(1 + \frac{\pi}{v_0}\Sigma(\eta)\right)^{-1}\left(1 + \frac{\pi}{v_0}\Sigma(-\eta)\right)^{-1} \int dp_x \int dp_y. \quad (19)$$

Substituting (18) and (19) in (8), summing over η and introducing I_0, the current in the absence of impurities, we obtain

$$I = I_0 \int_0^\infty \frac{d\omega}{2\pi}\left(\mathrm{th}\frac{\omega + eV}{2T} - \mathrm{th}\frac{\omega - eV}{2T}\right)\left(1 + \frac{\pi\Sigma(+)}{v_0}\right)^{-1}$$

$$\times \left(1 + \frac{\pi\Sigma(-)}{v_0}\right)^{-1}\left[\int_0^\infty \frac{d\omega}{2\pi}\left(\mathrm{th}\frac{\omega + eV}{2T} - \mathrm{th}\frac{\omega - eV}{2T}\right)\right]^{-1}. \quad (20)$$

When $T \ll eV$,

$$I = I_0\left(1 + \frac{\pi\Sigma(+, eV)}{v_0}\right)^{-1}\left(1 + \frac{\pi\Sigma(-, eV)}{v_0}\right)^{-1}. \quad (21)$$

Or[4)]

$$\frac{R(V)}{R_0} = \left(1 + \frac{\pi\Sigma(+, eV)}{v_0}\right)\left(1 + \frac{\pi\Sigma(-, eV)}{v_0}\right), \quad (22)$$

where

$$\Sigma(\eta, eV) \doteq \frac{p_0 m}{2\pi^2} S(S+1) N_\eta \left(\frac{j_\eta}{N}\right)^2 \left[1 + \frac{p_0 m}{\pi^2}\frac{j_\eta}{N}\ln\frac{\varepsilon_F}{eV}\right]^{-2} \quad (23)$$

It is seen from (23) that for antiferromagnetic coupling $j_\eta < 0$ the resistance increases with decreasing applied potential. Here it should be noted that near resonance the ratio (22) can attain rather large values compared with unity. Indeed, if we make a rather crude estimate[10] for the imaginary term in the resonance denominator of formula (23): $ij_\eta p_0 m/N\pi^2$, then we obtain for the maximum of this ratio

$$(R/R_0)_{max} = [1 + {}^1/_{24}\pi^2 S(S+1) c_+ p_0 z_+][1 + {}^1/_{24}\pi^2 S(S+1) c_- p_0 z_-]. \quad (24)$$

Here $c_\pm = 6\pi^2 n_\pm / p_0^3$ is the atomic concentration, and z_+ and z_- are the effective layers near the barrier in which paramagnetic impurities exist. The parameter $c_\pm p_0 z_\pm$ of order unity means that effectively one has a single atomic layer near the barrier which is completely filled with paramagnetic impurities.

In the case of ferromagnetic coupling the ratio of the resistances decreases with decreasing applied potential, and it is clear that this effect is much weaker.

It is easy to obtain from (20) the temperature dependence of the resistance for $T \gg eV$. It is clear (by integrating with logarithmic accuracy) that the dependence is the same as on the potential in the first limiting case $T \ll eV$.

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3) It should be noted that the solution of (16) is most easily obtained with the help of the linear canonical transformation [12].

$$G = \frac{1 - i\sigma_y}{\sqrt{2}}\begin{pmatrix} G^c & G^- \\ G^+ & \tilde{G}^c \end{pmatrix}\frac{1 + i\sigma_y}{\sqrt{2}} = \begin{pmatrix} 0 & G^a \\ G^r & F \end{pmatrix}.$$

4) We note that with logarithmic accuracy $I/V = dI/dV$.