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ABSTRACT

A hopping model of tunneling proposed by Caroli et al. is used to study electron-pseudofermion interaction in metal-insulator-metal junctions with magnetic impurity in either the insulator or the electrodes The contradiction between some earlier theories of zero-bias anomalies /Zawadowski et al. and Appelbaum et al./ is resolved. These theories appear as limiting cases of the hopping model theory of tunneling. Special attention is devoted to the study of the dependence of the conductance characteristic on the spatial distribution of the impurities.

АННОТАЦИЯ

На основе модели, разработанной Кароли с сотрудниками для объяснения эффекта туннелирования, нами было исследовано электрон-псевдофермионное взаимодействие в диодах металл-изолятор-металл содержащих либо в электроде, либо в изоляторном слое магнитные примеси. Разработанные ранее теории с одной стороны Завадовского, а с другой стороны Аппельбаума привели к противоречивым результатам. Наша обобщенная теория воспроизводит указанные теории как различные предельные случаи. Исследуется также зависимость вольт-амперной характеристики от пространственного распределения примесей.

KIVONAT

A Caroli és munkatársaiáltal az alagutjelenség értelmezésére felállitott modell felhasználásával az elektron-pszeudofermion kölcsönhatást tanulmányozzuk az elektródában vagy a szigetelőrétegben mágneses szennyezést tartalmazó fém-szigetelő-fém alagutdiódák esetén. Feloldjuk a zérus-feszültségü anomáliára Zawadowski és munkatársai illetve Appelbaum és munkatársai által korábban kidolgozott elméletek közötti ellentmondást. Ezek az elméletek a jelenlegi modell határeseteiként adódnak vissza. Tanulmányozzuk az áram-feszültség karakterisztikának a szennyezések térbeli eloszlásától való függését.

I. Introduction

Recently various theories have been proposed to explain zero-bias anomalies in the dynamical conductance--voltage characteristics of metal-metal oxid-metal tunnel junctions, which contain magnetic impurities in the vicinity of one of the electrode-barrier interfaces.

According to the approach of Appelbaum /Appelbaum 1966, 1967, Appelbaum et al. 1967, Appelbaum and Brinkman 197o/ the tunneling current contribution due to the tunneling process assisted by magnetic impurities shows a conductance peak in the case of antiferromagnetic interaction of the conduction electrons with the impurity spin this in turn becomes a resistance peak in the case of ferromagnetic coupling.

In another approach, that of Zawadowski /Zawadowski 1967, Sólyom and Zawadowski 1968 a, b, Mezei and Zawadowski 1971 a,b/ it was found that the amplitude of the tunneling current is determined by the local conduction-electron density of states /EDS/. In this theory influence of the paramagnetic impurities manifests itself as a strongly energy dependent depression of the local density of states compared to the unrenormalized one. The results are just the opposite of that of Appelbaum /1966, 1967/. The conductance maximum is obtained for ferromagnetic interaction while the giant resistance peak is due to antiferromagnetic coupling.

Recently a hopping model of tunnelling has been proposed by Caroli et al. /1967 a, b - referred to as CCNS in the following/. These authors have applied their theory to a few physical problems relevant to metal-insulator-metal /MIM/ tunnel junctions: tunneling though an impure barrier /Combescot 1971/, electron-phonon effects /Caroli et al. 1972/ and metal-semiconductor contacts /Combescot and Schreder 1973, 1974/. The hopping model is based on the nonequilibrium perturbation formalism of Keldysh /Keldysh 1965/ and does not rely on the transfer Hamiltonian approximation. Because of the simplicity of the basic concepts all the intermediate assumptions and simplifications can be easily and clearly controlled and discussed.

The purpose of the present article is to apply this hopping model of tunneling on MIM tunnel junctions containing magnetic impurities and to compare the obtained results with the two different afore-mentioned approaches.

In Sec. 2. this formalism is used to calculate the general expression for the self-energy and thereby the current up to the third order in perturbation theory. As the most simple case a one dimensional model with one magnetic impurity is treated. Using these self-energy expressions we considered first the case when the impurity is in the barrier. We studied also the dependence of the conductance on the position of the impuririty within the barrier. It was found that the hopping model approach is quite capable of including all contributions to the current obtained earlier from Zawadowski's and Appelbaum's

approaches, as well as to give the explicit expressions for Appelbaum's undetermined phenomenological parameters.

The case when the impurity is in one of the metal electrodes is considered in Sec. 3.

Our simple model is generalized to three dimensions and finite concentrations of impurities in Sec. 4. In the Appendix we discuss a square barrier potential for a continuous model.

We remark that the zero-bias anomalies are caused by Kondo-type impurity scattering /Anderson 1966, Appelbaum 1966, 1967/, which occurs when there is a magnetic moment on the d-level of the impurities /the contribution to the current due to the magnetic impurities shows logarithmic voltage dependence, which is a particular case of the Kondo effect/.

This means, that the zero-bias anomalies are particularly interesting for studying the Kondo effect - the energy and momentum dependence of the Kondo scattering amplitude. In the following publication we used the non--perturbative calculation for the scattering amplitude. There, we discussed in more detail the Kondo effect and made a comparison of the available experimental results and the theory.

2. Tunneling current in MIM contacts containing magnetic impurity.

2.1 Formulation

In this section we consider a simple one dimensional tunneling junction containing magnetic impurity at an arbitrary position. The CCNS formalism which has been developed at lenght in the four articles mentioned above is used throughout this work. We refer to Caroli et al. /1972/ and directly use some of their results.

For an MIM junction the system can be divided naturally into three parts.

Let α represent the last site of the left electrode, a the first site of the insulator, and similarly, b denotes the last site of the insulator and β the first site of the right electrode. Then, our Hamiltonian is

$$H = H_L + H_R + H_B + H_c + H_I \qquad /2,1/$$

where

$$H_L = \sum_{p,q} T_{pq} c_p^\dagger c_q \qquad p,q \leq \alpha \qquad /2.2/$$

$c_p^\dagger (c_p)$ is the electron creation /annihilation/ operator on site p. H_R and H_B are defined analogously with indices restricted to the right electrode and the barrier, respectively.

$$H_c = T\left(c_\alpha^+ c_a + c_a^+ c_\alpha\right) + T'\left(c_b^+ c_\beta + c_\beta^+ c_b\right) \qquad /2.3/$$

where T and T' are transfer matrix elements which describe the contacts between the electrodes and the barrier. We assumed that this H_c which couples different parts of the system, involves only nearest neighbour sites.

Assuming that a magnetic impurity with spin S is located on site i and interacts through a local exchange coupling with electrons on site i, this part of the Hamiltonian, using the Kondo type exchange coupling and Abrikosov's pseudo-fermion representation for the spin, can be written as follows

$$H_I = -J \sum_{\alpha\beta\gamma\delta} c_{i\alpha}^+ \vec{\sigma}_{\alpha\beta} c_{i\beta} a_\gamma^+ \vec{S}_{\gamma\delta} a_\delta \qquad /2.4/$$

$c_{i\alpha}^+$ and $c_{i\beta}$ are the electron operators taken at the impurity site, a_γ^+ and a_δ are the pseudo-fermion operators, $\vec{\sigma}_{\alpha\beta}$ and $\vec{S}_{\gamma\delta}$ are the Pauli matrix and the spin matrix, respectively.

The electronic current operator which describes the current across the barrier is given by

$$J = \frac{ie}{\hbar} T\left(c_\alpha^+ c_a - c_a^+ c_\alpha\right)$$

Introducing the correlation functions

$$G_{ij}^+(t,t') = i \left\langle c_j^+(t') c_i(t) \right\rangle$$

$$G_{ij}^-(t,t') = -i \left\langle c_i(t) c_j^+(t') \right\rangle \qquad /2.5/$$

which carry the information on the occupation of particle and hole states, the average current throught the junction may be written as

$$\langle J \rangle = \frac{e}{\hbar} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} T \left\{ G^{+}_{a\alpha}(\omega) - G^{+}_{\alpha a}(\omega) \right\} \qquad /2.6/$$

In calculating these correlation function in $\langle J \rangle$ we suppose that the junction was biased at $t = -\infty$ and H_c was switched on adiabatically.

In addition we shall need the Green's functions*

$$G^{+}_{ij}(t,t') = -i\,\Theta(t-t')\left\langle \left[c_i(t), c_j^{+}(t') \right]_{+} \right\rangle$$

$$G^{a}_{ij}(t,t') = i\,\Theta(t'-t)\left\langle \left[c_i(t), c_j^{+}(t') \right]_{+} \right\rangle \qquad /2.7/$$

which contain information on the distribution of available states, and causal and anticausal functions

$$G^{c}_{ij}(t,t') = -i \left\langle T\left(c_i(t) c_j^{+}(t') \right) \right\rangle$$

$$\tilde{G}^{c}_{ij}(t,t') = -i \left\langle \tilde{T}\left(c_i(t) c_j^{+}(t') \right) \right\rangle \qquad /2.8/$$

where T is usual time-ordering operator and $\tilde{T}$ orders the operators along the inverse branch of Keldysh's contour. This means that $\tilde{T}$ and T order the operators in just the opposite ways.

These functions are connected by the relations

$$G^{r} = G^{c} - G^{+} = -\tilde{G}^{c} + G^{-}$$

$$G^{a} = G^{c} - G^{-} = -\tilde{G}^{c} + G^{+} \qquad /2.9/$$

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* In the notation of Keldysh the definitions of G^{r} and G^{a} are permutted.

In the Keldysh formulation the Dyson eqations may be written as*

$$\begin{pmatrix} G^c & G^+ \\ G^- & \tilde{G}^c \end{pmatrix} = \begin{pmatrix} G_0^c & G_0^+ \\ G_0^- & \tilde{G}_0^c \end{pmatrix} + \begin{pmatrix} G_0^c & G_0^+ \\ G_0^- & \tilde{G}_0^c \end{pmatrix} \begin{pmatrix} \Sigma^c & -\Sigma^+ \\ -\Sigma^- & \tilde{\Sigma}^c \end{pmatrix} \begin{pmatrix} G^c & G^+ \\ G^- & \tilde{G}^c \end{pmatrix} \qquad /2.10/$$

Following Keldysh we make a linear canonical transformation of these matrices, for example the matrix $G = \begin{pmatrix} G^c & G^+ \\ G^- & \tilde{G}^c \end{pmatrix}$ becomes

$$G \to \frac{1 - i b_y}{\sqrt{2}} \begin{pmatrix} G^c & G^+ \\ G^- & \tilde{G}^c \end{pmatrix} \frac{1 + i b_y}{\sqrt{2}} = \begin{pmatrix} 0 & G^a \\ G^r & F \end{pmatrix} \qquad /2.11/$$

where b_y is the second of the three Pauli matrices

$$b_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad b_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad b_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$F = G^+ + G^- = G^c + \tilde{G}^c \qquad /2.12/$$

After that transformation equation /2,10/ reads as

$$\begin{pmatrix} 0 & G^a \\ G^r & F \end{pmatrix} = \begin{pmatrix} 0 & G_0^a \\ G_0^r & F_0 \end{pmatrix} + \begin{pmatrix} 0 & G_0^a \\ G_0^r & F_0 \end{pmatrix} \begin{pmatrix} \Omega & \Sigma^r \\ \Sigma^a & 0 \end{pmatrix} \begin{pmatrix} 0 & G^a \\ G^r & F \end{pmatrix} \qquad /2.13/$$

where

$$\Omega = \Sigma^+ + \Sigma^- = \Sigma^c + \tilde{\Sigma}^c \qquad /2.14/$$

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* Our definition of $\Sigma^{\pm}$ is opposite to that of Keldysh and corresponds to Caroli et al. /1972/.

Similar relations as /2.9/ hold also for the components of the self-energy matrix.

Dyson equations for $G^{r,a}$ and $G^{<}$ are then

$$G^{r} = G^{r}_{o} + G^{r}_{o}\Sigma^{r}G^{r}$$
$$G^{a} = G^{a}_{o} + G^{a}_{o}\Sigma^{a}G^{a} \qquad /2.15/$$

and

$$G^{<} = \left(1+G^{r}\Sigma^{r}\right)G^{<}_{o}\left(1+\Sigma^{a}G^{a}\right) + G^{r}\Sigma^{<}G^{a} \qquad /2.16/$$

We shall widely use these relations throughout this paper.

In calculating the current from /2.5/ we need $G^{<}$ which in turn will be calculated by treating H_c and H_I as perturbations. The complete propagator G is obtained from the zeroth order Green function g^{o} by including the exchange interaction $^{ex}\Sigma$ and the transfer matrix elements T and T'. Taking first the transfer matrix elements T and T' only and neglecting the exchange interaction, the renormalized Green function is denoted by G^{o}. This G^{o} is total propagator of the coupled non interacting system: T and T' are the elements of the self-energy $^{T}\Sigma$

$$^{T}\Sigma^{r}_{ij} = {}^{T}\Sigma^{a}_{ij} = T_{ij}, \quad {}^{T}\Sigma^{<}_{ij} = {}^{T}\Sigma^{>}_{ij} = 0$$

Taking now into account the interaction with the magnetic impurity, the self-energy due to the exchange interaction should be calculated by having G^{o} in the intermediate states. Let g denote the Green function where the self-energy corrections due to $^{ex}\Sigma$ are calculated with

renormalized G° functions. However there are no transfer matrix elements on the lines connecting the self-energy terms. This means that g propagator is defined with such diagrams in which the electron cannot cross the partition between different parts the system alone. However it is possible that the electron does that inside the self-energy $^{ex}\Sigma_{ij}$.

Since the interaction of conduction electrons with the localized spin is well localized /eq. (2.4)/, the self-energy $^{ex}\Sigma$ is local $^{ex}\Sigma_{ij} = {}^{ex}\Sigma_{ii}\delta_{ij}$ and is localized to site i where the magnetic impurity is situated. Then the electron propagator G°_{ij} which enters into the $^{ex}\Sigma_{ij}$ contains only an even number of elements T and even number of elements T'. This means that if the site p is on one side of the partition and the site q on another side, the electron propagator can cross the partition and connect the sites only via the transfer matrix elements T and T'. This is very important for the calculation, because if the self-energy were non-local connecting the sites on different sides of the dividing line, the theory would become very complicate. Futhermore it has to be emphasized that through the $^{ex}\Sigma$ the g propagator is a propagator for an out of equilibrium

system even if it is confined only to one electrode /for example $g^{\pm}_{dd}$ depends on the chemical potential μ_L of the left electrode and through $^{ex}\Sigma$ on the chemical potential μ_R of the right electrode./

Proceeding as in the paper by Caroli et al. /1972/ the current may be written as-

$$\langle J\rangle = \frac{e}{\hbar}\int_{-\infty}^{+\infty} T^2\left\{g^{+}_{dd}(\omega)G^{-}_{aa}(\omega) - g^{-}_{dd}(\omega)G^{+}_{aa}(\omega)\right\}\frac{d\omega}{2\pi} \quad /2.17/$$

Now it is possible to proceed on two different lines corresponding to two different regrouppings of the terms in $G^{\pm}_{aa}$. One is to expand $G^{\pm}_{aa}$ in powers of T, T' and g, which would lead to equation /13/ of Caroli et al. /1972/. In that equation the interaction still appers both in $g^{\pm}_{aa}$ and in $\Lambda\left(\Lambda = \frac{1}{1-T^2 g_{aa} g_{dd}}\right)$ /That expansion of $G^{\pm}_{aa}$ is of the form

$$G^{\pm}_{aa} = \Lambda^{r}\left(g^{\pm}_{aa} + g^{r}_{aa} T g^{\pm}_{dd} T g^{a}_{aa}\right)\Lambda^{a} \,/$$

In this section we will proceed on another line. That is just equation /17/ of Caroli et al. /1972/

$$G^{\pm}_{aa} = G^{r}_{aa} T g^{\pm}_{dd} T G^{a}_{aa} + G^{r}_{ab} T' g^{\pm}_{\beta\beta} T' G^{a}_{ba} + G^{r}_{ai}\,{}^{ex}\Sigma^{\pm}_{ij} G^{a}_{ja} \quad /2.18/$$

where i, j are any sites in the insulator. Its advantage is that it will enable us to see better the origin of different contributions to the current and compare these contributions with the corresponding

expression in the earlier theories of tunneling junctions with magnetic impurities, This expression for $G^{\pm}_{aa}$ was derived ba using the Dyson equation for $G^{\pm}$ /2.16/ and the fact that the energy integration in /2.17/ is confined to the region between μ_L and μ_R That range of the energy variable ω falls into the forbidden band of the insulator and so $g^{\pm}_{aa}=0$. This means that the requirement that $G^{\pm}_{ij}$ /i,j are two points in the insulator/ be different from zero, necessarily involves the trip of the electron into electrodes.

2.2 The magnetic impurity in the barrier.

2.2.1 The $\Sigma^{\pm}$ contribution to the dynamical current.

Let us consider now the case when the magnetic impurity is in the barrier and suppose that the interaction of conduction electrons with the localized spin is of the form /2.4/.

From equation /2.18/ and /2.17/ it follows that only the second and the third term in /2.17/ give non vanishing contribution to the current.

First, we shall discuss the contribution coming form the third term of equation /2.18/:

$$\langle \delta J_{\Sigma^{\pm}} \rangle = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} T^2 G^r_{ai}(\omega) G^a_{ia}(\omega) \left\{ g^+_{\mu\mu}(\omega) \Sigma^-_{ii}(\omega) - g^-_{\mu\mu}(\omega) \Sigma^+_{ii}(\omega) \right\} \quad /2.19/$$

In this paper we treat the exchange interaction in perturbation theory up to third order in J. /In a subsequent publication we shall use a non-perturbative expression for the scattering amplitude/. Since $^{ex}\Sigma$ appears explicitly in equation /2.19/ we may replace the factors G^r_{ai} and G^a_{ia} by G^{r0}_{ai} and G^{a0}_{ia} which are zeroth order with respect to $^{ex}\Sigma_{ii}$ but contain the transfer matrix elements T and T' / G^0 is obtained by inserting T and T' on the g^0 /. In the following text the notation $^{ex}\Sigma$ will be replaced by Σ /.

Since the impurity is supposed to lie in the barrier $g_{\mu\mu}$ and $g_{\beta\beta}$ become the free propagators $g^0_{\mu\mu}$ and $g^0_{\beta\beta}$/without T and T' and without self-energy effects/.

Let us calculate the second and third order contributions to the self-energy using Abrikosov's fictitious fermion operator technique and the nonequilibrium perturbation formalism of Keldysh. /It is possible to use Keldysh's formalism also for equilibrium problems and to get the same results in perturbation theory at finite temperature for Kondo scattering with Keldysh's real time Green functions as with complex time variables with thermodynamic Green functions./

The second and the third order contributions to the self-energy are represented in Figs. 1. and 2. a-b.

Making an expansion of the one particle electron Green function /for example G^c / in powers of H_c and H_I and using eq. /2.10/ we get / H_c is treated to all orders/

$$\Sigma^{(2)}(\omega) = J^2 S(S+1) e^{\beta\lambda} \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} \begin{pmatrix} G^{co}_{(\omega+\omega_1-\omega_2)} q^c(\omega_1) q^c(\omega_2) & -G^{+o}_{(\omega+\omega_1-\omega_2)} \bar{q}(\omega_1) q^+(\omega_2) \\ -G^{-o}_{(\omega+\omega_1-\omega_2)} q^+(\omega_1) \bar{q}(\omega_2) & \tilde{G}^{co}_{(\omega+\omega_1-\omega_2)} \tilde{q}^c(\omega_1) \tilde{q}^c(\omega_2) \end{pmatrix}$$

/2.20/

For the sake of simplicity we dropped the site indices from the self-energy and from the function G^o. /All G^o and Σ are taken at the position of impurity/. The fictitious fermion Green functions are given as

$$q^c(\omega) = \frac{1-f(\lambda)}{\omega-\lambda+i\delta} + \frac{f(\lambda)}{\omega-\lambda-i\delta}$$

$$\tilde{q}^c(\omega) = -\left(\frac{1-f(\lambda)}{\omega-\lambda-i\delta} + \frac{f(\lambda)}{\omega-\lambda+i\delta} \right)$$

$$q^r(\omega) = \frac{1}{\omega-\lambda+i\delta} \; ; \; q^a(\omega) = \frac{1}{\omega-\lambda-i\delta}$$

$$q^+(\omega) = 2\pi i \delta(\omega-\lambda) f(\lambda) \; ; \; q^-(\omega) = -2\pi i \delta(\omega-\lambda)(1-f(\lambda))$$

/2.21/

where λ is the energy of the pseudo-fermion, and in the final results $\lambda \to \infty$.

The same result can be achieved in another way which we sketch here. From Keldysh's paper we know that the Feynman rules remain intact in his technique, we only have to associate with every line not a single Green functions but a Green function matrix and with every point a vertex matrix, the form of which will depend on the type of interaction /two-particle, electron-phonon, etc./ . In addition we have to take into account the factor -1 for points on the inversed branch of the contour C . This means that in the present case we have to associate with each solid line a matrix $G^0 = \begin{pmatrix} G^{c0} & G^{+0} \\ G^{-0} & \tilde{G}^{c0} \end{pmatrix}$ and with each dotted line a matrix $D = \begin{pmatrix} D^c & D^+ \\ D^- & \tilde{D}^c \end{pmatrix}$ Our vertex matrix has to have four indices /because the vertex has four legs/ and every index may take only two values: 1 and 2 /these values correspond to the points on direct and inversed branch of the contour C , respectively/. In addition, this vertex matrix has to take into account the factor -1 for points on the inversed branch of C .

The elementary vertex matrix which satisfies the necessary conditions is of the form

$$\gamma^{kl}_{\alpha\beta} = J\,\delta_{\alpha\beta}(\sigma_z)_{\beta k}\,\delta_{kl} \qquad /2.22/$$

where the superscripts in γ correspond to pseudo-fermion lines and the subscripts to electron lines, σ_z is the

third Pauli matrix. For $k = 2$ this vertex matrix is negative and that takes into account the above mentioned factor -1.

So, to find the expression corresponding to a given diagram we need the usual Feynman rules extended with the prescription to use Green function and vertex matrices.

The usual Feynman rules for our diagrams are given in Abrikosov's paper /Abrikosov 1965/ and we shall write them again with only a slight modification /since we are dealing in the coordinate space/.

a./ Each dotted line has its own frequency, and one should integrate over these frequencies. The electron frequencies are determined by conservation rules.

b./ In calculating $\sum_{\alpha\alpha'}$ /α, α' are the spin indices of external electron lines/ one has to take the α, α' component of the product of electron spin operators in the order of their position on the electron line.

c./ All the dotted lines corresponding to one impurity atom form together a closed loop. A trace is taken of the product of the impurity spin operators in the order of their position along the loop.

Using these rules and Keldysh's prescription we get

$$\Sigma^{(2)}_{\alpha\beta}(\omega) = J^2 S(S+1) e^{\delta\lambda} \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} \gamma^{kl}_{\alpha\alpha'} g_{lm}(\omega_2) G^{0}_{\alpha'\beta'}(\omega+\omega_1-\omega_2) \gamma^{ms}_{\beta'\beta} g_{sk}(\omega_1) \qquad /2.23/$$

/the indices in this expression refer to matrix elements, the summation over the spin indices being already performed/

Using /2.22/ it is easy to see that equation /2.2o/ and /2.23/ are in fact equivalent. One can see from equation /2.2o/ that inside a self-energy correction the electron may cross the partition between different parts of the system, because in the intermediate states the function G^0 contain the transfer matrix elements T and T'. But, since the self-energy is local G^0 should contain even number of T and even number of T' vertices. From /2.2o/ and /2.21/ we get

$$\Sigma^{(2)\pm} = J^2 S(S+1) G^{\pm 0}(\omega) \qquad /2.24/$$

This result for Σ is independent of whether the impurity is in the electrodes or in the barrier.

The only difference will be in the form of G^0 functions.

If the impurity is in the barrier we have

$$G^{\pm 0}_{ii}(\omega) = T^2 \left| G^{r0}_{ia}(\omega) \right|^2 g^{\pm 0}_{\alpha\alpha}(\omega) + T'^2 \left| G^{r0}_{ib}(\omega) \right|^2 g^{\pm 0}_{\beta\beta}(\omega) \qquad /2.25/$$

/ i denotes the position of the impurity in the barrier/ The current up to second order in $\mathcal{J}$ may be cast into the form

$$\langle \delta J^{(2)}_{\Sigma^{\pm}} \rangle = \frac{4\pi e}{\hbar} \mathcal{J}^2 S(S+1) \int d\omega\, T^2 T'^2 \left| G^{r0}_{ai}(\omega) \right|^2 \left| G^{r0}_{ib}(\omega) \right|^2 \cdot$$

$$\cdot \rho^0_\alpha(\omega)\, \rho^0_\beta(\omega) \left(f_L(\omega) - f_R(\omega) \right) \qquad /2.26/$$

/From now on we write the expressions for the current and the conductance for both spin directions of the electron./

In deriving equation /2.26/ we used the fact that the propagators g^0 do not contain a crossing of the partition, so for them the two electrodes are separately in thermodynamic equilibrium with chemical potentials μ_L and μ_R. Then we can define densities of states at sites α and β by the relations

$$\rho^0_\alpha = -\frac{1}{\pi} \mathrm{Im}\, g^{r0}_{\alpha\alpha}$$

$$\rho^0_\beta = -\frac{1}{\pi} \mathrm{Im}\, g^{r0}_{\beta\beta} \qquad /2.27/$$

The spectral densities $g^{\pm 0}$ are related to the density of states as follows:

$$g^{+0}_{\alpha\alpha}(\omega) = 2\pi i\, \rho^0_\alpha(\omega) f_L(\omega) \qquad g^{+0}_{\beta\beta}(\omega) = 2\pi i\, \rho^0_\beta(\omega) f_R(\omega)$$

$$g^{-0}_{\alpha\alpha}(\omega) = -2\pi i\, \rho^0_\alpha(\omega) (1 - f_L(\omega)) \qquad g^{-0}_{\beta\beta}(\omega) = -2\pi i\, \rho^0_\beta(\omega) (1 - f_R(\omega)) \qquad /2.28/$$

where f_L and f_R are the Fermi factors on the left and right hand side of the barrier, respectively. This contribution to the current corresponds to an elastic process. /We note that in the case of an electron-phonon interaction the contribution to the current comming from $\Sigma^{\pm}$ corresponds to an inelastic process, in which a real phonon is emitted during the tunneling event./

The reason of this difference is that for a single magnetic impurity without external magnetic field no energy is required to change the direction of the spin.

The factor $G^{ro}_{ai} G^{ro}_{ib} G^{ao}_{bi} G^{ao}_{ia}$ describes the following physical situation: the electron goes from site a to site i with energy ω, interacts elastically with the magnetic impurity, and then goes to site b with the same energy; the return trip is just the reversed one because the exchange interaction is well localized.

The expression $U^{\uparrow} = TT' G^{ro}_{ai} G^{ro}_{ib}$ is the effective coupling between the two electrodes. It is energy dependent and very small. The square of that expression is essentially the "transparency" of the barrier.

The two electrodes enter symmetrically in equation /2.26/ for the current, as it should be.

If we want to consider in some detail the frequency dependence of the various factors in equation /2.26/, then we could repeat the discussion by Caroli et al. /1972/. Exprimentally zero bias anomalies appear in the range of lo-loo mV around V=0 either as a conductance or a giant resistance peak. These energies are much smaller than both the barrier height and the Fermi energy for ordinary MIM junctions. We may therefore neglect the frequence dependence of ρ^0_α , ρ^0_β and the effective coupling matrix element for biases of interest for these anomalies. The change in the dynamical conductance $\delta G^{(2)}_{\Sigma^\pm}$ due to the third term of /2.18/ is given by

$$\delta G^{(2)}_{\Sigma^\pm} = \frac{d\langle \delta J^{(2)}_{\Sigma^\pm} \rangle}{dV} = \frac{4\pi e^2}{\hbar} \int S(S+1) T^2 T'^2 |G^{r0}_{ai}|^2 |G^{r0}_{ib}|^2 \rho^0_\alpha \rho^0_\beta \qquad /2.29/$$

where $-\frac{\partial f(\varepsilon-\omega)}{\partial \varepsilon}$ is approximated by $\delta(\varepsilon-\omega)$ and $eV = \mu_L - \mu_R$ Equation /2.29/ always corresponds to an increase of the conductance.

If we compare that expression for the second order conductance with the corresponding one in the papers by Appelbaum /1967/ or Appelbaum et al. /1967/,

we see easily that instead of their undetermined parameter T_l^2 we have an explicit expression for the effective coupling matrix element. /Knowing the wave functions of electrons in the electrodes and the insulator, and working in the continuous representation as described in the Appendix, we can calculate directly this effective coupling matrix element/.

As to the dependence of the conductance on the position of the impurity in the barrier it can be shown that the expression $G^{ro}_{ai} G^{to}_{ib}$ is roughly independent of l /this is because G^{ro} is an exponentially decreasing function of the positions in the barrier/. It follows that the tunneling efficiency of an impurity in second order is roughly independent of its location in the insulator.

The expression for the third order self-energy corrections corresponding to diagram /2a/ from Fig. 2. may be obtained from the afore-mentioned diagram rules.

$$\Sigma^{(3a)}_{\alpha\beta}(\omega) = i J^3 S(S+1) e^{\beta\lambda} \int \frac{d\omega_1 d\omega_2 d\omega_3}{(2\pi)^3} \gamma^{kl}_{\alpha\alpha'} \varrho_{em}(\omega_1) G^0_{\alpha'\beta'}(\omega+\omega_3-\omega_1) \cdot$$

$$\cdot \gamma^{ms}_{\beta'\delta'} \varrho_{sn}(\omega_2) G^0_{\delta'\kappa}(\omega+\omega_3-\omega_2) \gamma^{nr}_{\kappa\beta} \varrho_{rk}(\omega_3) \qquad /2.30/$$

The indices refer to the matrix elements./

Explicitly it is

$$\Sigma^{(3a)}(\omega) = i J^3 S(S+1) e^{\beta\lambda} \int \frac{d\omega_1 d\omega_2 d\omega_3}{(2\pi)^3} \cdot$$

$$\Big(G^{co}(\omega+\omega_3-\omega_1) G^{co}(\omega+\omega_3-\omega_2) q^c(\omega_1) q^c(\omega_2) q^c(\omega_3) - G^{+o} G^{-o} q^+ q^- q^c \quad - G^{co+o} q^c q^+ q^- + G^{+o\tilde{}co} G \, q^+ \tilde{q}^c q^-$$

$$- G^{-o} G^{co} q^- q^c q^+ + \tilde{G}^{co} G^{-o} \tilde{q}^c q^- q^+ \quad \tilde{G}^{co\tilde{}co} \tilde{q}^c \tilde{q}^c \tilde{q}^c - G^{-o} G^{+o} q^- q^+ \tilde{q}^c \Big)$$

/2.31/

In the same way as for $\Sigma^{(2)}$ we did not write the site indices.

The self energy can be calculated very easily from /2.31/ because $q^{\pm}(\omega)$ are proportional to $\delta(\omega-\lambda)$

$$\Sigma^{\pm(3a)}(\omega) = i J^3 S(S+1) G^{\pm o}(\omega) \left[2P \int \frac{d\varepsilon}{2\pi} \frac{G^{+o}(\varepsilon)}{\omega-\varepsilon} - 2i \, \mathrm{Re}\, G^{\tau o}(\omega) \right]$$

/2.32/

/ P denotes the principal value of the integral.#

The expression in the bracket of /2.32/ came from

$$\int \frac{d\omega_1}{2\pi i}\left(\frac{G^{co}(\omega+\lambda-\omega_1)}{\omega_1-\lambda+i\delta}+\frac{\tilde{G}^{co}(\omega+\lambda-\omega_1)}{\omega_1-\lambda-i\delta}\right)$$

by using /2.9/, the analytical properties of the function $G^{r,a}$ and the dispersion relations for $G^{r,a}$. In this calculation we did not specify the position of the impurity and the same expressions are valid for the case when the impurity is in the electrodes. The only difference is in the form of the G^{o} functions. Substituting /2.32/ with $G^{\pm o}$ given by /2.25/ into /2.19/ we see that as before only the second part of /2.25/ will contribute to the current. We obtain

$$\langle \delta J^{(3a)}_{\Sigma^t} \rangle = \frac{4\pi e}{\hbar} i S(S+1) J^3 \int d\omega\, T^2 T'^2 \left|G^{ro}_{ai}(\omega)\right|^2 \left|G^{ro}_{ib}(\omega)\right|^2 \rho^{o}_{\alpha}(\omega)\rho^{o}_{\beta}(\omega)$$
$$\left(f_L(\omega)-f_R(\omega)\right)\left[2P\int \frac{d\varepsilon}{2\pi i}\frac{G^{+o}_{ii}(\varepsilon)}{\omega-\varepsilon}-2i\,\mathrm{Re}\,G^{+o}_{ii}(\omega)\right]. \qquad /2.33/$$

Because of the discontiunity of $G^{\pm o}$ at the Fermi level the factor $P\int \frac{d\varepsilon}{2\pi i}\frac{G^{+o}(\varepsilon)}{\omega-\varepsilon}$ contains the dominant voltage and temperature dependence and accounts for the zero bias conductance anomalies.

Now, to perform the integration over ε in /2.33/ a cut-off parameter E_o should be introduced. At this point there arises a question about the range of E^o and related with it the physical origin of that cut-off parameter. There are two sources which may de-

termine the cut-off energy: the momentum dependence of the exchange coupling constant $J_{kk'}$/which was neglected in the form of the exchange interaction that we used/ or the energy dependence of the bulk electron density of states. The problem of the momentum dependence of the exchange coupling constant is carefully discussed by Mezei and Zawadowski /1971 a,b/ . They introduced two parameters Δ and D . Δ is width of the energy region where $J_{kk'}$ changes and a cut-off energy D reflects the band structure /the conduction electron bandwidth/. In terms of these parameters we shall make qualitative discussion about the range of our cut-off energy E_0 .

Let us suppose for the moment that we start from the beginning with momentum dependent exchange coupling constant $J_{kk'}$. / That can be taken into account following the approach of Zawadowski and Mezei /1971 a,b//

For one impurity which lies well inside the insulator, the interaction of conduction electrons with the impurity spin is then very well localized. Because of that localization the matrix elements are non-vanishing even for big momentum transfer and therefore there is no cut-off coming from $J_{kk'}$. But, on the other hand

we know that our $G^{\pm 0}$ is proportional to the density of states in the electrodes. So, the best what we can do for the case of one impurity deeply inside the barrier, is to perform really the integration in eq. /2.33/ by taking the cut-off energy E_0 to be D, and to suppose that in that energy interval J and ϱ^0 are contants. If the impurity lies inside the metal, because of the overlapping of the neighbouring Wannier functions $J_{kk'}$ will change essentially in the region Δ which is much smaller than D. This means that in the case of one impurity in the metal we would need to take the cut-off energy E_0 to be determined by Δ, and J and ϱ^0 to be constant in that region.

Since in our calculation we did not take into account the momentum dependence of the exchange coupling constant we shall simply restrict the principal value integral in eq. /2.33/ to an energy region of width $2E_0$ centered at the Fermi energy ε_F /all energies are measured from ε_F/. E_0 has to be taken as $\Delta \ll \varepsilon_F$ for an impurity in the metal and as $D \simeq \varepsilon_F$ for an impurity in the barrier. In both cases, if we are interested only in a simple logarithmic term and want to make comparison with previous theories, we have to neglect the energy dependence of all factors in G^{+0} /in the range of $2E_0$/

except the energy dependence of the Fermi function. /In fact that assumption is not so drastic since these factors, the energy dependence of which have been neglected, are not singular anywhere in the range $2E_0$ and moreover they are slowly varying function of ε in that range/

Then, this principal value integral gives logarithmic dependence. We may drop other terms which do not contain $f(\varepsilon)$ such as $\mathrm{Re}\, G^{r0}_{ii}$ in eq. /2.33/ since these terms are small compared to terms with $f(\varepsilon)$ and they cannot give logarithmic dependence.

Taking the derivative with respect to the voltage and neglecting the frequency dependence of $\rho^0_\alpha, \rho^0_\beta$ and U^r in the integration over ω /that is quite justified since the range of ω is between μ_L and μ_R which is very small/ we may write the change in the dynamical conductance due to $\Sigma^{\pm(3)}$ in the form

$$\delta G^{(3)}_{\Sigma^\pm} = \frac{16\pi e^2}{h} S(S+1) J^3 |U^r|^2 \rho^0_\alpha \rho^0_\beta \left(T^2 |G^{r0}_{ia}|^2 \rho^0_\alpha F(eV) + T'^2 |G^{r0}_{ib}|^2 \rho^0_\beta F(eV) \right) \qquad /2.34/$$

where

$$F(eV,T) = -\int_{-\infty}^{+\infty} d\varepsilon' \frac{\partial f(\varepsilon'-eV)}{\partial \varepsilon'} P\int_{-E_0}^{E_0} d\varepsilon \frac{f(\varepsilon)}{\varepsilon-\varepsilon'} \,. \qquad /2.34\ a/$$

An interpolative approximation for $F(eV,T)$ is

$$F(eV,T) \simeq -\ln\left(\frac{e|V|+nkT}{E_0}\right) \qquad \text{where } n = 1{,}35$$

/Appelbaum 1967, Shen and Rowell 1968/

/ Recently Wyatt and Wallis /1974/ have discussed this approximation for $F(eV,T)$ and performed numerical integration of eq. /2.34 a/ for different temperatures and showed that the interpolation function is most inadequate when $eV \simeq 3kT$. /

We find again that the contribution to the dynamical conductance coming from $\Sigma^{\pm}$ corresponds to the Appelbaum expression /Appelbaum 1967/ and gives a zero bias conductance peak for $J<0$ i.e. the antiferromagnetic coupling. Note again that we have an explicit expression for his phenomenological parameters.

Let us now consider the dependence of that contribution to the conductance on the position of the megnetic impurity in the barrier. As was mentioned before $|U|^2$ is relatively independent of i - the position of impurity -, but the factors in the bracket of eq. /2.33/ strongly depend on it. If the impurities are only on one

side of the barrier, let us say on the left side near the barrier metal interface, than $T^2|G^{ro}_{ia}|^2 \simeq T^2|G^{ro}_{aa}|^2$. When the impurities are deeply in the barrier the conductance drops off rapidly with distance from the barrier--metal interface /$|G^{ro}_{ia}|^2 \propto e^{-KL}$ for an impurity in the center of the barrier/.

After having discussed the contribution to the current from the $\Sigma^{\pm}$ term in detail we now return to equations /2.17/ and /2.18/.

2.2.2 The $\Sigma^{r,a}$ contribution to the dynamical current

The second term in /2.16/ gives the following contribution to the current /the first term in /2.18/ does not give any contribution/

$$\langle \delta J \rangle = \frac{4\pi e}{h}\int d\omega\, T^2 T'^2 |G^{r}_{ab}(\omega)|^2 \rho^{o}_{a}(\omega)\rho^{o}_{b}(\omega)\left(f_L(\omega) - f_R(\omega)\right) \qquad /2.35/$$

Since the impurity is in the barrier we have replaced $g^{\pm}_{\alpha\alpha}$ ($g^{\pm}_{\beta\beta}$) by their zeroth order values $g^{\pm o}_{\alpha\alpha}$ ($g^{\pm o}_{\beta\beta}$) and used relations /2.27/ and /2.28/ in deriving /2.35/.

Making an expansion of $|G^r_{ab}|^2$ to third order in the electron-pseudofermion interaction we get

$$|G^r_{ab}|^2 \simeq \left\{ G^{r0}_{ai} G^{r0}_{ib} G^{a0}_{ba} \left(\Sigma^{r(2)}_{ii} + \Sigma^{r(3)}_{ii} \right) + G^{r0}_{ab} G^{a0}_{bi} G^{a0}_{ia} \left(\Sigma^{a(2)}_{ii} + \Sigma^{a(3)}_{ii} \right) \right\} \qquad /2.36/$$

In order to calculate the second order contribution to /2.35/ and /2.36/ we need $\Sigma^{r(2)}_{ii}(\omega)$ to second order in J. Knowing that $\Sigma^r = \Sigma^c - \Sigma^+$, using the relations /2.2o/ or /2.23/ and performing the integration over ω_1 and ω_2 in Σ^c /for that integration we only have to use the analytical properties of G^o and relations /2.21/ we get

$$\Sigma^{r(2)}_{ii}(\omega) = J^2 S(S+1) G^{r0}_{ii}(\omega) \qquad /2.37/$$

Another way to achieve the same result is to use Keldysh's linear canonical transformation /2.11/ after which the matrix G^o transforms to $G^{To} = \begin{pmatrix} 0 & G^{a0} \\ G^{r0} & F^o \end{pmatrix}$, Σ transforms to $\Sigma^T = \begin{pmatrix} \Omega & \Sigma^r \\ \Sigma^a & 0 \end{pmatrix}$ and the vertex $\gamma^{kl}_{\alpha\beta}$ transforms to

$$\gamma^{T_{11}}_{\alpha\beta} = \gamma^{T_{22}}_{\alpha\beta} = \frac{1}{2}(\delta_x)_{\alpha\beta}$$

$$\gamma^{T_{12}}_{\alpha\beta} = \gamma^{T_{21}}_{\alpha\beta} = \frac{1}{2}\delta_{\alpha\beta} \qquad /2.38/$$

We may write Σ^T as

$$\Sigma^T_{\alpha\beta} = e^{\beta\lambda} J^2 S(S+1) \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} \gamma^{Tkl}_{\alpha\alpha'} \varrho^T_{lm}(\omega_2) G^{oT}_{\alpha'\beta'}(\omega+\omega_1-\omega_2) \gamma^{Tms}_{\beta'\beta} \varrho^T_{sk}(\omega_1) \qquad /2.39/$$

/T means the transformed matrix./

Sometimes it is easier to make integration, in the transformed form using the analytical properties of $G^{r(a)o}$

The second order contribution to the dynamical conductance may be written as

$$\delta G^{(2)} = \frac{4\pi e^2}{k} J^2 S(S+1) \rho^o_\alpha \rho^o_\beta T^2 T'^2 \left\{ G^{ro}_{ai} G^{ro}_{ib} G^{ao}_{ba} G^{ro}_{ii} + G^{ro}_{ab} G^{ao}_{bi} G^{ao}_{ia} G^{ao}_{ii} \right\} \qquad /2.40/$$

Using relations

$$G^{ro}_{ai} G^{ro}_{ib} = G^{ro}_{ab} G^{ro}_{ii} \qquad /2.41/$$

we get

$$\delta G^{(2)} = \frac{4\pi e^2}{k} J^2 S(S+1) \rho^o_\alpha \rho^o_\beta T^2 T'^2 |G^{ro}_{ab}|^2 \left((G^{ro}_{ii})^2 + (G^{ao}_{ii})^2 \right) \qquad /2.42/$$

We note that the expression in front of the bracket is just the conductance for the pure contact /without impurities/

and the expression in the bracket is therefore the change due to impurities.

The total second order contribution to the conductance is given by

$$G^{(2)}(V) = \frac{4\pi e^2}{\hbar} \int^2 S(S+1) T^2 T'^2 |G^{r0}_{ab}|^2 \left\{ |G^{r0}_{ii}|^2 + \left[(G^{r0}_{ii})^2 + (G^{a0}_{ii})^2 \right] \right\} \rho^0_a \rho^0_b \qquad /2.43/$$

Where the first term $|G^{r0}_{ii}|^2$ is due to $\Sigma^{\pm}$.

Let us discuss now the dependence of $G^{(2)}(V)$ on the impurity position in the barrier. In a recent work Appelbaum, and Brinkman /1970/ using a simple model for MIM contacts pointed out that if the impurity is found in the first atomic layer of the barrier, the interaction depresses the current. On the other hand the impurities deeper inside the barrier enhance the current. It is easy to get the same result from our calculations if we go to the continuous representation of this discrete model /see Caroli et al. /1971//. Moreover, we are able to figure out where these two different contributions come from and how far from the barrier-metal interface is the factor which gives a depression of tunneling current still effective. The different expressions for the propagators in the continuous limit for the simple square barrier model are given in the Appendix. To simplify the calculation we shall divide our system into two halves only and locate the partition well inside the insulator

/we now consider the case when impurities are on the left side only near the contact between the left electrode and the insulator/. Then, in the discrete representation we may write.

$$G^{\tau 0}_{ii} = g^{\tau 0}_{ii} + \frac{T^2 \left(g^{\tau 0}_{i\gamma}\right)^2 g^{\tau 0}_{cc}}{1 - T^2 g^{\tau 0}_{\gamma\gamma} g^{\tau 0}_{cc}}$$

/2.44/

γ and c denote the sites on either side of the new partition, g^0 denotes the free one sided propagator. The propagator g^0 for the left-electrode+the half of the barrier is easily expressed in terms of the corresponding g^0 for the metal M and insulator I alone simple algebra gives

$$g^{\tau 0}_{ii} = g^0_{ii} + \frac{T^2 g^0_{ia} g^0_{ai} g^{\tau 0}_{\alpha\alpha}}{1 - T^2 g^0_{aa} g^{\tau 0}_{\alpha\alpha}}$$

/2.45/

Let us first see what happens when the impurity is at the contact between the left electrode and the insulator. Then, we may retain in /2.44/ $g^{\tau 0}_{ii}$ only. In the continuous representation this becomes

$$g^{\tau(a)0}\left(\tfrac{l}{2}, \tfrac{l}{2}\right) = -\frac{2m}{\hbar^2} \frac{1}{K \mp iq}$$

/2.46/

/where $\hbar q = (2m\omega)^{\frac{1}{2}}$; $\hbar K = (2m(V_B - \omega))^{\frac{1}{2}}$, l is the interatomic distance.

The signs - and + in the denominator of /2.46/ refer to retarded and advanced $\mathcal{G}^0$ functions respectively./

The first factor in the wavy bracket of the equation /2.43/ /which is the $\Sigma^{\pm}$ contribution/ becomes

$$|\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})|^2 = \left(\mathrm{Re}\,\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 + \left(\mathrm{Im}\,\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 =$$

$$= \left(-\frac{2m}{\hbar^2}\right)^2 \frac{K^2}{(K^2+q^2)^2} + \left(-\frac{2m}{\hbar^2}\right)^2 \frac{q^2}{(K^2+q^2)^2} = \left(-\frac{2m}{\hbar^2}\right)^2 \frac{1}{K^2+q^2} \qquad /2.47/$$

This factor always enhances the current.

On the other hand

$$\left(\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 + \left(\mathcal{G}^{a0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 = 2\left[\left(\mathrm{Re}\,\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 - \left(\mathrm{Im}\,\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2\right] =$$

$$= \left(-\frac{2m}{\hbar^2}\right)^2 \frac{2(K^2-q^2)}{(K^2+q^2)^2} \qquad /2.48/$$

Since, usually $q > K$, this factor is negative and reduces the current.

The sum of the equations /2.47/ and /2.48/

$$|\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})|^2 + \left(\mathcal{G}^{r0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 + \left(\mathcal{G}^{a0}(\tfrac{1}{2},\tfrac{1}{2})\right)^2 = \left(-\frac{2m}{\hbar^2}\right)^2 \frac{3K^2-q^2}{(K^2+q^2)^2}$$

can be positive or negative, depending on the ratio $\frac{K_F}{q_F}$.

If $\frac{K_F}{q_F} < \frac{1}{\sqrt{3}}$ the absolute value of the negative term is larger than positive one, and therefore the sum is negative

The opposite case is for $\frac{K_F}{q_F} > \frac{1}{\sqrt{3}}$

If the impurity is deeply in the barrier, then

$$G^{ro}_{ii} = G^{ao}_{ii} \simeq g^{o}_{ii}; \quad |G^{ro}_{ii}|^2 \simeq (g^{o}_{ii})^2, \quad (G^{ro}_{ii})^2 + (G^{ao}_{ii})^2 \simeq 2(g^{o}_{ii})^2$$

Both terms are now positive for all values of the ratio $\frac{K_F}{q_r}$ / g^{o}_{ii} in these expressions denotes only the real part of the propagator since there is no density of states in the barrier in the energy range of interest. Then $g^{ro}_{ii} = g^{ao}_{ii} = g^{co}_{ii} = g^{o}_{ii}$ /

The condititon which gives the distance of the impurity from the electrode-barrier contact, so that the negative term is in absolute value just equal to the positive term, may be written as follows

$$|\varphi^{ro}_{ii}|^2 = -\left[(\varphi^{ro}_{ii})^2 + (\varphi^{ao}_{ii})^2\right] \qquad /2.49/$$

or in the continuous representation,

$$\left|\varphi^{ro}\left(\tfrac{L}{2} - nl, \tfrac{L}{2} - nl\right)^2\right|^2 = -\left[\left(\varphi^{ro}\left(\tfrac{L}{2} - nl, \tfrac{L}{2} - nl\right)\right)^2 + \left(\varphi^{ao}\left(\tfrac{L}{2} - nl, \tfrac{L}{2} - nl\right)\right)^2\right].$$

n is the number of the interatomic distances measured from the metal-barrier interface.

This yields

$$\frac{qK}{\sqrt{3}} = \left(K^2 \operatorname{ch} Knl + q^2 \operatorname{sh} Knl\right) e^{Knl} \qquad /2.50/$$

or

$$n_o l = \frac{1}{2K} \ln \frac{q^2 - K^2 + \frac{2qK}{\sqrt{3}}}{K^2 + q^2} \qquad /2.51/$$

The curve $n_0(x = \frac{k_F}{q_F})$ defines the dividing line between the region in which the sum $|G^{r0}_{ii}|^2 + (G^{r0}_{ii})^2 + (G^{a0}_{ii})^2$ is positive and the region in which this sum is negative. This negative sum is in accordance with the Sólyom-Zawadowski theory.
They attributed the depression of the tunneling current to the corresponding depression of the electronic density of states in the neighbourhood of the impurities.

Going on to the third order contribution to /2.35/ we have to calculate $\Sigma^{r(3)}(\omega)$. $\Sigma^{+(3)}(\omega)$ is already known, $\Sigma^{c(3)}(\omega)$ can be calculated easily from /2.31/. So using the relation $\Sigma^r = \Sigma^c - \Sigma^+$ we obtain

$$\Sigma^{r(3)}(\omega) = 2\gamma^3 S(S+1)\left\{2i G^{r0}(\omega)\int \frac{d\varepsilon}{2\pi} \frac{G^{+0}(\varepsilon)}{\omega-\varepsilon} - 2i\int \frac{d\varepsilon}{2\pi} \frac{\mathrm{Re}G^{r0}(\varepsilon) G^{+0}(\varepsilon)}{\omega-\varepsilon} + \right.$$

$$\left. + (G^{r0}(\omega))^2 + i G^{+0}(\omega)\,\mathrm{Im}\, G^{r0}(\omega)\right\}$$

/2.52/

The same exspression may be obtained by making the integration in the transformed Σ^T matrix which is given by expression /2.30/, where all matrices are replaced by the transformed ones.

The terms which contain the dominant voltage

and temperature dependence are

$$4i\mathcal{J}^3 S(S+1)\left[G^{r0}_{(\omega)}\int\frac{d\varepsilon}{2\tilde{\pi}}\frac{G^{+0}(\varepsilon)}{\omega-\varepsilon}-\int\frac{d\varepsilon}{2\tilde{\pi}}\frac{\mathrm{Re}\,G^{r0}_{(\varepsilon)}G^{+0}_{(\varepsilon)}}{\omega-\varepsilon}\right]$$

Introducing the cut-off energy E_0 and using the same arguments as in derivation of the $\Sigma^{\pm}$ contribution we get

$$\langle\delta\mathcal{J}^{(3)}\rangle=-\frac{32\tilde{\pi}e}{\hbar}i\mathcal{J}^3S(S+1)\int d\omega\rho^0_\alpha(\omega)\rho^0_\beta(\omega)\,T^2T'^2\,|G^{r0}_{ab}(\omega)|^2\cdot$$

$$\cdot\left(f_L(\omega)-f_R(\omega)\right)\cdot\left(\mathrm{Im}\,G^{r0}_{ii}(\omega)\right)^2\cdot\int\frac{d\varepsilon}{2\tilde{\pi}}\frac{G^{+0}(\varepsilon)}{\omega-\varepsilon} \qquad /2.53/$$

Adding the $\Sigma^{\pm}$ contribution we get the total third order contribution to the conductance from an impurity confined to the barrier as follows

$$G^{(3)}(V,T)=\frac{16\tilde{\pi}e^2}{\hbar}\mathcal{J}^3S(S+1)|U^1_0|^2\rho^0_\alpha\rho^0_\beta\left(T^2\rho^0_\alpha|G^{r0}_{ia}|^2+\right.$$

$$\left.+T'^2\rho^0_\beta|G^{r0}_{ib}|^2\right)\left((\mathrm{Re}\,G^{r0}_{ii})^2-(\mathrm{Im}\,G^{r0}_{ii})^2\right)F(eV)$$

$$U^r_0=TT'G^{r0}_{ab} \qquad /2.54/$$

Here there is a factor similar to that which determined whether the tunneling current is depressed or enhanced in $G^{(2)}$. Therefore, a similar discussion concerning the dependence of the sign of $G^{(3)}$ on the position of the impurity is valid here /only $|G^{r0}_{ii}|^2+(G^{r0}_{ii})^2+(G^{a0}_{ii})^2=3(\mathrm{Re}\,G^{r0}_{ii})^2-(\mathrm{Im}\,G^{r0}_{ii})^2$ which appears in /2.43/ is replaced by $(\mathrm{Re}\,G^{r0}_{ii})^2-(\mathrm{Im}\,G^{r0}_{ii})^2$ in /2.54// Also during the treatment of the $\Sigma^{\pm}$ contribution we have seen that due to the expression in last bracket in /2.54/ the total conductance will drop off rapidly with the distance of the

impurity from the I-M or I-M' contacts.

3. The magnetic impurity in the electrode

From equations /2.17/ and /2.18/ it follows that the current through junction in the case when the impurity is confined to the electrodes may be written as

$$\langle J \rangle = \frac{2e}{\hbar} \int \frac{d\omega}{2\pi} \left| U^{\tau'}(\omega) \right|^2 \left(g^{+}_{\alpha\alpha}(\omega) g^{-}_{\beta\beta}(\omega) - g^{-}_{\alpha\alpha}(\omega) g^{+}_{\beta\beta}(\omega) \right) \qquad /3.1/$$

where the effective coupling matrix element is

$$U^{\tau'} = T T' G^{\tau}_{ab}$$

It was already mentioned that $g^{\pm}_{\alpha\alpha}$ corresponds to such events that in the intermediate state described by G° the electron may cross the partition going to the right electrode. This means that $g^{\pm}_{\alpha\alpha}$ depends both on μ_L and μ_R. The contribution of those processes where this crossing really takes place is proportional to $|G^{\tau}_{ab}|^2$. Because G^{τ}_{ab} is an exponentially decreasing function of the width of the barrier, the above mentioned factor is very small and we may neglect this contribution. Then $g_{\alpha\alpha}$ and $g_{\beta\beta}$ are the propagators of two isolated regions in thermal equilibrium with chemical potentials μ_L and μ_R respectively.

From this consideration it follows that we may use relations /2.27/ and /2.26/ for the g propagators and write equation /3.1/ in the form

$$\langle J \rangle = \frac{4\pi e}{h} \int d\omega \, T^2 T'^2 |G^r_{ab}|^2 \rho_\lambda(\omega) \rho_\mu(\omega) \{ f_L(\omega) - f_R(\omega) \} \qquad /3.2/$$

Now, we can proceed exactly in the way as it was done by Caroli et al. /1972/ by making an expansion of G^r_{ab} in powers of g and T.

Instead of that we shall follow for the sake of illustration another way, which leads to the same result with the same effective density of states $\tilde{\rho}_\lambda$ as theirs. The difference is that we make an expansion of G^r_{ab} in powers of G^0 and Σ instead of expanding in powers g and T. Up to third order in the exchange interaction

$$|G^r_{ab}|^2 = G^r_{ab} G^a_{ba} = G^{r0}_{a\lambda} \Sigma^{r[(2)+(3)]}_{\lambda\lambda} G^{r0}_{\lambda b} G^{a0}_{ba} +$$
$$+ G^{r0}_{ab} G^{a0}_{b\lambda} \Sigma^{a[(2)+(3)]}_{\lambda\lambda} G^{a0}_{\lambda\lambda} \qquad /3.3/$$

where $\Sigma^{r,a[(2)+(3)]} = \Sigma^{r,a(2)} + \Sigma^{r,a(3)}$ and λ is the

position of impurity in the left electrode. If the impurity were in the right electrode, we would have had a similar expression.

$$\rho_\alpha = \rho^0_\alpha + \delta\rho_\alpha$$
$$\delta\rho_\alpha = -\frac{1}{\pi}\,\mathrm{Im}\,\delta g^r_{\alpha\alpha} \qquad /3.4/$$

$$\delta g^r_{\alpha\alpha} = g^{r0}_{\alpha\lambda}\sum^{r[(2)+(3)]}_{\lambda\lambda} g^{r0}_{\lambda\alpha} = \left(g^{r0}_{\alpha\lambda}\right)^2 \sum^{r[(2)+(3)]}_{\lambda\lambda} \qquad /3.5/$$

Using the relations

$$G^{r0}_{\lambda b} = T\, g^{r0}_{\lambda\alpha} G^{r0}_{ab}$$
$$G^{a0}_{b\lambda} = T\, G^{a0}_{ba}\, g^{a0}_{\alpha\lambda} \qquad /3.6/$$

$$G^{r0}_{a\lambda} \simeq \frac{T\, g^0_{aa}\, g^{r0}_{\alpha\lambda}}{1 - T^2 g^0_{aa}\, g^{r0}_{\alpha\alpha}} \qquad /3.7/$$

and the symmetry properties $G^{a0}_{\lambda a} = G^{a0}_{a\lambda}$ /which follows from the time reversal invariance of g^0 propagators/, we may cast equation /3.3/ into the form

$$|G^r_{ab}|^2 = |G^{r0}_{ab}|^2 T^2 g^0_{aa}\left(\frac{\delta g^r_{\alpha\alpha}}{1-T^2 g^0_{aa} g^{r0}_{\alpha\alpha}} + \frac{\delta g^a_{\alpha\alpha}}{1-T^2 g^0_{aa} g^{a0}_{\alpha\alpha}}\right) \quad /3.8/$$

After some algebra, the contribution to the dynamical current due to impurities in the left electrode may be written as

$$\langle \delta J_L \rangle = \frac{4\pi e}{h}\int d\omega |TT' g^0_{ab}(\omega)|^2 \delta\tilde{\rho}^0_\alpha(\omega)\cdot\tilde{\rho}^0_\beta(\omega)\left\{f_L(\omega)-f_R(\omega)\right\} \quad /3.9/$$

where we introduced the effective densities of states $\tilde{\rho}^0_\alpha$, ρ^0_β and the correction $\delta\rho_\alpha$ as in Caroli et al. /1972/

$$\tilde{\rho}^0_\alpha = \frac{\rho^0_\alpha}{|1-T^2 g^{r0}_{\alpha\alpha} g^0_{aa}|^2} = -\frac{1}{\pi T^2 g^0_{aa}} Im\left[\frac{1}{1-T^2 g^0_{aa} g^{r0}_{\alpha\alpha}}\right] \quad /3.10/$$

$$\delta\tilde{\rho}_\alpha = -\frac{1}{\pi} Im \frac{\delta g^r_{\alpha\alpha}}{(1-T^2 g^0_{aa} g^{r0}_{\alpha\alpha})^2} \quad /3.11/$$

The second order contribution to the conductance may then be written in the form

$$\delta G^{(2)}_L = \frac{4\pi e^2}{h}|\tilde{u}^r|^2 \tilde{\rho}^0_\beta \delta\tilde{\rho}^{(2)}_\alpha \quad /3.12/$$

where $\tilde{u}^r = TT' g^{r0}_{ab}$ and $\delta\tilde{\rho}^{(2)}_\alpha = -\frac{1}{\pi} Im \frac{\delta g^{r(2)}}{(1-T^2 g^0_{aa} g^{r0}_{\alpha\alpha})^2} = -\frac{1}{\pi} Im\left(G^{r0}_{\lambda\lambda}\right)^2 \Sigma^{r(2)}_{\lambda\lambda}$

and $\Sigma^{r(2)}_{\lambda\lambda}(\omega) = J^2 S(S+1) G^{r0}_{\lambda\lambda}(\omega)$.

In the continuous representation of the simple square barrier model as discussed in the Appendix we would be able to plot the curve $\delta G^{(2)}$ as a function of the impurity position. Instead of that the main feature of the behaviour of that curve may be seen from the quite general discussion presented by Caroli et al. /1972/. We shall repeat in main lines their arguments to have complete consideration of the effect of impurities confined to the electrode.

All the differences with respect to the case when the impurities are confined to the oxide barrier arise from the fact that in a metal $g^{r0}_{\lambda\lambda}$ is oscillatory, /with rapid changes of the phase of $g^{r0}_{\lambda\lambda}$ on the scale of $\frac{1}{2_F}$ / The effective density of states and also $\langle \delta \jmath_L \rangle$ will contain some combination of $Re\,\Sigma^r_{\lambda\lambda}$ and $Im\,\Sigma^r_{\lambda\lambda}$. The coefficients of $Re\,\Sigma^r_{\lambda\lambda}$ and $Im\,\Sigma^r_{\lambda\lambda}$ are $Im\,\frac{(g^{r0}_{\lambda\lambda})^2}{(1-T^2 g^{r0}_{\lambda\lambda} g^0_{aa})^2}$ and $Re\,\frac{(g^{r0}_{\lambda\lambda})^2}{(1-T^2 g^{r0}_{\lambda\lambda} g^0_{aa})^2}$ respectively. These coefficients are energy independent /between μ_L and μ_R / for MIM junctions. They have approximately the same value which depends very strongly on the special model used for junction. This consideration is applicable not only to $\delta \varsigma_L^{(2)}$ but in the same way to $\delta \varsigma_L^{(3)}$ as well /where this oscillatory behaviour implies a variation of the sign of the

logarithmic conductance anomaly with the position of the impurity in the electrode/, since the conclusions above were drawn from the form of $\delta\tilde{\rho}_\lambda$ i.e. $\delta g^r_{\alpha\lambda}$.

The third order contribution to the current from the impurities confined to the left electrode may by written as

$$\langle \delta\gamma_L^{(3)} \rangle = \frac{16\pi e}{\hbar} J^3 S(S+1) \int d\omega \left| T T' g^0_{ab} \right|^2 \tilde{\rho}^0_\beta \left\{ f_L(\omega) - f_R(\omega) \right\} \cdot$$

$$\cdot \left(-\frac{1}{\pi}\right) \mathrm{Im} \left\{ \frac{(g^{r0}_{\alpha\lambda})^2}{(1 - T^2 g^{r0}_{\alpha\alpha} g^0_{aa})^2} \cdot 2 \left(G^{r0}_{\lambda\lambda}(\omega) \int \frac{\mathrm{Im} G^{r0}_{\mu\mu}(\varepsilon) f_L(\varepsilon)}{\omega - \varepsilon} \frac{d\varepsilon}{2\pi} - \right. \right.$$

$$\left. \left. - \int \frac{d\varepsilon}{2\pi} \frac{\mathrm{Im} G^{r0}_{\lambda\lambda}(\varepsilon) \mathrm{Re} G^{r0}_{\lambda\lambda}(\varepsilon) f_L(\varepsilon)}{\omega - \varepsilon} \right) \right\} \quad /3.131$$

We already isolated here the term which contains the dominant voltage and temperature dependence, and in the integral over ε used the relation $G^{+0}_{\lambda\lambda}(\varepsilon) \simeq -2i f_L(\varepsilon) \mathrm{Im} G^{r0}_{\lambda\lambda}(\varepsilon)$ which is valid for impurities confined to the left electrode. In calculating the integrals we have to use a cut-off, similarly as in the derivation if equation /2.34/ from /2.33/.

Neglecting the energy dependence of $\mathrm{Im}\, G^{r0}_{\lambda\lambda}(\varepsilon)$ $\mathrm{Re}\, G^{r0}_{\lambda\lambda}(\varepsilon)$ in the integral over ε and that of $\tilde{\rho}^0_\beta, \tilde{U}^r, G^{r0}_{\alpha\lambda}$ and $G^{r0}_{\lambda\lambda}$ in the integral over ω, we shall again obtain a logarithmic behaviour in the conductance.

4. Generalization to three dimensions and finite impurity concentration.

As in the paper by Caroli et al. /1972/ H_c which describes the coupling between the electrodes and the barrier is assumed to be translationally invariant in the direction parallel to the interface. It means that the momentum component $\vec{k}_{\parallel}$ is conserved during the transition from site α to site a and from site b to site β. This approximation was carefully discussed by Combescot and Schreder /1973/ and they showed that as long as the tunneling involves small spreads of $\vec{k}_{\parallel}$ and ω with respect to the Brillouin zone and the band width the interface scattering gives a tunneling current which differs from the specular one / $\vec{k}_{\parallel}$ is conserved/ by a multiplicative constant of the order of unity.

The transfer electrode-barrier coupling is then taken as

$$H_c = \sum_{a,\alpha} T_{\alpha a} \left(c_\alpha^+ c_a + c_a^+ c_\alpha \right) + \sum_{\beta,b} \left(c_\beta^+ c_b + c_b^+ c_\beta \right) \qquad /4.1/$$

where $\alpha(\beta)$ lies in the first atomic plane of $M(M')$ and $a(b)$ in the first /last/ atomic plane of the insulator. Let us first consider an impure junction with magnetic impurities located inside the barrier, with a random distribution in the (yz) direction /plane parallel to the interface./ Making an averaging on the impurity distribution in the (yz) plane the system becomes

translationally invariant along that plane and the density of impurities is a function of one space coordinate only, that of X . This distribution is given in the discrete site representation as C_i and is kept undetermined in the calculation. We also confine ourselves to the case of low impurity concentration so we suppose that the magnetic moments are independent of each other. Expression /2.19/ may be written as

$$\langle \delta J_{\Sigma^{\pm}} \rangle = \frac{2e}{\hbar} \int \frac{d^2\vec{k}_{\parallel}}{(2\pi)^2} \int \frac{d\omega}{2\pi} T^2(\vec{k}_{\parallel}) \left| G^{r0}_{ai}(\vec{k}_{\parallel}) \right|^2 \sum_i C_i \cdot$$

$$\cdot \left\{ g^{+0}_{\alpha\alpha}(\vec{k}_{\parallel}) \sum_{ii}^{-[(2)+(3)]} - g^{-0}_{\alpha\alpha}(\vec{k}_{\parallel}) \sum_{ii}^{+[(2)+(3)]} \right\} \qquad /4.2/$$

where we took into account that the propagators g^0 and G^0 are translationally invariant. $\sum^{\pm}_{ii}$ is the contribution to the self-energy of one impurity at the place $\vec{r}_i$ and it does not depend on $\vec{k}_{\parallel}$. Here we used the Fourier transforms with respect to y and z

$$T(\vec{k}_{\parallel}) = \sum_{\alpha,a} T_{\alpha a} e^{i\vec{k}_{\parallel}(\vec{R}_{\alpha} - \vec{R}_a)}$$

$$G^0_{ij}(\vec{k}_{\parallel}, \omega) = \sum_{\vec{r}_{\parallel}, \vec{y}_{\parallel}} G^0_{\vec{R}_i \vec{R}_j} \exp\left\{ i\vec{k}_{\parallel}(\vec{r}_{\parallel} - \vec{y}_{\parallel}) \right\} \qquad /4.3/$$

The other contribution to the current can be obtained from a generalization of /2.35/ and /2.36/

$$\langle \delta J \rangle = \frac{4\pi e}{\hbar} \int \frac{d^2\vec{k}_{\parallel}}{(2\pi)^2} \int d\omega T^2(\vec{k}_{\parallel}) T'^2(\vec{k}_{\parallel}) \rho_{\alpha}(\vec{k}_{\parallel}) \rho_{\beta}(\vec{k}_{\parallel}) \left(f_L(\omega) - f_R(\omega) \right) \cdot$$

$$\cdot \sum_i C_i \left[G^{r0}_{ab}(\vec{k}_{\parallel}) G^{a0}_{bi}(\vec{k}_{\parallel}) \sum_{ii}^{a[(2)+(3)]} G^{a0}_{ia}(\vec{k}_{\parallel}) + G^{a0}_{ba}(\vec{k}_{\parallel}) G^{r0}_{ai}(\vec{k}_{\parallel}) \sum_{ii}^{r[(2)+(3)]} G^{r0}_{ib}(\vec{k}_{\parallel}) \right] \qquad /4.4/$$

In the case when the impurities are inside the left /or right/ electrode, their contribution to the current may be written as

$$\langle \delta j_L \rangle = \frac{4\pi e}{k} \int \frac{d^2\vec{k}_\parallel}{(2\pi)^2} \int d\omega\, T^2(\vec{k}_\parallel) T'^2(\vec{k}_\parallel) \left| g^0_{ab}(\vec{k}_\parallel) \right|^2 \tilde{g}^0_{\beta}(\vec{k}_\parallel) \cdot$$

$$\cdot \sum_\lambda c_\lambda \operatorname{Im}\left(G^{r0}_{\alpha\lambda}(\vec{k}_\parallel) \right)^2 \cdot \sum_{\lambda\lambda}^{r[(2)+(3)]} \qquad /4.5/$$

where c_λ is the concentration in the λ -th atomic plane in the left electrode.

In perturbation theory which we used throughout this article the first order self-energy $\Sigma^{(1)}$ is equal to zero. Therefore up to third order in j the electrode and barrier effects are simply additive.

We know that the range of parallel momentum which is involved mostly in tunneling is very small i.e. only the electrons with energies near the Fermi energy and with $\vec{k}_\parallel \simeq 0$ play an important role in the tunneling process. That follows because the wave function of other electrons is damped more strongly in the barrier. All the main features seen in 1-D case and for one impurity will therefore remain intact. This can be easily verefied going on to the continuous representation and performing the integration over the parallel momentum. For impurities confined to the barrier there is no destructive interference as in the metallic region, for the evanescent wave function has a constant phase G(V,T) is negative for impurities very close to the interface.

otherwise it is positive. However, if the impurities are situated in the electrode region some question arise. One question in how far from the metal-barrier interface the impurities may be /assuming a layer-like distribution parallel to the junction surface at distance from M-I contact/ so that the contact still "feels" their effect in the conductance. This question is connected with the problem of a coherence lenght and of spatial dependence of the electron density of states around the impurity layer. /We note that actually in expression /4.5/ there is some renormalized density of states at the place of M-I contact i.e. $\delta \tilde{\rho}_\alpha$ /. To the extent that there is no damping factor in the free electron propagators in the metal / $g^{r0}_{\alpha\lambda}$ /, the renormalized density of states and the conductance due to the magnetic impurities will be an oscillating function of position. If we take into account the momentum dependence of the exchange coupling $J_{kk'}$ and introduce correspondingly a cut-off Δ /wich will give the coherence lenght $\xi_\Delta = \frac{v_F}{\Delta}$ / then the propagator $g^{r0}_{\alpha\lambda}$ will not be a simple oscillating function of the position λ but will contain some damping factors. This damping will cause the renormalized density of states will consist of two parts, an oscillating and non-oscillating one. These results are in agreement with Mezei and Zawadowski/1971 a.b./.

For further discussion about the range and relative importance of these two parts in the renormalized density of states and their effect in tunneling anomalies we refer to Mezei and Zawadowski.

Appendix

Caroli et al. (1972) illustrated the general behaviour of the propagator g^{o} for the region comprising one electrode and half the barrier by considering a square barrier potential for a continuous model. We will solve the equations for the free propagators in the barrier alone and in the electrode alone, and show on one example how to go from an expression in the discrete representation to the corresponding expression in the continuous model using these free propagators.

For the free propagators in the barrier alone we have to solve the equation

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)-\omega\right)g^{o}(x,y,\omega)=\delta(x-y) \qquad (A.1)$$

with the boundary condition that $g^{o}=0$ if x or $y = 0$ and $g^{o} = 0$ if X or $y = L$. The general solution is

$$g^{o}(x,y) = A_{\pm}\exp\{Kx\}+B_{\pm}\exp\{-Kx\} \qquad (A.2)$$

The coefficients $A_{\pm}$ $B_{\pm}$ refer respectively to $x>y$ and $x<y$. They are determined by the boundary conditions and the condition that g^{o} is continuous at $x = y$, while $\frac{\partial g^{o}}{\partial x}$ has a discontinuity $-\frac{2m}{\hbar^2}$. The result may be written as

$$g^{o}(x,y)=\begin{cases}-\frac{2m}{\hbar^2K}\frac{\sinh K(L-y)}{\sinh KL}\sinh Kx & x<y\\ -\frac{2m}{\hbar^2K}\frac{\sinh Ky}{\sinh KL}\sinh K(L-x) & y<x\end{cases} \qquad (A.3)$$

Solving the equations

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-\omega\right)g^{ro}(x,y)=\delta(x-y) \qquad (A.4)$$

with the boundary condition $g^{ro}(x,y)=0$ if x or $y = 0$ we will get the free propagators in the metal alone.

The general solution is

$$g^{ro}(x,y) = \alpha_{\pm}(y) \exp\{iqx\} + \beta_{\pm}(y) \exp\{-iqx\} \qquad (A.5)$$

G^{ro} has to satisfy the following conditions

(i) $g^{ro} = 0$ for $X = 0$

(ii) g^{ro} must be analytic when continued into the upper half of the ω plane; it means that for $x > y$, $\beta_{+} = 0$. (iii) g^{ro} is continuous at $x = y$ while $\frac{\partial g^{ro}}{\partial x}$ has a discontinuity $-\frac{2m}{\hbar^2}$. These conditions are fulfilled by

$$g^{ro}(x,y) = \begin{cases} -\frac{2m}{\hbar^2 q} \sin qx \cdot \exp\{iqy\} & x<y \\ -\frac{2m}{\hbar^2 q} \sin qy \cdot \exp\{iqx\} & x>y \end{cases} \qquad (A.6)$$

Now, we are able to transform every propagator, G^{o}_{ij}, given in the discrete model into the continuous form, using for example the free propagators of the specific continuous model discussed here.

Let consider g^{ro}_{ii} as a simple example.

In the discrete model g^{ro}_{ii} is given by the equation (2.45)

$$g^{ro}_{ii} = g^{o}_{ii} + \frac{T^2 g^{o}_{ia} g^{o}_{ai} g^{ro}_{\alpha\alpha}}{1 - T^2 g^{o}_{aa} g^{ro}_{\alpha\alpha}}$$

The continuous g^{ro} is given by

$$g^{ro}(x_i,x_i) = \lim_{l\to 0} g^{ro(l)}_{ii} \quad \text{where} \quad g^{ro}_{ii} = l\, g^{ro(l)}_{ii} \tag{A.7}$$

Then

$$l\, g^{ro(l)}_{ii} \simeq \frac{T^2 l^3 g^{o(l)}_{ia}\, g^{ro(l)}_{\alpha\alpha}\, g^{o(l)}_{ai}}{1 - T^2 l^2 g^{o(l)}_{aa}\, g^{ro(l)}_{\alpha\alpha}} \tag{A.8}$$

l is the interatomic distance and going on from discrete to continuous representation we need the "normalized" Green function $G = lG^{(l)}$ (for the detailed discussion see Caroli et al. (1971b). The transfer terms T or T´ are $-\frac{\hbar^2}{2ml^2}$ Taking the limit $l \to 0$ and introducing our free propagators in the continuous model given by (A.4) and (A.7) into (A.9) we obtain the continuous $g^{ro}(x_i,x_i)$

$$g^{ro}(x_i,x_i) = \left(-\frac{2m}{\hbar^2}\right) \frac{1}{2K} \left[1 + \frac{K+iQ}{K-iQ}\, e^{-2Kx_i}\right] \tag{A.9}$$

This propagator is the same as the one sided propagator obtained by Caroli et al (1971b) (Their formula (A.4)).
In the same way we could evaluate the continuous 'non-equilibrium" propagator $G^{ro}(x_i,x_j)$.

5. Conclusions

In order to treat the effect of exchange scattering of tunneling electrons on magnetic impurities in a tunnel junction, we have used the CCNS theory and Abrikosov´s

fictitious fermion operator technique. We find that when the magnetic impurities are situated in the barrier region there are two different contributions. The first one (which is due to the $\sum^{\pm}$ term in the self-energy) leads to an enhancement of the tunneling current to order J^2 (eq.(2.29)) and to a zero bias conductance peak for $J<0$ in the third order of perturbation theory (eq.2.34)) Comparison with Appelbaum's theory (1967) shows that this contribution is just equal to his result (with one important difference that we have an explicit expression for his phenomenological parameters). The second contribution (which is due to the $\sum^{r,a}$ term in the self-energy) is not always of the same sign. The region in which this contribution has the sign opposite to that of the $\sum^{\pm}$ contribution depends on the ratio $\frac{K_F}{2_F}$ and is not larger than one atomic layer. Therefore only for impurities which are situated in the barrier close to the metal-insulator interface (not further than one atomic layer) the total second order (or third order) contribution to the current may be negative and reduce the current. This negative sum corresponds to the Sólyom--Zawadowski theory.

Regarding the relationship of these two contributious to the calculations by Appelbaum and by Zawadowski and Sólyom we have to make several remarks.

Appelbaum's (1966, 1967) theory considers the magnetic impurities in the barrier as providing an easy way for the electron tunneling through the barrier and describes it by adding a phenomenological term to the conventional tunneling Hamiltonian. In the case of antiferromagnetic interaction the current obtained with such a procedure is always positive and that supported the idea of a "new channel". (A microscopic

basis of this idea has been suggested by Anderson (1966)).

Considering only the Σ^{+-} contribution to the current for impurities in the barrier we have obtained exactly the same results as Appelbaum (with the same numerical factors) but with explicit expressions for his phenomenological parameters). We note that we used a microscopic theory which does not contain phenomenological parameters .

From the theory for electron-phonon interaction in the barrier (Caroli et al. (1972) we know that the Σ^{+-} term corresponds to an inelastic process in which a real phonon is emitted during the tunneling event. Furthermore, in the case of electron-phonon interaction (for phonons in the barrier not close to one of the electrodes) this inelastic current $\langle J_{in} \rangle$ which stems from Σ^{+-} dominates over the elastic current $\langle \delta J_{el} \rangle$ which stems from $\Sigma^{r,a}$.

In our case of electron-magnetic impurity interaction we have found that, for impurities in the barrier not too close to one of the electrodes, there are again two contributions to the current: one from $\Sigma^{r,a}$ and another one from Σ^{+-}. But both terms now correspond to elastic processes (if the magnetic moments are non interacting as we supposed) and in the second order of J both lead to an enhancement of the tunneling current (the impurities are farther than one atomic layer from the insulator-metal contact) and they are of the same order of magnitude. If the impurities are still in the barrier but situated very close to one electrode the $\Sigma^{r,a}$ term in the second order of J changes sing and becomes bigger than the Σ^{+-} term (which is always positive).

In the third order of J the $\Sigma^{\pm}$ contribution leads to a zero bias conductance peak for $J<0$. On the other hand the $\sum^{r,a}$ term leads (for each position of the impurity) to a zero bias conductance dip for $J<0$. But this $\sum^{r,a}$ contribution in the third order of J is proportional to $\left(\mathrm{Im}\, G^{ro}_{ii}\right)^2$ (see (2.53)) and therefore becomes negligible except for the impurities which are very close to the metal-insulator contact.

This consideration shows that Appelbaum's original (1966, 1967) calculation of the current is incorrect since it does not include all important contributions to the current. Moreover, it follows that the notion of "assisted tunneling" is not well defined. In what follows we will show that the terminology as "non local effect or assisted tunneling" and "local effect or the change of electronic energy spectrum" is also incorrect and that it is impossible to make such a distinction.

Appelbaum et al. (1967) using a Green's function decoupling scheme derived two terms, one negative term (which corresponds to our $\sum^{r,a}$ term) and one positive term (which corresponds to our $\sum^{\pm}$ contribution), which means that their calculation gives correct results for impurities very near to one electrode (but not for impurities well inside the insulator). In their derivation they again introduced phenomenologically the impurity spin-assisted tunneling channel as suggested by Appelbaum (1966, 1967).

In contradistinction, Zawadowski (1967) derived an expression for the current assuming that the electron interaction with impurities shows a local character. His calculation is microscopic, and no phenomenological parameters are introduced.

Starting from the expression for the current Sólyom and Zawadowski (1968 a,b) found that the amplitude of the tunneling current can be expressed in terms of the local density of states. They supposed that the exchange interaction coupling constant is momentum dependent and introduced an energy cut-off parameter which was assumed to be small compared to the Fermi energy. The assumption that the cut-off parameter is small led them to neglect the real part of the free propagators with respect to the imaginary part. As a consequence of that approximation they obtained only a depression in the electron density of states and a corresponding depression in the tunneling current. The same calculations as that of Zawadowski was made by Appelbaum and Brinkman (1970) in their recent coordinate representation version of the transfer Hamiltonian theory. Without using a small cut-off in the calculations of the free propagators, they succeeded in deriving correctly all terms for impurities confined to the electrode region or to the barrier (but not for the case when the impurities are so deeply in the barrier that we have to take both electrodes into account simultaneously and on equal footing. All these considerations can be easily illustrated on the second order contribution to the current. Let us write the total second order contribution in the form

$$\langle j^{(2)} \rangle = \frac{4\pi e}{\hbar} J^2 S(S+1) \int d\omega \left(f_L(\omega) - f_R(\omega) \right) \rho^0_\alpha(\omega) \rho^0_\beta(\omega) \cdot$$
$$\cdot T^2 T'^2 |G^{ro}_{ab}|^2 \left\{ |G^{ro}_{ii}|^2 + \left[(G^{ro}_{ii})^2 + (G^{ao}_{ii})^2 \right] \right\} \tag{5.1}$$

where

$$G^{ro}_{ii} = g^{o}_{ii} + g^{o}_{ia} T g^{ro}_{\alpha\alpha} T G^{ro}_{ai} + g^{o}_{ib} T' g^{ro}_{\beta\beta} T' G^{ro}_{bi} \qquad (5.2)$$

and "i" is the position of the impurity in the barrier. From (5.2) one may see that G^{ro}_{ii} is the propagator for a non-equilibrium system since it contains contribution from both electrodes, which have different chemical potentials. The term in wavy bracket $|G^{ro}_{ii}|^2$ is due to the $\sum^{L}$ contribution and $(G^{ro}_{ii})^2 + (G^{ao}_{ii})^2$ is due to the $\sum^{r,a}$ contribution. Their sum may be written as

$$|G^{ro}_{ii}|^2 + \left[(G^{ro}_{ii})^2 + (G^{ao}_{ii})^2\right] = 3\left(\mathrm{Re}\, G^{ro}_{ii}\right)^2 - \left(\mathrm{Im}\, G^{ro}_{ii}\right)^2 \qquad (5.3)$$

Let us suppose now that the impurity is closer to the left electrode. In that case the third term in (5.2) will be of the order of $\exp\{-2KL\}$ (L is the depth of the barrier). Since in (5.1) there is already a term $|G^{ro}_{ab}|^2 \alpha \exp\{-2KL\}$, the third term of (5.2) may be neglected with respect to the first two terms. G^{ro}_{ii} may then be written as

$$G^{ro}_{ii} \simeq g^{ro}_{ii} = g^{o}_{ii} + \frac{T^2 g^{o}_{ia} g^{ro}_{\alpha\alpha} g^{o}_{ai}}{1 - T^2 g^{o}_{aa} g^{ro}_{\alpha\alpha}} \qquad (5.4)$$

In this approximation G^{ro}_{ii} does not contain the spectral density of the right electrode. Writing equation (5.4) in the continuous representation for the square barrier potential model one has

$$G^{ro}(x_i, x_i) \simeq \left(-\frac{2m}{\hbar^2}\right) \frac{1}{2K} \left[1 + \frac{K+iq}{K-iq} \exp\left\{-2K\left(\frac{L}{2} - x_i\right)\right\}\right] = \qquad (5.5)$$

$$= g^{ro}(x_i, x_i)$$

(x_i is the position of the impurity and $x = 0$ is taken in the middle of the barrier). In that form $G^{ro}(x_i, x_i)$ is exactly the same as the free propagator used by Sólyom and Zawadowski but written in coordinate representation, (See equation (8) by Sólyom-Zawadowski (1968) with functions given by their equation (11) and (A.I.2)), or it is the same as Appelbaum-Brinkmann's left hand side propagator taken at the place of the impurity. (Equation (2.18) by Appelbaum-Brinkmann (1970)[x]). We may call $G^{ro}(x_i, x_i)$ written in the form (5.5) the one sided propagator and denote it as $g^{ro}(x_i, x_i)$. Sólyom and Zawadowski did not use $g^{ro}(x_i, x_i)$ in the coordinate representation but went instead to the momentum representation and neglecte the real part of the free propagator. Therefore, instead of equation (5.3) which we may now write with the one sided propagators as

$$\left| g^{ro}(x_i, x_i) \right|^2 + \left[\left(g^{ro}(x_i, x_i) \right)^2 + \left(g^{ro}(x_i, x_i) \right)^2 \right] = 3 \left(\mathrm{Re}\, g^{ro}(x_i, x_i) \right)^2 - \left(\mathrm{Im}\, g^{ro}(x_i, x_i) \right)^2$$

they get only $- \left(\mathrm{Im}\, g^{ro}(x_i, x_i) \right)^2$

(We note that the similar factor, namely $\left(\mathrm{Re}\, g^{ro}(x_i, x_i) \right)^2 - \left(\mathrm{Im}\, g^{ro}(x_i, x_i) \right)^2$ appears also in front of the logarithmic function in the third order of perturbation calculation). On the other hand Appelbaum and Brinkmann's theory (that is nothing else than the coordinate version of Zawadowski's theory without neglecting the real part of th the free propagators) gives the sum $3 \left(\mathrm{Re}\, g^{ro}(x_i, x_i) \right)^2 - \left(\mathrm{Im}\, g^{ro}(x_i, x_i) \right)^2$ in the second order of J or $\left(\mathrm{Re}\, g^{ro}(x_i, x_i) \right)^2 - \left(\mathrm{Im}\, g^{ro}(x_i, x_i) \right)^2$ in the third order of J correctly. It means that the Sólyom-

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[x] There is a difference in the numerical factors of $G^{ro}(x_i, x_i)$ given by (5.5) and Appelbaum-Brinkman's G_0^L given by their equation (2.18) which comes from different definition of the propagators.

-Zawadowski theory (or its improvement the Appelbaum-Brinkman theory) is correct for those impurities for which we may replace G^{ro}_{ii} given by (5.2) with one side propagator $\mathcal{G}^{ro}_{ii}$ given by (5.4) or (5.5). If the impurities are at approximately the same distance from both electrodes than the second and the third term in (5.2) are of the same order of magnitude. The problem has to be treated as a true nonequilibrium problem in all steps and it is not possible to replace eq.(5.2) by (5.4).

Another useful illustration of these ideas may be achieved if in our calculation we divide the system from the beginning into two halves (instead of three parts as we had) by a partition located in the middle of the insulator).

Then, starting with equation (2.17) and making an expansion of $G^{\pm}$ in powers of T and $\mathcal{G}^{o}$, we may write the second order contribution coming from an impurity situated close to the boundary between the left electrode and the barrier (either in the electrode or in the barrier) as

$$\langle \mathcal{J}^{(2)} \rangle = \frac{8e}{\hbar} \int \frac{d\omega}{2\pi} \frac{T^2}{|1 - T^2 \mathcal{G}^{ro}_{cc} \mathcal{G}^{ro}_{\gamma\gamma}|^2} (f_L - f_R) \cdot \mathrm{Im}\, \mathcal{G}^{ro}_{cc} \cdot \mathrm{Im} \left(\mathcal{G}^{ro}_{\gamma i} \Sigma^{\pi(2)}_{ii} \mathcal{G}^{ro}_{ir} \right) \qquad (5.6)$$

γ and c denote the sites on either side of the new partition and $\mathcal{G}$ denotes the one sidéd propagator.

/ $\mathcal{G}^{\tau 0}_{ii}$ is the same as $G^{\tau 0}_{ii}$ given by /5,4/ or $\mathcal{G}^{\tau 0}(x_i, x_i)$ in the continuous representation. We assumed that the impurities are only on the left side of the partition and in the demoninator we replaced $\mathcal{G}^{\tau}_{cc}$ and $\mathcal{G}^{\tau}_{\delta\delta}$ /which contain the interaction/ by $\mathcal{G}^{\tau 0}_{cc}$ and $\mathcal{G}^{\tau 0}_{\delta\delta}$, since the corrections to $\mathcal{G}^{\tau}_{cc}$ $\mathcal{G}^{\tau}_{\delta\delta}$ are of the order of $\exp\{-2KL\}$ This form of the current is quite similar to Zawadowski's and Appelbaum and Brinkmann's expression for the current. If it is calculated in the continuous representation, we will get

$$\langle j^{(2)}_{\delta} \rangle = \frac{4e}{\pi k} \int d\omega \, \frac{4K^2}{(K^2+q^2)^2} \, e^{-2KL} \cdot q^2 (f_L - f_R) \Big\{ \Big(-\frac{2m}{k^2}\Big)^2 J^2 S(S+1) \cdot \frac{1}{4K^2} \cdot$$

$$\Big[\Big(2 + 4 \, \frac{K^2-q^2}{K^2+q^2} \, e^{-2K\left(\frac{L}{2}-x_i\right)} + 2 \, \frac{e^{-4K\left(\frac{L}{2}-x_i\right)}}{(K^2+q^2)^2} \Big((K^2-q^2)^2 - 4q^2K^2 \Big) \Big)$$

$$+ \Big(1 + 2 \, \frac{K^2-q^2}{K^2+q^2} \, e^{-2K\left(\frac{L}{2}-x_i\right)} + \frac{e^{-4K\left(\frac{L}{2}-x_i\right)}}{(K^2+q^2)^2} \cdot$$

$$\cdot \Big((K^2-q^2)^2 + 4q^2K^2 \Big) \Big) \Big] \Big\} \qquad /5.7/$$

The same result follows from equation /5.1/ using the one side propagators /5,4/ or /5.5/ instead of /5.2/.

The expression in front of the wavy bracket gives the current for the case without an impurity and expression inside the wavy bracket is the change due to the impurity.

The first summand in the square bracket is due to the $\Sigma^{r,a}$ contribution $\left((\mathcal{G}^{ro}_{ii})^2 + (\mathcal{G}^{ao}_{ii})^2 \right)$ and the second one is due to the Σ^{+-} term $|\mathcal{G}^{ro}_{ii}|^2$. /From Appelbaum and Brinkmann's equations exactly the same expression may be derived for $\langle \mathcal{J}^{(2)} \rangle$ since the propagators are the same/.

We remark that $\Sigma^{r(2)}$ in /5.6/ is $\Sigma^{r(2)} = \mathcal{J}^2 S(S+1) \cdot G^{ro}_{ii}$ but for an impurity very near to the FM contact we may replace G^{ro}_{ii} by the left side propagator $\mathcal{G}^{ro}_{ii}$. This remark shows that for one impurity close to the contact the self-energy cannot sample simultaneously the chemical potentials in the left and the right electrode since the propagation in the barrier is exponentially decreasing with distance into the barrier. In this way we came to the main point of this discussion, namely the fact that the notions "assisted tunneling" and "local self-energy effects" have actually no physical meaning in this problem and emerged only from approximate treatments of the nonequilibrium problem.

If the impurity is close to the electrode-barrier interface and the self-energy cannot lump together μ_L and μ_R, than the equation /5.1/ which collects the Σ^{+-} and $\Sigma^{r,a}$ contributions may be replaced by eq. /5.6/ in where only real and imaginary part of Σ^{r} appear.

Therefore, for such an impurity it is not possible to distinguish between the $\Sigma^{\pm}$ and $\Sigma^{r,a}$ contributions Because of that we cannot say that the $\Sigma^{\pm}$ contribution /which corresponds exactly to that what Appelbaum calls "assisted tunneling" /describes some "assisted tunneling" and that it opens a new "channel". If the impurity is deeply in the barrier then we have to retain equation /5.1/ with η_{ii}^{r0} given by /5.2/, but again we cannot distinquish the $\Sigma^{\pm}$ term and $\Sigma^{r,a}$ since they have the same sign and /in the second order of γ / they are of the same order of magnitude.

In addition we discuss briefly the relative importance of the impurities situated in the barrier and in the electrodes. Carefull discussion and comparison with experiments will be made in a future publication, in which the non-perturbative expression for the scattering amplitude is used instead of $\Sigma^{(2)} + \Sigma^{(3)}$.

The contribution of the impurities confined to the barrier region is to order γ^2, approximately independent of the position and always positive /exscept for the first atomic layer./ When the impurities move into the metal, there will be a rapid /on atomic distances/ spatial oscillation in the dynamical conductance. These oscillations will produce a destructive interference and a sizeable reduction of the conductance. It means that if the impurities are randomly distributed with respect to the

metal-barrier interface the contribution of the impurities situated in the barrier will be much bigger than the J^2 contribution of the impurities confined to the electrode region. The situation to order J^3 is different. It was shown that the J^3 terms drop off rapidly with increasing distance into the barrier /since the logarithmic function is multiplied by a factor of the form $|G^{\tau 0}_{ia}|^2$ which falls off very rapidly/. Therefore, the barrier impurities will not show such a dominant role in the logarithmic anomaly as they do in the second order term.

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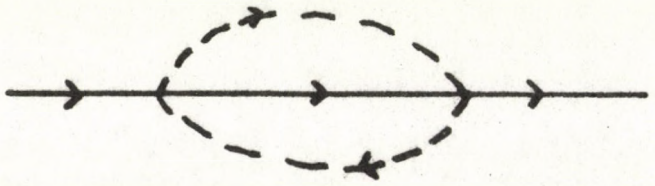


Fig. 1

Self-energy diagram in second order. The propagators of fictions fermions are represented by dotted lines while the solid lines stand for the electron propagators G^{o}_{ii} */i is the position of the impurity/.*

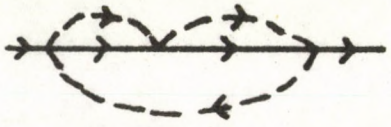


Fig. 2.a

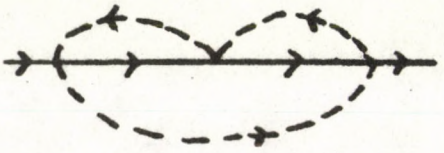


Fig. 2.b

Self-energy diagrams in third order.

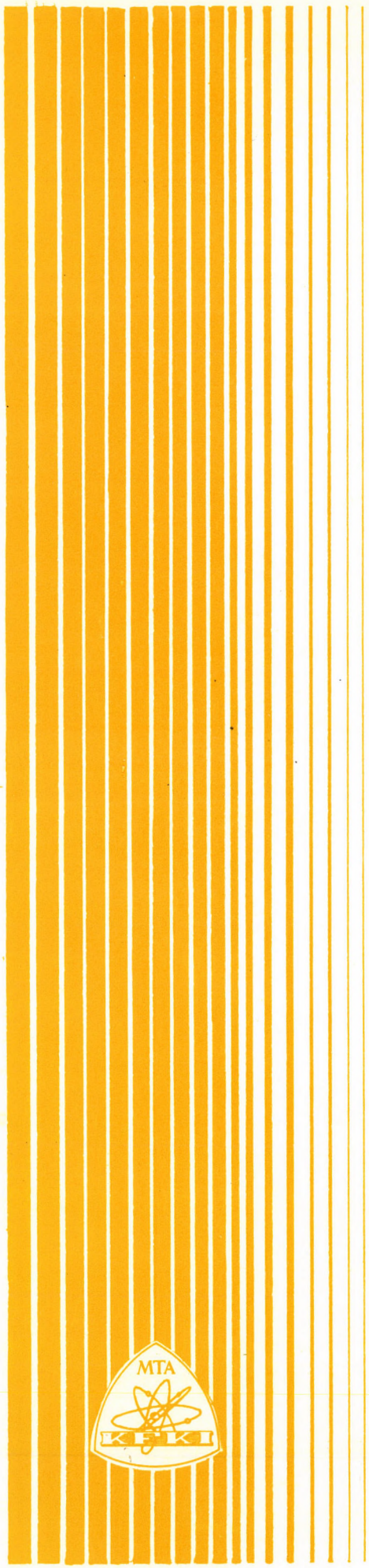
Fig. 1

Self-energy diagram in second order. The propagators of fluctuations fermions are represented by dotted lines while the solid lines stand for the electron propagators $G_{ii'}$. It is the position of the impurity.

Fig. 2.a

Fig. 2.b

Self-energy diagrams in third order.



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