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THEORY OF ZERO BIAS ANOMALIES DUE TO PARAMAGNETIC IMPURITIES

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Summary.

Using Zawadowski's approach to the tunneling phenomena the anomalous tunneling due to paramagnetic impurities is investigated. The tunneling current is expressed in terms of the local density of states at the barrier which in turn is given in terms of the life-time of the conduction electrons. To take into account the effect of the Kondo scattering of electrons on paramagnetic impurities different solution for the life-time /e.g. resonant state or quasi-bound state solutions/ are assumed and the resulting possible voltage-current characteristics are discussed and compared with the experimental results. The role played by the impurities lying at different positions relative to the metal-oxide interface is thoroughly investigated.

1. Introduction

Zero bias anomalies on transition metal - transition metal ox
normal /non-transition/ metal diodes have been observed by Wyatt [1] a
Rowell and Shen [2]. Anderson [3], Appelbaum [4] and Suhl [5] have sugg
that the paramagnetic atoms inside the barrier play an important role in bringing about these anomalies.

One of the authors [6] has proposed that diodes composed of metal - metal oxide - small amount of evaporated paramagnetic impurities - metal be investigated with regard to possible zero bias anomalies. This type of diodes has been studied by Wyatt and Lythall [7] and Mezei [8] and they found anomalies similar to the ones observed on transition metal - transition metal oxide - normal metal diodes. Their experiments indicate that the magnetic impurities at the barrier surface are responsible for a large variety of the zero bias anomalies. The aim of the present paper is to give a theoretical interpretation of the phenomena observed in diodes of the second type, where the positions of those magnetic atoms which play an important role in the effects are rather well determined.

The first accound of zero bias anomalies, observed on semiconductor tunnel junctions [9], [10], is due to Hall, Racette and Ehrenreich [9]. They treated the problem in terms of the bulk density of states, which is supposed to be modified by the existence of polaron states. Later it was shown by Duke and Mahan [11] that this picture is incorrect.

Various theories have been developed to explain different tunneling anomalies, but it is common among them that the barrier and its surrounding are the scence of the phenomena. Anderson [3], Appelbaum [4] and independently Suhl [5] proposed an interpretation that emphasizes the importance of the bound or resonant state on the magnetic impurity. They suggested that the localized magnetic states in the barrier represent an easy route for tunneling. This theory can explain zero bias anomalies with small relative amplitude, but cannot explain the giant resistivity maximum observed by Rowell and Shen [2] on Cr-CrO-Ag diodes and by Wyatt and Lythall [7] and Mezei [8] on junctions containing magnetic impurities at the barrier. An entirely different mechanism has been suggested by Duke, Silverstein and Bennett [12]; they assume that the electron tunneling process is associated with creation or annihilation of some quasiparticles, such as phonons and magnons. The phonon processes have been studied by Mahan [13] too. However, the estimated amplitudes of the magnon process are too small to account for the observed effects. New anomalies have been observed by Jaklevic and Lambe [14] on junctions containing organic or inorganic molecules. According to the theory developed by Marcus and Scalapino [15] to explain these anomalies, the excitations of the molecules give the important contribution to the anomalous tunneling current. All the above mentioned theories deal with tunneling processes associated with some elementary excitation which is rather well localized at the barrier.

A different approach, which emphasizes the change of the electronic energy spectrum in the barrier, has been suggested by the authors [6], [16]. The change is the effect of the Kondo resonant scattering or the existance of bound states on the magnetic impurities near the barrier. The contribution of the Kondo effect to the energy spectrum is essential only in the neighbourhood of the Fermi level; therefore, it may give rise to an observable effect at zero bias. The theory also can account for the giant resistivity maxima. This approach was first used by the authors [16] to calculate the tunneling current. More recently similar results have been obtained by Appelbaum, Phillips and Tzouras [17]. Anderson [18] has also pointed out, although from a quite different point of view, that the change in the electron spectrum at the paramagnetic impurities could be responsible for the anomalies.

The two approaches outlined above are not mutually exclusive; they rather correspond to physically different situations, which might be classified into two groups:

1. Non-local effect or assisted tunneling.

During the tunneling some quasiparticles /phonons, magnons/, molecular vibrations, or localized magnetic states are excited. It will be shown that these processes are important only if the selfenergy operator corresponding to the excitations is non local in space. This is the case if the subsequent interactions described by the higher order terms take place at different points of the barrier or on different sides of the barrier. A typical diagram corresponding to a second order contribution is given in Fig.1. [1]. The assisted tunneling processes appear as a new channel through the barrier[2].

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[1] This type of diagram has been calculated in ref. [12] and [13] considering the phonon assisted tunneling.

[2] The importance of non-local effects in zero bias anomalies have been emphasized by Appelbaum et al [17].

2. Local effect or the deformation of the electronic energy spectrum at the barrier.

In this case the interaction of the conduction electrons with the localized impurity excitations leads to change of the electronic energy spectrum in the neighbourhood of the impurities /Fig. 2/. If the energy spectrum changes at the barrier, then the amplitudes of the electrons penetrating into the barrier also change. Therefore, the overlap of the wave functions of the left and right electrons will be modified. This effect may be described by strongly energy dependent tunneling matrix elements or by the local /i.e. not bulk/ density of states at the barrier.

The distinction of local and non-local effects is rather idealistic. However, the above classification points out necessity for two different theoretical treatments in the physically different cases. The aim of the present paper is to work out the theory for local effects.

In the first part of this paper we investigate the physical meaning of the density of states, ρ , in the formula

$$I \sim \int \rho_{left}(E)\, \rho_{right}(E+eV) \left[n_F(E) - n_F(E+eV) \right] dE \qquad /1/$$

where I is the tunneling current and n_F is the Fermi distribution function. The density of states is usually determined from the experimental results, using eq. /1/. Our investigation is based on a generalization of Bardeen's tunneling theory [19]. This theory [2o], which takes into account many body effects by using Green functions is outlined in Sec. 2. The Green functions are built up from the solutions of two particular problems corresponding to the metals on the left and right hand side of the barrier. The calculation of the Green functions is given in Sec. 3. In the calculation the interaction with the impurities in the vicinity of the barrier is described by a local self-energy operator. In Sec. 4 we obtain a new expression for ρ , the effective density of states appearing in formula /1/. ρ is related to ρ_o , the bulk density of states, by

$$\rho = \rho_o Z \qquad /2/$$

where Z is a renormalization factor. This function describes the energy spectrum of the electrons at the barrier; it is expressed by the conduction electron life time corresponding to the scattering on the impurities. In Sec. 5 an average over the positions of the impurities is taken and the dependence of the energy spectrum at the barrier on the distribution of the impurities is carefully investigated. The coherence length introduced by the authors [21] is discussed. It is found that the impurities inside the coherence length measured from the barrier are the most effective /Fig.2./.

In the second part of this paper the characteristics of the tunneling diodes are investigated, assuming different scattering amplitudes for the electron-paramagnetic impurity scattering. The relationship between the assumed scattering amplitudes and the resulting diode characteristics is discussed. No final conclusion can be drawn, since the problem of the Kondo scattering [22] is not yet solved. The known approximations /e.g. the Abrikosov-Suhl resonance [23] and the Kondo bound state [24]/ give quite different results[3]. Further experimental investigation of this type of diodes, however, could give information on the scattering amplitudes. This information is not available from the measurements of other parameters /e.g. bulk resistivity/, because most of those parameters depend on the average of the scattering amplitudes taken over an energy interval of few times the temperature around the Fermi energy.

In Sec. 6. some general properties of the diode characteristics are given. The most frequently discussed scattering amplitudes are listed in Sec. 7. The results derived in the perturbation theory of the third order are summarized in Sec. 8. In Sec. 9. the characteristics are calculated on the basis of different scattering amplitudes listed in Sec. 7. Also in Sec. 9. the connection between the renormalized density of states and the relaxation time is pointed out and the main features of the selfconsistent theory are outlined. In Sec. 1o. the effect of external magnetic field is shortly discussed. The comparison of the experimental results and the present theory is given in Sec. 11. In Sec. 12. the possibility of the determination of the scattering amplitudes from the tunneling measurements is discussed and the comparison of the present theoretical results and other theories is given.

BASIC FORMULATION

2. General current formula

One of the authors [2o] developed an approach to the tunneling phenomena for metal-metal oxide-metal tunnel diodes. The Green functions of this problem are constructed from the Green functions corresponding to two particular problems, in which the metal on the left hand side /or right

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[3] Further literature can be found in ref. [25]

hand side/ is replaced by an insulator. The corresponding particular problem is called the right hand side problem /or left hand side problem/. The one-particle causal Green functions are introduced for finite temperatures by

$$G_{s,s';\alpha}(x,x') = -i \langle T\{\psi_s(x)\,\psi^+_{s'}(x')\}\rangle, \qquad \alpha = r,l \qquad /3/$$

where r and l stand for the right hand problem and left h.p., respectively, and s is the spin index. The expression of the current /at point x/ can be considered as a response to the tunneling rate /at point y/. Thus the expression for the i^{th} component of the current has been found to be

$$j_i(x) = (C \to R)\, e \sum_{s,s'} \left\{ \int_S df_{\vec{y},i} \int dy_0 \lim_{\vec{x} \to \vec{x}'} \right.,$$

$$\left. \left(\frac{\overrightarrow{\nabla}_{\vec{x}} - \overleftarrow{\nabla}_{\vec{x}}}{2m} \right)_i G_{s,s';l}(x,y) \left(\frac{\overrightarrow{\nabla}_{\vec{y}} - \overleftarrow{\nabla}_{\vec{y}}}{2m} \right)_j G_{s',s;r}(y,x') - (r \leftrightarrow l) \right\} \qquad /4/$$

where the direction of an arrow above a differential operator indicates the operand and the cyclic rule is to be followed in the absence of an adjacent operand. The surface integral is to be taken on an arbitrary surface S^4 in the barrier with surface element $df_{y,i}$ /see Fig.3./. The symbol /C → R/ stands for the replacement of the causal response function by the retarted one. For the space-time vectors the four-component notation is applied, $y = /y_0, \vec{y}/$ and the operation /r↔l/ stands for the exchange of the right and left indices.

The particular Green functions satisfy equations in which the potentials are as illustrated in Fig.4./a,b. The potential of the right hand problem is the same as that of the original one as shown in Fig.4/c excepting the region of the metal on the left hand side. The selfenergy operator Σ_r of the right hand problem is a sum of the self-energy Σ^e_r of the electron gas on the right hand side and the additional self-energy Σ_B coming from the region of the barrier and its neighbourhood

$$\Sigma_\alpha(x,x') = \Sigma^e_\alpha(x,x') + \Sigma_B(x,x')$$

In the derivation of the current formula, eq. /4/ it is supposed that the self-energy is a local function of the space variables inside

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[4] The value of the current density calculated by formula /4/ is independent of the choice of the surface S up to the second order of the tunneling rate, as it is shown in ref. 2o .

the barrier

$$\Sigma_B(x,x') = \Sigma_B(\vec{x};\, x_0 - x_0')\,\delta(\vec{x}-\vec{x}') \qquad /5/$$

The locality condition is well fulfilled, when the barrier self-energy is due to the interaction of conduction electrons with localized spins via the exchange interaction, given by the Kondo Hamiltonian [22]

$$H_k = -\frac{J}{N}\sum_i \sum_{s,s'} \psi_s^+(\vec{R}^{(i)})\,\sigma_{s,s'}\,\psi_{s'}(\vec{R}^{(i)})\, S^{(i)} \qquad /6/$$

where $\frac{J}{N}$ is the coupling constant, σ and S are the spin matrices of the conduction electrons and localized spins, respectively. The summation index i labels the different impurities. The electron field operator $\psi(R^{(i)})$ is taken at the position of the i^{th} impurity. The exchange interaction spreads over about one atomic distance and therefore the locality condition is realistic. The spin-spin correlation of different impurities is neglected. If the self-energy is non-local, eq. /4/ does not hold and the present method cannot be applied without any modification. This is the case, when tunneling is assisted by some quasiparticle or molecular vibration excitation which has been called "non-local barrier effect" in the introduction.

3. Determination of the particular Green functions

The Green function equations for the particular problems are

$$\left\{ i\frac{\partial}{\partial x_0} + \frac{\Delta_{\vec{x}}^2}{2m} - V_\alpha(\vec{x}) \right\} G_{s,s';\alpha}(x,x') - \sum_{s''}\int \Sigma_{s,s'';\alpha}(x,y)\, G_{s'',s'}(y,x')\, d^4y =$$

$$= \delta(x-x') \quad , \alpha = l,r \qquad /7/$$

which have to be solved approximately.

We are interested in the effect of the paramagnetic impurities put into the barrier or its neighbourhood. The particular Green functions can be determined in two steps namely taking into account

1, the self-energy Σ_α^e corresponding to the electron-electron interaction,

2, the effect of the impurities.

The electron-electron interaction seems to be not important for the zero bias anomalies [4], therefore it can be taken into account e.g. in Hartree-Fock approximation. The Green function can be given in the first step as

$$G^{(o)}_{s,s';\alpha}(\vec{x},\vec{x}\,';E)=\sum_{\lambda}\chi_{\lambda;\alpha}(\vec{x})\,G^{(o)}_{\lambda,s,s';\alpha}(E)\,\chi^{*}_{\lambda;\alpha}(\vec{x})$$

/8/

where the one-particle wave function $\chi_{\lambda,\alpha}$ satisfy the following Schrödinger equation

$$\left\{-\frac{\Delta_{\vec{x}}^{2}}{2m}+V_{\alpha}(\vec{x})\right\}\chi_{\lambda;\alpha}=\varepsilon_{\lambda;\alpha}\chi_{\lambda;\alpha}$$

/9/

with eigenvalues $\varepsilon_{\lambda,\alpha}$. The energy dependent term is

$$G^{(o)}_{\lambda,s,s';\alpha}(E)=\left(\frac{1-n_F(\varepsilon_{\lambda,\alpha})}{E-\varepsilon_{\lambda,\alpha}+i\varepsilon}+\frac{n_F(\varepsilon_{\lambda,\alpha})}{E-\varepsilon_{\lambda,\alpha}-i\varepsilon}\right)\delta_{s,s'}$$

/10/

where n_F is the Fermi distribution function.

For the sake of simplicity we suppose that the barrier is translational invariant in the directions y and z. The wave vector parallel to the plane of the barrier $\vec{k}_{\parallel}$ is a good quantum number. The wave functions $\chi_{\lambda;\alpha}$ may be written in the form

$$\chi_{\lambda;\alpha}(\vec{x})=\frac{1}{\sqrt{\Omega_{\alpha}}}\,e^{i\vec{k}_{\parallel}\vec{x}}\,f^{\alpha}_{\vec{k}_{\parallel},\nu}(x)$$

/11/

where $f_{\vec{k}_{\parallel},\nu}$ /x/ is the longitudinal component of the wave function, ν is a further quantum number and Ω_{α} is the volume of the metal on side α. Furthermore inside the barrier

$$f_{\vec{k}_{\parallel},\alpha}(x)\sim e^{\mp\varkappa_{\perp}x}\qquad x\in B,\ \alpha=l,r$$

/12/a/

with the damping factor $k_{\perp}$ given by

$$\varkappa_{\perp} \approx \sqrt{2m\left[V + \frac{k_{\parallel}^{2}}{2m} - E_F\right]} \qquad /12/b/$$

where E_F is the Fermi energy and the potential V is the height of the barrier taken to be constant. As it is well known only the electrons with energy near the Fermi energy and with $\vec{k}_{\parallel} \sim 0$ play an important role in the tunneling phenomena, because the wave function of other electrons is damped much more strongly in the barrier.

The next step is the determination of the Green functions in the presence of paramagnetic impurities. There is a representation of the Green function similar to the previous one given by eq /8/, but also off-diagonal elements occur, i.e.

$$G(\vec{x},\vec{x}\,';E) = \sum_{\lambda,\lambda'} \chi_{\lambda}(\vec{x})\, G_{\lambda,\lambda'}(E)\, \chi^{*}_{\lambda'}(\vec{x}\,') . \qquad /13/$$

The matrix element $G_{\lambda,\lambda'}(E)$ can be given in terms of the spectral function $\rho_{\lambda,\lambda'}(E)$ as

$$G_{\lambda,\lambda'}(E) = \int_{-\infty}^{\infty} \rho_{\lambda,\lambda'}(E') \left\{ \frac{1-n_F(E')}{E-E'+i\varepsilon} + \frac{n_F(E')}{E-E'-i\varepsilon} \right\} dE' \qquad /14/$$

Perturbation theory gives incorrect results if it is applied to the time-dependent Green functions at finite temperatures[5], therefore we have to turn to the thermodynamic Green functions with complex time variables [26], τ $(x = \{\vec{x},\tau\})$

$$\mathcal{G}_{\omega;\, s,s';\alpha}(\vec{x},\vec{x}\,') = -\int \langle T\{\psi_s(x)\,\psi^{+}_{s'}(x')\}\rangle_{\alpha}\, e^{i\omega_n(\tau-\tau')} \cdot d(\tau-\tau') \qquad /15/$$

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[5] The application of the thermodynamic Green functions with real time variables may give wrong result in some special canes. Using them the obtained life time is given by the correct one multiplied by an incorrect factor $/1-2n_F/E//$.

where $\omega = i\omega_n = i2\pi T(2n+1)$ with n an integer. The spectral representation of the thermodynamic Green functions is

$$\mathcal{G}_{\omega;\alpha}(\vec{x},\vec{x}') = \sum_{\lambda,\lambda'} \chi_{\lambda;\alpha}(\vec{x})\,\mathcal{G}_{\omega;\alpha}(\lambda,\lambda')\,\chi^{*}_{\lambda';\alpha}(\vec{x}')$$

/16/a/

with

$$\mathcal{G}_{i\omega_n;\alpha}(\lambda,\lambda') = \int \frac{\rho_{\lambda,\lambda';\alpha}(E')}{i\omega_n - E'}\,dE'$$

/16/b/

where the spectral functions $\rho_{\lambda,\lambda';\alpha}(E)$ are the same as in eq./14/.

In absence of impurities the spectral function is obtained by comparing eqs. /lo/ and /14/ as

$$\rho^{(o)}_{\lambda,\lambda';\alpha}(E) = \delta_{\lambda,\lambda'}\,\delta(E-\varepsilon_{\lambda,\alpha})$$

/17/

from which the Green function $\mathcal{G}^{(o)}$ is readily determined. The relation of $\mathcal{G}$ to $\mathcal{G}^{(o)}$ is expressed by the Dyson equation in symbolic notation as

$$\mathcal{G}_{\omega;\alpha} = \mathcal{G}^{(o)}_{\omega;\alpha} + \mathcal{G}^{(o)}_{\omega;\alpha}\,\Sigma_{B,\omega}\,\mathcal{G}_{\omega;\alpha}$$

/18/a/

The concrete form of the self-energy Σ_B due to the impurities will be discussed later. We only mention here that its imaginary part exhibits the energy dependence characteristic to the Kondo scattering while its real part is a smooth function of energy, which might be included in the scalar potential V_α . Thus we keep only the imaginary part of Σ_B in the following.

For the sake of simplicity a random distribution of the impurities is supposed in the planes parallel to the barrier. The self-energy averaged over the positions of the impurities, $\bar{\Sigma}_B$ depends only on the component x of the space variable. The parallel momentum $\vec{k}_{\parallel}$ is conserved. Calculating the matrix elements of the Dyson equation, eq. /18/a/, with the functions χ , we have

$$\mathcal{G}_{\omega;\alpha}(k_{\parallel};\nu,\nu')=\mathcal{G}^{(0)}_{\omega,\alpha}(k_{\parallel},\nu)\delta_{\nu,\nu'}+\frac{1}{L_\alpha}\sum_{\nu''}\mathcal{G}^{(0)}_{\omega;\alpha}(k_{\parallel},\nu'')\bar{\Sigma}_{B,\omega}(k_{\parallel};\nu,\nu'')\mathcal{G}_{\omega,\alpha}(k_{\parallel};\nu'',\nu')$$

/18/b/

The matrix element of the self-energy is

$$\frac{1}{L_\alpha}\bar{\Sigma}_{B,\omega;\alpha}(k_{\parallel};\nu,\nu')=\int d^3x\,\chi_{k_{\parallel},\nu;\alpha}(\vec{x})\;\bar{\Sigma}_{B,\omega}(x)\,\chi^{*}_{\vec{k}_{\parallel},\nu';\alpha}(\vec{x})=$$

$$=\frac{1}{L_\alpha}\int dx\, f^{\alpha}_{\vec{k}_{\parallel},\nu}(x)\,\bar{\Sigma}_{B,\omega}(x)\,f^{\alpha}_{\vec{k}_{\parallel},\nu'}(x)$$

/19/

where the thickness of the metal sandwich is denoted by L_α. /$f_{\vec{k}_{\parallel},\nu}(x)$ can be chosen to be real and positive in the barrier./

The contribution of an impurity to the matrix element given by eq. /19/ is very sensitive to the relative position of the impurity and the barrier, namely

1, if the impurity is inside the barrier or on its surface the factor $f_{\vec{k}_{\parallel},\nu}(x)\,f_{\vec{k}_{\parallel},\nu'}(x)$ /$x \in$ B/ depends only on the energies ε_ν and $\varepsilon_{\nu'}$. This dependence is very weak and the contribution is purely imaginary,

2, if the impurity is in the metal sandwich its contribution to the matrix element is an oscillating function of its distance from the barrier. The most slowly oscillating part of the matrix element is proportional to

$$a\cos[(k_\perp-k_\perp')x]+b\sin[(k_\perp-k_\perp')x]$$

/2o/

as it is shown in Appendix I. These matrix elements are important only if they are taken between electron states lying in an interval of width ΔE around the Fermi energy, where ΔE is the energy region from which the largest contribution to the Kondo scattering comes.

We can introduce a coherence length similarly to the superconductivity

$$\xi_{\Delta E}=\frac{\pi v_F}{\Delta E}$$

/21/

where $v_F = \frac{k_F}{m}$ is the Fermi velocity[6]. If the impurity lies much nearer the barrier than the coherence length $\xi_{\Delta E}$, then the factor given by eq. /2o/ is positive and independent of indexes k_l and k_l' for matrix elements taken between the interesting electron states discussed above.

Thus the matrix elements given by eq. /19/ can be regarded to be independent of the indices ν and ν', if the impurities are inside the barrier or in the metal not far from the metal-metal oxide interface. In this section we investigate the former case. The role played by the impurities lying in the metal will be discussed in Sec. 5. From eq. /19/ we get

$$\overline{\Sigma}_{B,\omega;\alpha}(\vec{k}_{\parallel},\nu,\nu') \approx$$

$$\approx \int \bar{f}^{\alpha\,2}_{\vec{k}_{\parallel}}(x)\,\overline{\Sigma}_{B,\omega}(x)\,dx = \int \bar{f}^{\alpha\,2}_{\vec{k}_{\parallel}}(x)\,\Sigma_{\omega}(x)\,c(x)\,dx \qquad /22/$$

where $\bar{f}$ is an averaged wave function taken at the Fermi energy and c/x/ stands for the impurity concentration. It is supposed to depend only on the distance from the surface of the barrier. $\Sigma_{\omega}(x)$ is the contribution to the self-energy of one impurity in the space point x.

For the calculation of the current given by eq. /4/ the Green functions G or $\mathcal{G}$ with space variables lying in the barrier are needed, which may be written as

$$\mathcal{G}_{\omega;\alpha}(\vec{x},\vec{x}') = \frac{1}{\Omega_{\alpha}}\sum_{\vec{k}_{\parallel},\nu,\nu'} e^{i\vec{k}_{\parallel}(\vec{x}-\vec{x}')} f^{\alpha}_{\vec{k}_{\parallel},\nu}(x)\, f^{\alpha}_{\vec{k}_{\parallel},\nu'}(x')\,\mathcal{G}_{\omega;\alpha}(\vec{k}_{\parallel},\nu,\nu') \approx$$

$$\approx \frac{1}{F_{\alpha}}\sum_{\vec{k}_{\parallel}} e^{i\vec{k}_{\parallel}(\vec{x}-\vec{x}')}\,\bar{f}^{\alpha}_{\vec{k}_{\parallel}}(x)\,\bar{f}^{\alpha}_{\vec{k}_{\parallel}}(x')\,\overline{\mathcal{G}}_{\omega;\alpha}(\vec{k}_{\parallel}) \qquad /23/$$

where we have made use of eqs. /11/ and /16/a/, moreover

$$F_{\alpha} = \frac{\Omega_{\alpha}}{L_{\alpha}} \quad \text{and} \quad \overline{\mathcal{G}}_{\omega;\alpha}(\vec{k}_{\parallel}) = \frac{1}{L_{\alpha}}\sum_{\nu,\nu'}\mathcal{G}_{\omega;\alpha}(\vec{k}_{\parallel},\nu,\nu') \qquad /24/$$

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[6] The spin polarization around the impurity becomes negligible outside of a similar distance. See Nagaoka's work, ref. [24]

Taking the matrix elements of the Dyson equation, eq. /18/a/ and averaging according to eq. /24/, by making use of eq. /19/ we have

$$\overline{\mathcal{G}_{\omega;\alpha}(\vec{k}_{\parallel})} = \overline{\mathcal{G}^{(0)}_{\omega;\alpha}(\vec{k}_{\parallel})} + \overline{\mathcal{G}^{(0)}_{\omega;\alpha}(\vec{k}_{\parallel})}\;\overline{\Sigma_{B,\omega}(\vec{k}_{\parallel})}\;\overline{\mathcal{G}_{\omega;\alpha}(\vec{k}_{\parallel})}$$

/25/

where

$$\overline{\mathcal{G}^{(0)}_{\omega;\alpha}(\vec{k}_{\parallel})} = \frac{1}{L_{\alpha}} \sum_{\nu} \mathcal{G}^{(0)}_{\omega;\alpha}(\vec{k}_{\parallel};\nu)$$

/26/

The solution of equation /25/ is

$$\overline{\mathcal{G}_{\omega;\alpha}(\vec{k}_{\parallel})} = \overline{\mathcal{G}^{(0)}_{\omega;\alpha}(\vec{k}_{\parallel})} \quad \frac{1}{1 - \overline{\Sigma}_{B,\omega;\alpha}(\vec{k}_{\parallel})\;\overline{\mathcal{G}^{(0)}_{\omega;\alpha}(\vec{k}_{\parallel})}}$$

/27/

The spectral representation of the averaged Green function is

$$\overline{\mathcal{G}_{\omega;\alpha}(\vec{k}_{\parallel})} = \int \frac{\overline{\varrho_{\alpha}(k_{\parallel};E')}}{i\omega - E'}\, dE'$$

/28/

Comparing eq. /28/ with eqs. /16/a/ and /24/ we get

$$\overline{\varrho_{\alpha}(\vec{k}_{\parallel};E)} = \frac{1}{L_{\alpha}} \sum_{\nu,\nu'} \varrho_{(\vec{k}_{\parallel},\nu)(\vec{k}_{\parallel},\nu');\alpha}(E) > 0$$

which is positive because it is symmetrical in the indices. /29/

The spectral function can be obtained from eq. /28/ by the spectral theorem

$$\overline{\varrho_{\alpha}}(\vec{k}_{\parallel}) = -\frac{1}{2\pi i}\left\{ \overline{\mathcal{G}(\vec{k}_{\parallel})}_{i\omega = E + i\varepsilon;\alpha} - \overline{\mathcal{G}(\vec{k}_{\parallel})}_{i\omega = E - i\varepsilon;\alpha} \right\}$$

/30/

The unperturbed averaged Green function, given by eq. /26/ can be calculated easily

$$\overline{\mathcal{G}^{(0)}(\vec{k}_{\parallel})}_{i\omega = E \pm i\varepsilon;\alpha} = \frac{1}{L_{\alpha}} \sum_{\nu} \frac{P}{E - \varepsilon_{\vec{k}_{\parallel},\nu;\alpha}} \mp i\pi\, \varrho_{0;\alpha}(\vec{k}_{\parallel};E)$$

/31/

where $\rho_{0;\alpha}(\vec{k}_\parallel,E)$ is the partial density of states for a given wave vector $\vec{k}_\parallel$. The first sum gives only a small contribution for $E \ll E_F$ and thus can be neglected. A detailed discussion of this approximation will be given in Sec. 5. In this way we have

$$\overline{G^{(0)}_{i\omega=E\pm i\varepsilon;\alpha}(\vec{k}_\parallel)} = \mp i\pi\rho_{0;\alpha}(\vec{k}_\parallel) \qquad /32/$$

where $\rho_{0;\alpha}(k_\parallel) = \rho_{0;\alpha}(k_\parallel; E=0)$ i.e. a weak dependence of the density of states on the energy is assumed.

Comparing eqs. /32/ and /27/ and using the spectral theorem, eq./30/, we get the following expression of the averaged perturbed spectral function

$$\overline{\rho_\alpha(\vec{k}_\parallel;E)} = \frac{\rho_{0;\alpha}(\vec{k}_\parallel)}{1+\pi\rho_{0;\alpha}(\vec{k}_\parallel)\dfrac{1}{2\tau_\alpha(\vec{k}_\parallel;E)}} \qquad /33/$$

where τ_α, which is a quantity of relaxation time type, is defined through the purely imaginary self-energy as

$$\overline{\Sigma_{B,i\omega=E\pm i\varepsilon;\alpha}(\vec{k}_\parallel)} = \mp i\,\frac{1}{2\tau_\alpha(\vec{k}_\parallel;E)} \qquad /34/$$

The derivation of formula /33/ is one of the crucial points of our theory. Its generalization to the case in which there are impurities also in the metal will be given in Sec. 5.

4. Expression of the total current

The total current can be determined by inserting the particular Green functions given by eqs. /14/, /16/a/, /29/ and /33/ into the general current formula, eq. /4/. As it is shown in Appendix II the current may be expressed by the spectral functions $\rho_\alpha(\vec{k}_\parallel;E)$ /α =l,r/ in the following way

$$T(V) = 4\pi e\sum_{\vec{k}_\parallel}|T(\vec{k}_\parallel)|^2\int dE\,\bar{\rho}_l(\vec{k}_\parallel;E)\,\bar{\rho}_r(\vec{k}_\parallel;E+eV)\cdot\left\{n_F(E)-n_F(E+eV)\right\} \qquad /35/$$

where $T(\vec{k}_\parallel)$ is the tunneling matrix element and V is the applied bias. This formula is a generalization of the one valid in the free electron model.

The spectral function $\rho_\alpha(\vec{k}_{\parallel};E)$ has different physical interpretations for different systems as illustrated in Table I.

TABLE I

Physical interpretation of the spectral function for different systems

Formula	Physical interpretation	System
$\rho_0(\vec{k}_{\parallel};E)$	one particle density of states	free electron model
$\rho_{tun}(\vec{k}_{\parallel};E) = \sum_{k_\perp}\rho(\vec{k}_{\parallel},k_\perp;E)$	tunneling density of states [27]	strong coupling superconductors
$\rho_{local}(\vec{k}_{\parallel};E) = \rho_0(\vec{k}_{\parallel};E)Z(\vec{k}_{\parallel};E)$	local density of states	local barrier effects

The tunneling density of states has been introduced by Schrieffer, Scalapino and Wilkins [27] for strong coupling superconductors. As this quantity reflects the spectrum of the bulk material, the summation index ν may be replaced by the wave vector perpendicular to the barrier surface $k_\perp$. This density of states may be essentially different from the usual one calculated from the dispersion relation of the one particle excitations which enters the thermodynamic quantities of an interacting electron gas[7].

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[7] Recently is has been pointed out, that heat capacity of dilute magnetic alloy in homogeneously polarized state is determined by the tunneling density of states instead of the thermodynamic one, if the Kondo Hamiltonian assumed. J.Sólyom and A.Zawadowski, physica status solidi, to be published.

In the case discussed here the spectral function cannot be replaced by the bulk one, because it is depressed near the barrier due to paramagnetic impurities. The measure of the depression is the renormalization factor

$$Z(\vec{k}_{\parallel}; E) = \frac{\rho(\vec{k}_{\parallel}; E)}{\rho_0(\vec{k}_{\parallel}; E)} \qquad /36/$$

which in the present case according to eq. /33/ is

$$Z_{\alpha}(\vec{k}_{\parallel}; E) = \frac{1}{1+\pi\rho_{0;\alpha}(\vec{k}_{\parallel})\,\dfrac{1}{2\tau_{\alpha}(\vec{k}_{\parallel}; E)}} \qquad /37/$$

As it has been mentioned before, it is only the states with $\vec{k}_{\parallel} \approx 0$ that contribute appreciably to the total current, therefore the renormalization constant can be replaced by its value for $\vec{k}_{\parallel} = 0$, i.e.

$$Z_{\alpha}(E) = Z_{\alpha}(\vec{k}_{\parallel} = 0; E) = \frac{1}{1+\pi\rho^{(0)}_{\parallel;\alpha}\,\dfrac{1}{2\tau_{\alpha}(E)}} \qquad /38/$$

where $\tau_{\alpha}(\vec{k}_{\parallel} = 0; E) = \tau_{\alpha}(E)$

The corresponding density of states is

$$\rho^{(0)}_{\parallel;\alpha} = \rho_{0;\alpha}(\vec{k}_{\parallel} = 0) = \frac{1}{\pi}\,\frac{m}{p_0} = \rho_0\,\frac{1}{N_s z} \qquad /39/$$

where p_0 is the Fermi momentum, $\rho_0 = \frac{p_0 m}{2\pi^2}$ is the density of states at the Fermi level, N_s is the surface density of atoms which is defined taking a surface orthogonal to one of the crystallographic axes in a cubic crystal and z is a number of order unity.

Inserting eq. /39/ into eq. /38/ wo get the final results

$$Z_{\alpha}(E) = \frac{1}{1+\rho_0\,\dfrac{\pi}{N_s z}\,\dfrac{1}{2\tau_{\alpha}(E)}} \qquad /40/$$

It is worth mentioning that the renormalization factor always leads to a depression of the density of states at the barrier and never to an enhancement. /See Fig. 2/b./

5. Dependence of the renormalization factor on the positions of the impurities

The renormalization constant Z/E/, given by eq. /4o/ depends on the relaxation time τ , which is determined by the matrix element /19/. This matrix element is composed of the imaginary part of the self-energy, $Im\,\Sigma_{\omega}(R)$, corresponding to one impurity.

$Im\,\Sigma_{\omega}(R)$ is a functional of the energy spectrum $\rho(\vec{R};E)$ of the electron density at the impurity site $\vec{R}$ through the intermediate states. Using the Kondo Hamiltonian, eq. /6/, we get the following structure

$$Im\,\Sigma_{\omega}(\vec{R}) = \frac{J}{N} s_{\omega}\left(\left\{\frac{J}{N}\rho(\vec{R};E)\right\}\right) \qquad /41/$$

where s is a function of ω and a functional of its argument. Inserting eq. /41/ into eq. /22/ we have

$$\frac{1}{2\tau(\vec{k}_{\parallel};E)} = Im\,\overline{\Sigma_{B,\,i\omega=E-i\varepsilon}(\vec{k}_{\parallel})} = \frac{J}{N}\int f_{\vec{k}}^{-2}(x)\, \underset{i\omega=E-i\varepsilon}{s}\left(\left\{\frac{J}{N}\rho(x;E)\right\}\right) c(x)\, dx \qquad /42/$$

In eq. /42/ the longitudinal components of the wave functions have been replaced by the average value $\bar{f}$ taken at the Fermi level. This is a good approximation provided the impurities lie nearer the barrier than the coherence length $\xi_{\Delta E}$ introduced in eq. /21/. The energy dependence of the density of states at the impurity site $\vec{R}$ can be determined from the Green function $\mathcal{G}$ as

$$\rho(\vec{R};E) = \frac{1}{\pi} Im\,\mathcal{G}_{i\omega=E-i\varepsilon}(\vec{R},\vec{R}) \qquad /43/$$

Making use of eq. /16/a-b/, /11/ and /29/ we obtain

$$\rho(\vec{R};E) = \int \frac{d^2\vec{k}_{\parallel}}{(2\pi)^2}\, \bar{\rho}(\vec{k}_{\parallel};E)\, \bar{f}^{\,2}_{\vec{k}_{\parallel}}(\vec{R}) \qquad /44/$$

We have derived a coupled system of equations consisting of eqs. /33/, /42/ and /44/ for the renormalization factor Z/$\vec{k}_{\parallel}$;E/ and for $\bar{\rho}$/$k_{\parallel}$;E/. We should determine $\bar{\rho}\,(k_{\parallel};E)$ from this system of equations in a selfconsistent way which is important in all cases, where the relative amplitude of the effect is not small /e.g. if Z/E/< 0,8 at some energy values/.

For the investigation of the dependence of the renormalization factor on the position of the impurities relative to the barrier we have to recall that when solving the Dyson equation, eq. /18/b/ it has been supposed that the matrix element $\bar{\Sigma}_{B,\omega}(k_{\parallel},\nu,\nu')$ given by eq./22/ is independent of the indices ν and ν' in an energy region near the Fermi level. If the impurities lie inside the metal, the distance d of the impurity from the surface of the barrier and the energy interval ΔE where the matrix element is independent of ν and ν' are connected by a relation similar to eq. /21/. We require this independency for an energy interval larger than kT, eV and kT_K, where kT_K[8] is the energy interval in which the Kondo scattering is effective. If the impurities lie nearer the metal-metal oxide interface than the Kondo coherence length ξ_{kT_K}, given by

$$\xi_{kT_K} = \frac{\pi v_F}{kT_K} \qquad /45/$$

the above supposition holds and this makes possible to write the second term on the rigth hand side of eq. /25/ as a product.

The problem can be greatly simplified if the real part of $\bar{q}^{(0)}$ in eq. /31/ vanishes, i.e.

$$\sum_{\nu} \frac{P}{E-\varepsilon_{\nu}} \approx 0$$

This is true if the summation over ν extends to an energy interval ΔE^{*} at least an order of magnitude larger than the energy intervals discussed above, $kT_K \ll \Delta E^{*}$. Therefore we require that the matrix element $\bar{\Sigma}_{B,\omega}(k_{\parallel},\nu,\nu')$ be independent of the indices ν and ν in the energy interval ΔE^{*} around the Fermi energy. According to the above considerations the maximal distance d_{max} of the impurities from the surface of the barrier is limited by the condition

$$d_{max} \ll \xi_{\Delta E} \ll \xi_{kT_K} \qquad /46/$$

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[8] The definition of the Kondo temperature is $kT_K=1.14E_0$, where E_0 is given by /55/.

where $$\xi_{\Delta E^{*}} = \frac{\pi v_F}{\Delta E^{*}}$$

This means that the distance d_{max} must be smaller than the Kondo coherence length ξ_{kT_K} by at last one order of magnitude.

If the thickness of the impurity layer on the barrier satisfies the condition /46/, then the matrix element /22/ of the self-energy is proportional to the impurity concentration. The amplitude of the zero bias anomalies can be increased by evaporating more impurity atoms. It can be shown, however, that in the limit when the metal on one side is a dilute alloy with homogeneously distributed impurities the tunneling density of states does not change due to the impurities. The present theory can not be applied to the case in which the thickness of the impurity layer is larger than d_{max}.

It seems reasonable that there is an optimal thickness of the impurity layer, i.e. when the effect of the impurities is the largest.

In a dilute alloy the self-energy averaged over the positions of impurities is independent of the space variables and according to eq./19/ it is diagonal in the indices. The Dyson equation, eq. /18/b/ is

$$\mathcal{G}_{\omega,\alpha}(\vec{k}_{\parallel},r,r') = \mathcal{G}^{(o)}_{\omega,\alpha}(\vec{k}_{\parallel},r)\delta_{r,r'} + \mathcal{G}^{(o)}_{\omega,\alpha}(k_{\parallel},r)\bar{\Sigma}_{B,\omega}(\vec{k}_{\parallel},r)\mathcal{G}_{\omega,\alpha}(\vec{k}_{\parallel},r,r') \qquad ./47/$$

where $\Sigma_{B,\omega}(\vec{k}_{\parallel},r) = \Sigma_{B,\omega}(\vec{k}_{\parallel},r,r)$. Now the first term in the expression of $\bar{\mathcal{G}}^{(o)}_{\omega}$ given by eq. /31/ cannot be neglected. Assuming that the exhange coupling constant is independent of the momenta the self-energy of the electrons in a dilute alloy depends only on the energy. The spectral function $\rho_{\lambda;\alpha}(E)=\delta_{\lambda,\lambda'}=\rho_{\lambda,\lambda';\alpha}(E,r,r')$ given by eq. /16/b/ can be calculated using the spectral theorem, eq. /30/, and we get

$$\rho_{\lambda;\alpha}(E) = \frac{1}{\pi}\,\frac{Im\,\bar{\Sigma}_{\omega;\alpha}}{(E-\varepsilon_{\lambda}-Re\,\bar{\Sigma}_{\omega;\alpha})^2+(Im\,\bar{\Sigma}_{\omega;\alpha})} \qquad /48/$$

The tunneling density of states given in Table I is

$$\rho_{tun;\alpha}(k_{\parallel};E) = \frac{1}{\pi}\sum_{r}\frac{Im\,\bar{\Sigma}_{\omega,\alpha}}{(E-\varepsilon_{\vec{k}_{\parallel},r}-Re\,\bar{\Sigma}_{\omega;\alpha})^2+(Im\,\bar{\Sigma}_{\omega;\alpha})^2} \qquad /49/$$

Neglecting the energy dependence of the unrenormalized density of states we get

$$\rho_{tun;\alpha}(\vec{k}_{\parallel};E)=\rho_{o;\alpha}(\vec{k}_{\parallel}) \qquad /5o/$$

Thus there is no bulk effect in the tunneling density of states due to the impurities. This result suggests that the amplitude of the effect becomes smaller if the dependence of the matrix elements /19/ on the indices v , v' starts to set in.

The problem of the impurities in the barrier is much more simple. The deeper the impurity is in the barrier the more the averaged amplitude of the electron wave function decreases. This amplitude occure in the self-energy, eq. /42/ explicitly and in the argument of the function s through the density of the intermediate states. Because the function s is of higher order in the coupling constant, the impurities in the barrier far from the surface do not give an essential contribution to eq. /42/. A rough estimate of the averaged wave function $\bar{f}$ as a function of the space variable measured from the barrier surface shows that the impurities in the second atomic layer of the barrier cause already very small effect.

This we may conclude that only the impurities found in the metal sandwich inside the Kondo coherence length[9] and in the first and second atomic layers of the barrier are important from the point of view of the local tunneling anomalies.

This change in the local energy spectrum of the conduction electrons appears only in the range of the coherence length. This statement can be proved using the accurate expression of the local energy spectrum

$$\rho_{\alpha}(\vec{R};E)=\frac{1}{L_{\alpha}}\sum_{v,v'}\int\frac{d\vec{k}_{\parallel}^{2}}{(2\pi)^{2}}f_{\vec{k}_{\parallel},v;\alpha}(\vec{R})\rho_{\alpha}(\vec{k}_{\parallel},v,v';E)f_{\vec{k}_{\parallel},v\;;\alpha}(\vec{R}) \qquad /51/$$

The product of the two wave functions is given by eq. /22/. They can be replaced by the averaged wave functions if the space variable $\vec{R}$ is inside of the coherence length. Outside of the coherence length the effect of the impurities is destroyed by the interference of the wave functions as illustrated in Fig. 2/b.

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[9] As we have seen homogeneously distributed impurities cause no effect in the tunneling density of states. Therefore the inhomogeneous part ot the distribution function appearing inside of the coherence length contributes to the zero bias anomalies.

CHARACTERISTICS

6. General behaviour of the characteristics

Now let us discuss the formula /35/ of the current There are two possible construction of the samples. Namely, if

1, there are impurities only on one side of the barrier,

2, there are impurities on both sides of the barrier.

The first possibility is realized in experiments where paramagnetic impurities are evaporated on one of the surfaces of the barrier [7],[8] while the second one is the case of junctions with oxide layer consisting of paramagnetic atoms or ions [1],[2].

At zero temperature the current formula, eq. /35/ is simplified to the following one

$$I(V)\sim\int_0^{eV} dE\,\rho_{0;l}(E)Z_l(E)\rho_{0;r}(E+eV)Z_r(E+eV) \qquad /52/$$

where all quantities are taken $\vec{k}_{\parallel}\sim 0$ as in eqs. /38-4o/.

An essential simplification appears, if there are impurities only on one side of the barrier and the bulk density of states of the metals can be taken to be constants. Thus we get

$$I(V)\sim\rho_{0;l}\,\rho_{0;r}\int_0^{eV} dE\,Z_l(E) \qquad /53/$$

In general dynamical conductance can be determined by taking the derivative of the current, eq. /35/. At finite temperatures this derivative, however, contains integrals, which in general can be calculated only by a computer. The case discussed above is an exception and we get the following simple expression for dynamical conductance and resistivity from eq. /53/

$$G(V)=\frac{dI(V)}{dV}=Z_l(eV) \qquad R(V)=G(V)^{-1}=\frac{1}{Z_l(eV)} \qquad /54/$$

and

This is a good approximation at finite temperatures too, provided $eV \gg kT$ and the variation of the renormalization constant Z/E/ is small enough in intervals of the order kT, i.e. if

$$\left.\frac{\partial Z_\ell}{\partial E}\right|_{E=eV} \cdot kT \ll Z_\ell(eV)$$

7. Scattering amplitudes

For the calculation of the renormalization constant eq. /38/ and the characteristics we need analitical forms of the scattering amplitudes. Here we do not want to give a critical discussion of the Kondo problem and the determination of the scattering amplitude[10]. Our aim is to give the most important features of the dynamical conductance /or resistivity/ for the typical scattering amplitudes, found in the current literature.

The simplest form of the scattering amplitude can be obtained in the third order of perturbation theory, the applicability of which, however, is very limited [23]. We shall discuss this case in Sec. 9.

Using nonperturbative methods a great variety of theoretical results have been derived. These results especially for antiferromagnetic coupling lead to different physical consequences. We restrict ourselves to three types here.

1. Abrikosov type [23]: The scattering amplitude shows maxima at energies $\pm E_0$ corresponding to resonant scattering. The energy of the resonance is

$$E_o = E_c \exp\left\{ + \frac{N}{2 J \rho_o} \right\} \qquad /55/$$

where E_c is a cut-off energy determined by the band width and locality of the interaction in space. The usually accepted values lie in the interval loo meV $< E_c <$ lo eV, where the upper limit corresponds to the band width and the lower one to the locality [28]. The imaginary self-energy due to one impurity at site $\vec{R}$, is

$$\operatorname{Im} \Sigma_{i\omega = E \pm i\varepsilon}(\vec{R}) = \mp \frac{1}{2\tau_o(\vec{R})} \left\{ \left[1 + \frac{2J\rho^{(o)}(\vec{R})}{N} \ln \frac{E_c}{|E|} \right]^2 + \left(\frac{2J\rho^{(o)}(\vec{R})}{N} \right)^2 x^2 \right\}^{-1} \qquad /56/$$

where

$$\frac{1}{2\tau_o(\vec{R})} = \left(\frac{J}{N} \right)^2 S(S+1)\, \pi \rho^{(o)}(\vec{R}) \qquad /57/$$

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[10] See the current literature in ref. [23-25].

As compared to the original Abrikosov's one this expression has been completed by a further term containing the parameter $\varkappa^2$ to avoid the occuring divergence. The parameter $\varkappa^2$ has been estimated by Yosida and Okiji [29] and found to be $\varkappa^2 = S(S+1)\frac{\pi^2}{4}$ [11]. The validity of the scattering amplitudes, eq. /56/, is questioned this time for low temperatures $kT < E_0$, because of the apperance of an inadmissible complex pole of the scattering amplitude on the physical sheet.

When calculating the characteristics for different models we will accept the scattering amplitude in eq. /56/ for the resonant scattering model.

2, Suhl-Wong type [23]: There is a sharp maximum in the scattering amplitude, but its energy is always comparable with the temperature.

3, Nagaoka type [24]: At low enough temperatures a quasibound state of the localized spin and a conduction electron occurs. The transition temperature corresponding to the formation of the quasibound state is

$$kT_c \approx 1,14\, E_0 \qquad /58/$$

and the imaginary self-energy is given by

$$Im \sum_{i\omega = E \pm i\varepsilon} (\vec{R}) = \mp \frac{1}{\pi \rho^{(0)}(\vec{R})} \frac{E_0^2}{E_0^2 + E^2}. \qquad /59/$$

where, in Nagaoka's notation, $E_0 = \Delta$

This solution exhibits a maximum in the scattering amplitude at zero energy and it might be regarded as some type of resonance with zero energy.

The different imaginary self-energies are plotted in Fig. 3/a-c/.

8. Characteristics in perturbation theory

We treat the renormalization constant up to third order of perturbation theory. This problem has been investigated by Appelbaum applying the tunneling Hamiltonian method [3], [4] and by one of the authors in the way presented here [6]. The use of perturbation theory can be expected to be justified if at all only for ferromagnetic coupling in which case the problem of a resonant or bound state does not arise. It will be seen in the next section that the validity of the results calculated up to third order is restricted to high energies, the region of applicability, however, can be extended by replacing the coupling constant and other parameters by

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[11] Further discussion can be found in Appendix III.

effective values. Appelbaum's and the present results are compared in Sec. 12.

For the determination of the self-energy we have to apply the thermodynamic Green functions with complex time variables[12]. The self-energy operator Σ is calculated in Abrikosov's fictitious fermion operator technique [23]. The second and third order contributions to the self-energy are given in Figs. 4/a-b/, respectively. In these diagrams the propagators of fictious fermions are represented by dotted lines while the solid lines stand for the electron propagators.

After the analytical continuation in the energy variable the self-energy up to third order is given by

$$Im\, \Sigma^{(3)}_{i\omega = E \pm i\varepsilon;\, \sigma, \sigma'}(\vec{R}) =$$

$$= \mp \delta_{\sigma,\sigma'} \frac{1}{2\tau_0(\vec{R})} \left(1 - \frac{4J}{N} \rho^{(0)}(\vec{R}) \ln \frac{E_c}{|E|} \right) \qquad /60/$$

where eq. /57/ has been used. E_c stands for the cutoff energy.

The density of states at the site $\vec{R}$ of the impurity is expressed by the averaged amplitude of the wave functions of the intermediate states at the Fermi level as

$$\rho^{(0)}(\vec{R}) = \sum_{\alpha = l,r} \overline{|f_\alpha(\vec{R})|^2}\, \rho_{0;\alpha} \qquad /61/$$

where

$$\rho^{(0)}_\alpha \overline{|f_\alpha(\vec{R})|^2} = \int \frac{d\vec{k}_{\parallel}^{2}}{(2\pi)^2} \rho_\alpha(\vec{k}_\parallel, E - E_F) \overline{|f_{\vec{k}_\parallel, v_F}(\vec{R})|^2} \qquad /62/$$

and v_F is defined by $\varepsilon(k_\parallel, v_F) = 0$

The electrons on both sides contribute to the density of the intermediate states as shown by eq. /6o/. As only the impurities at the barrier surfaces are effective, $\vec{R}$ has to be near one of the surfaces and the contribution of the electrons on the opposite side of the junction can be neglected.

Hitherto the impurity site $\vec{R}$ has been fixed and now an average over the possible impurity sites will be taken. It is worth mentioning that in Abrikosov's approach each self-energy term containing a fictitious fermion loop is averaged separately.

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[12] The application of the time dependent Green function technique is responsible for the occurence of some incorrect factors $/1-2n_F/E//$ in the works of ref. [6] and [16].

According to eq. /4o/, using the self-energy correction, eq. /6o/, the first correction to the renormalization constant Z/E/ is

$$Z(E) = 1 - \frac{\pi}{N_s Z}\,\rho_o \cdot \frac{1}{2\tau^{(3)}(E)} \qquad /63/$$

where, from eq. /22/

$$\frac{1}{2\tau^{(3)}(E)} = \int dR\, c(R)\, \bar{f}^{-2}_{\vec{k}_\parallel = 0}(R)\, \frac{1}{2\tau_o(R)} \left\{ 1 - \frac{4J}{N}\rho^{(o)}(R) \log\frac{E_c}{|E|} \right\} \qquad /64/$$

Only the part of the renormalization constant containing the logarithmic term characteristic to the Kondo effect is interesting. Using eqs. /63-64/ and /57/ this part, as generalized to finite temperatures, is approximately given by

$$\Delta Z^{(3)}(E) = \frac{4\pi}{N_S^{Z}}\,\rho^{(o)} S(S+1)\left(\frac{J}{N}\right)^3 \int dR\, c(R)\, \bar{f}^{-2}_{\vec{k}_\parallel = 0}(R)\, \rho^{(o)2}(R) \log\frac{E_c}{|E| + \alpha kT} \qquad /65/$$

The term $\log\frac{E_c}{|E|}$ has been replaced by $\log\frac{E_c}{|E| + \alpha kT}$, which is a good approximation with the value $\alpha = 1$ as pointed out by Appelbaum [4]. The anomalous tunneling current due to the energy dependence of the renormalization constant is

$$\Delta I^{(3)}(V) \sim \rho_{0;l}\,\rho_{0;r} \int \left(n_F(E) - n_F(E + eV) \right) \left\{ \Delta Z_l^{(3)}(E) + \Delta Z_r^{(3)}(E + eV) \right\} dE \qquad /66/$$

If there are impurities only on one side of the barrier, the anomalous part of the conductance for large bias eV > kT, using eq. /54/, becames

$$\Delta G^{(3)} \sim \Delta Z^{(3)}(eV) \qquad /67/$$

Using eq. /65/, we get the following ratio

$$\frac{\Delta G^{(3)}}{G_o} = \frac{4\pi}{Z} S(S+1)\, \frac{N^{(3)}_{i,eff}}{N_S} \left(\frac{J}{N}\right)^3 \rho_o^{\,3} \log\frac{E_c}{|eV|} \qquad /68/$$

where the effective surface density of impurities, $N_{i,eff}$, is given by

$$N^{(3)}_{i,eff} = \int \bar{f}^{-2}_{\vec{k}_\parallel = 0}(R) \left\{ \overline{|f(R)|^2} \right\}^2 c(R)\, dR \qquad /69/$$

This is the actual density of impurities if the impurities are on the surface of the barrier or in the metal.

The temperature dependence of the anomaly at zero bias can be obtained if a new variable of integration, $x = \frac{E}{kT}$, , is introduced in the current formula, eq. /66/. Using eq./65/ we get

$$\frac{\Delta G^{(3)}}{G_0}\bigg|_{V=0} = 4\pi S(S+1) \sum_{\alpha=l,r} \left(\frac{J_\alpha}{N_\alpha}\right)^3 \varrho^3_{0;\alpha} \frac{1}{Z_\alpha} \frac{N^{(3)}_{i,eff;\alpha}}{N_{S,\alpha}}$$

$$\left\{ \int \frac{dn(x)}{dx} \log(x+1)\, dx - \log \frac{kT}{E_{c;\alpha}} \right\} \qquad /70/$$

which shows a logarithmic dependence on the temperature. This result corresponding to a conductance maximum for ferromagnetic and resistivity maximum for antiferromagnetic coupling. This derivation suffers from the weakness that the expression of the renormalization constant, eq. /40/, and the imaginary self-energy, eq. /56/, have been expanded into a power series. These approximations are correct only for high energies or large bias.

9. Characteristics in nonperturbative treatment

In the last section we obtained results containing logarithmic terms, which are not small for energies near the Fermi energy and thus showing the need of nonperturbative treatment, as has been pointed out by the authors [16].

In this section the current-voltage characteristics are discussed using different expressions for the electron life-time. Our aim is to find the connection between the life-time and the characteristics.

a, Abrikosov type formula

The life-time corresponding to the resonance scattering can be described by Abrikosov's formula eq. /5/, which can be written in a more practical form as

$$Im \Sigma_{i\omega = E \pm i\varepsilon}(\vec{R}) = \mp \frac{\pi}{4} S(S+1) \frac{1}{\rho^{(0)}(\vec{R})} \left[\left(\log \frac{E_0(\vec{R})}{|E| + kT} \right) + x^2 \right]^{-1} \qquad /71/$$

where the characteristic energy $E_0/\vec{R}/$ is defined similarly to eg. /55/

$$E_0(\vec{R}) = E_C \exp \left\{ \frac{N}{2J\rho^{(0)}(\vec{R})} \right\}$$

According to eqs. /34/ and /22/ the imaginary part of the self-energy occuring in the renormalization factor, eq. /4o/, is

$$\frac{1}{2\tau_{k_{\parallel}=0}(E)}=\frac{\pi}{4}S(S+1)\int dR\ c(R)\ f^{-2}_{\vec{k}_{\parallel}=0}(R)\frac{1}{\left(\log\frac{E_0(R)}{|E|+kT}\right)^2+\varkappa^2}\ \frac{1}{\rho^{(0)}(R)}$$

/73/

Considering impurities only inside of the metal we get $\rho^{(0)}(R)=\rho_0$ from eq. /61/ and $E_0/R/=E_0$ from eqs. /55/ and /72/. The corresponding expression for the renormalization factor is

$$Z(E)=\left\{1+\frac{1}{2}\frac{\pi^2}{4}S(S+1)\frac{N_i}{N_s}\frac{1}{\left[\log\frac{E_0}{|E|+\alpha kT}\right]^2+\varkappa^2}\right\}^{-1}$$

/74/

where N_i is the surface density of impurities. By introducing the following notations

$$t=\frac{kT}{E_0},\quad v=\frac{eV}{E_0},\quad \varepsilon=\frac{|E|}{E_0},\quad a^2=\frac{1}{2}\frac{\pi^2}{4}S(S+1)\frac{N_i}{N_s}$$

/75/

eq. /74/ goes over to the somewhat simpler form

$$Z(E)=\frac{\log^2(\alpha t+\varepsilon)+\varkappa^2}{\log^2(\alpha t+\varepsilon)+\varkappa^2+\alpha^2}<1.$$

/76/

Z/E/ is plotted for the cases of ferromagnetic and antiferromagnetic coupling on Figs. 7/a-b/, respectively. Let'us discuss first the ferromagnetic case.

1, Ferromagnetic coupling: J > 0. From the definition of the parameter E_0, eq. /55/, follows that $E_0 \gg E_c$, because $\frac{2|J|\rho_0}{N}\approx 0{,}01-0{,}2$. On the other hand $|E|<E_c$ therefore $\varepsilon\ll 1$ and $t\ll 1$. According to eq. /76/ Z/E/ is a monotonically decreasing function of the energy. For t=o Z/E/ assumes its maximal value, MaxZ/E/=1, at $\varepsilon=0$ and its minimal one,

MinZ/E/=$1-\frac{a^2}{(\log\frac{E_c}{E_0})^2+\varkappa^2+a^2}$, at the cut-off energy, E_c. We can estimate MinZ/E/ substituting reasonable values for the parameters, namely $\varkappa^2=2$, in the case of a monoatomic impurity layer $a^2=5-10$ and $\left(\log\frac{E_c}{E_0}\right)^2>25-100$. Thus we get MinZ/E/ > 0,9 or at least MinZ/E/ > 0,75. The energy dependence of the renormalization factor is very smooth and the relative amplitude of the effect is small.

Two typical conductance curves corresponding to impurities on one and both sides of the barrier are shown on Fig. 8/a-b/. The dynamical conductance is plotted against the logarithm of the voltage in Fig. 9 and the zero bias conductance against the temperature in Fig. lo. It can be seen that the conductance does not show an exact logarithmic behaviour as a function of bias and temperature, though it can be approximated by simple logarithmic functions in restricted intervals, for the renormalization factor, eq. /76/, is constructed from logarithmic functions.

In the following the possibility of fitting the non-perturbative results, eq. /76/, by the perturbative ones, eqs. /68/ and /7o/, is discussed. First we determine the intervals of the variables in which the results of third order perturbation theory are valid.

As it has been mentioned before the condition that the imaginary part of the self-energy as well as the renormalization factor Z/E/ can be expanded into a series in powers of the coupling constant is

$$\frac{2|J|\,\rho^{(0)}(R)}{N}\;ln\frac{E_c}{|E|} << 1 \qquad /77/$$

The energy interval, in which this condition is fulfilled, depends on the value of the coupling constant. If the effective coupling constant $\frac{J\rho}{N}$ is large, eq. ~ 0,1 this condition is so strong that no energy region of physical interest is included.

On the other hand a formal fit might be derived which is valid for a rather wide energy and temperature interval. Let us introduce an other characteristic energy parameter $E_{c,eff}$ lying somewhere in the middle of the actually investigated energy interval. $E_{c,eff}$ satisfies the following inequality $E_{c,eff} << E_c$. The typical logarithmic term in eq. /76/ can be written in the following form

$$log\,(\varepsilon + \alpha t) = log\frac{|E| + \alpha kT}{E_o} =$$

$$= log\frac{|E| + \alpha\cdot kT}{E_{c,eff}} + log\frac{E_{c,eff}}{E_o} \qquad /78/$$

where from the choice of $E_{c,eff}$ follows that

$$\left| log\frac{|E| + \alpha kT}{E_{c,eff}} \right| \ll \left| log\frac{E_{c,eff}}{E_o} \right| \qquad /79/$$

On the basis of eq. /79/ eq. /76/ can be expanded in powers of $\left| log\frac{|E| + \alpha kT}{E_{c,eff}} \right|$ and to the first order we get

$$Z(E) = 1 - \frac{a^2}{\left(\log \frac{E_{c,eff}}{E_0}\right)^2 + a^2 + x^2} \left(1 - 2\frac{\log \frac{E_0}{E_{c,eff}}}{\left(\log \frac{E_{c,eff}}{E_0}\right)^2 + a^2 + x^2} \log \frac{E_{c,eff}}{|E| + \alpha kT}\right) \qquad /8o/$$

This can be compared with the expression of Z/E/ given by eq. /68/ after having it generalized to finite temperature. Namely eq. /8o/ can be brought to the same form as eq. /68/ provided the parameters in eq. /68/ are replaced by effective ones. In this way we get the following expression

$$\Delta Z(E) = 4\pi^2 S(S+1)\left(\frac{J_{eff}}{N}\right)^3 \frac{1}{z}\, \rho_0^3 \frac{N_i}{N_s} \log \frac{E_{c,eff}}{|E| + \alpha kT} \qquad /81/$$

with

$$\frac{2J_{eff}\rho_0}{N} = \sqrt[3]{\frac{\log \frac{E_0}{E_{c,eff}}}{\left[\left(\log \frac{E_0}{E_{c,eff}}\right)^2 + a^2 + \varkappa^2\right]^2}} \approx \left(\log \frac{E_0}{E_{c,eff}}\right)^{-1} \qquad /82/$$

where it has been supposed that $\left|\log \frac{E_{c,eff}}{E_0}\right| \gg 1,\ \varkappa^2, a^2$

Though $E_{c,eff}$ is much smaller than E_c, J_{eff} is of the same order of magnitude as J. The conclusion is, that the parameters, especially E_c, obtained by fitting the perturbative formula to the experimental data are not realistic.

2, <u>Antiferromagnetic coupling: J< 0.</u> According to eq. /55/ the characteristic energy E_0 has a very small value, $E_0 \ll E_c$, and also can be smaller than the temperature kT. The renormalization factor Z/E/ is plotted in Fig. 7/b. From eq. /76/ follows that

$$\lim_{E \to 0} Z(E) = \lim_{E \to \infty} Z(E) = 1 \qquad \text{for } T=0 \qquad /83/$$

The minimum of Z/E/ occurs at $E=E_0$ and the minimal value is

$$\operatorname{Min} Z(E) = \frac{\varkappa^2}{\varkappa^2 + a^2} \qquad /84/$$

The larger the constant a^2 or the higher the impurity concentration, the deeper the minimum.

Using the current formula, eq. /35/, and eq. /76/ for the renormalization constant the dynamical resistivity has been calculated by numerical integration. Typical characteristics are plotted on Fig. 11 for diodes with impurities on one side of the barrier. These curves show that the minimum in the resistivity at zero bias corresponding to the maximum of Z/E/ at E=0 can be observed only in those cases in which $3kT < E_0$ because otherwise the characteristics are smoothed out. A characteristic resistivity curve is given in Fig. 12 for large bias on logarithmic scale. While the occurence of a resistivity maximum which may have quite a large value is a common feature of the curves shown on Figs. 11 and 12, the occurrence of the local minimum depends on the parameter values.

The resistivity maximum is a consequence of the depression of the density of electrons around the Fermi energy. If the depression is large the change in the energy spectrum of the electrons can be expected to cause an essential modification of the scattering amplitude too. Therefore a selfconsistent solution would be necessary which is, however, not feasible due to the fact that no analytical form of the scattering amplitude is available for energy dependent density of states.

To illustrate the consequences of the selfconsistency we will treat the problem in a crude approximation.

The scattering amplitude of an electron with energy E depends on the density of states and especially on that of the most probably excited intermediate states, whose energies are close to the incoming energy E. We will consider the approximation in which the density of states in the scattering amplitude at energy E is replaced by the renormalized density of states taken at the same energy. This approximation is good if the dependence of the renormalization factor on the energy is weak. The characteristic constant E_0 appearing in eq. /73/ becomes energy dependent

$$E_o(Z) = E_c \exp\left\{-\frac{N}{2|J|\rho_o Z(E)}\right\} \qquad /85/$$

as a consequence of the energy dependence of the density of states. In this way from eq. /74/ we get

$$Z^{-1}(E) = 1 + \frac{a^2}{\left(\log\frac{E}{E_o(Z)}\right)^2 + \varkappa^2} \qquad /86/$$

Solving eq. /86/ for the energy we obtain

$$\log\frac{E}{E_o} = -\frac{N}{2|J|\rho_o}\left(\frac{1}{Z} - 1\right) + \sqrt{\frac{a^2 Z}{1-Z} - \varkappa^2} \qquad /87/$$

where eq. /85/ has been used. In the energy region where the effect of the renormalization is large i.e. Z/E/ ≪ 1, eq. /87/ can be simplified to

$$Z(E) = - \frac{N}{2|J|\rho_0} \; \frac{1}{\log \frac{E}{E_0}} \qquad /88/$$

The dynamical resistivity at zero temperature can be obtained using eqs. /54/ and /88/ as

$$R(v) \sim \frac{1}{Z(eV)} = - \frac{2|J|\rho_0}{N} \log \frac{eV}{E_0} \qquad /89/$$

A logarithmic voltage dependence has been obtained, but its validity is very limited due to the crudeness of the approximation made here.

The effect of the selfconsistency is illustrated on Fig. 13, where schematic plots of the renormalization factor with and without taking into account selfconsistency are shown. By comparing the two curves the following conclusions can be drawn:

1, the low energy region of the unrenormalized curve /$E < E_0$/ shrinkes to so narrow a region that this part of the unrenormalized curve plays only an essentially restricted role in the formation of the selfconsistent curve, and as a consequence,

2, in the case of the giant effect only the maximum of the resistivity can be observed at zero bias independently of the type of the scattering amplitude used,

3, the low energy region of the scattering amplitude should be studied by experiments with very small relative resistivity increase /in which case a selfconsistent treatment is not necessary/.

As to the temperature dependence of the giant resistivity maximum at zero bias, on the basis of thermal smearing effect in an energy interval of a few kT the following can be expected. The height of the resistivity maximum is decreasing as the temperature is increasing in such a way that the top of the maximum has an energy width of about a few kT, as it is shown on Fig. 14. Moreover the dependence of the resistivity on the voltage at T=0 and on the temperature at zero bias can be expected to be the same.

b. Suhl-Wong type formula.

A difference between the scattering amplitudes given by Abrikosov, eq. /56/ and Suhl and Wong [23] appears only for antiferromagnetic coupling.

In this case the maximum of the scattering amplitude occurs at energies comparable with the temperature. Thus, as we have seen before, the maximum of the renormalization factor at E=o is smoothed out and only a simple resistivity maximum appears in the characteristics.

c. Nagaoka type formula.

The determination of the renormalization factor using Nagaoka's scattering amplitude, eq. /59/, follows the line of the previous calculations. Similar to eq. /73/ it is obtained that

$$\frac{1}{2\tau_{\vec{k}_{\parallel}=0}(E)} = \frac{1}{\pi}\int dR\, c(R)\, f^{-2}_{\vec{k}_{\parallel}=0}(R)\, \frac{E_0^2}{E^2+E_0^2}\quad \frac{1}{\rho^{(o)}(R)} \qquad /90/$$

and the renormalization factor is given by

$$Z_{Nagaoka}(E) = \left\{1 + \frac{1}{z}\,\frac{N_i}{N_s}\,\frac{E_0^2}{E^2+E_0^2}\right\}^{-1} \qquad /91/$$

which leads to a resistivity maximum at zero bias. The relative amplitude of this maximum is

$$Min\left(Z_{Nagaoka}\right) = \frac{1}{1+\frac{1}{Z}\frac{N_i}{N_s}} \qquad /92/$$

The selfconsistent equation corresponding to eq. /91/ reads

$$Z^{-1}(E) = 1 + \frac{1}{Z}\,\frac{N_i}{N_s}\,\frac{E_0^2(Z)}{E^2+E_0^2(Z)} \qquad /93/$$

where E_0 has been replaced by the energy dependent characteristic constant $E_0/Z/$, given by eq. /85/. The solution of eq. /93/ in the approximation $Z/E/\ll 1$ is

$$\log\frac{E}{E_o} = \frac{N}{2\pi\rho_o}\,Z + O\left(\frac{1}{Z},\ \log Z\right) \qquad /94/$$

which gives for the resistivity

$$R(V) = \frac{2\pi\rho_o}{N}\,\log\frac{eV}{E_o} \qquad /95/$$

We have obtained just the same voltage dependence as in the case of Abrikosov's scattering amplitude, eq. /89/. This result supports one of the conclusions of the last section, namely that the giant resistivity maximum is not sensitive to the actual form of the scattering amplitude at low energies.

Finally it is worth mentioning that Appelbaum, Phillips and Tzouras [15] using a different method, have derived an expression for the conductance in which the term due to the impurities is of the same form as the expression obtainable from eq. /93/. However, the term obtained by them increases the conductance of the junction as compared to the case without impurities, while in our case the total conductance is less than the conductance of the pure junction. We will discuss this question in more detail in the "Conclusions".

10. Characteristics in a magnetic field.

Appelbaum [4] has shown in perturbation theory that the effect of an external magnetic field is the splitting of the peak at zero bias. The new peaks appear at voltages $\pm g\mu H$. A correct treatment of this problem would require the knowledge of the scattering amplitude in an external magnetic field. This problem has been treated by Abrikosov [23] in a rough approximation with the result that the peak is broadened instead of split. The only available results have been derived in the third order of perturbation theory and their validity is very limited as it has been discussed before. This theory gives just the same dependence on the magnetic field as it has been obtained by Appelbaum. Moreover the dependence on the voltage is also the same provided the asymetrical terms which should not occur are left from Appelbaum's formula.

The main features of the effect of magnetic field might be understood in a qualitative manner as it has been pointed out by Appelbaum [4] . The most important energy dependent terms of the scattering amplitude are due to spin-flip scattering processes. These processes might be frozen in by the magnetic field if the magnetic energy is larger than the electronic energy. This may reduce the effect of the magnetic impurities on the renormalization factor in the energy range $E<\mu gH$ leading to a splitting of the resistivity or conductance peak at zero bias.

In the case of the giant effect the importance of the electronic intermediate states with very small energies is reduced as a consequence of the deep minimum in the renormalization factor Z/E/ at small energies as we have seen in connection with the selfconsistent treatment. On the other hand the magnetic field is effective at small energies $E<\mu gH$ and therefore the smaller the renormalization factor at small energies /or the larger the resistivity maximum at zero bias/ the weaker the magnetic field dependence of the characteristics.

11. Comparison of the experimental and theoretical results.

In this section the result of the experiments performed until now will be discussed. It will be seen that the available results cannot decide between the different scattering amplitudes discussed above. Altough the recent measurements by Mezei [8] show that resistivity maxima or minima can be found on similarly prepared junctions depending on the impurity concentration, for the sake of clarity the small conductance maxima and the giant resistivity maxima will be treated separately.

a./ Conductance maximum at zero bias.

Studying transition metal-transition metal oxide-metal diodes Wyatt [1] , Rowell and Shen [2] have reported a series of experiments in which zero bias conductance maxima have been observed at zero bias. In these measurements the relative increase of the conductance has been smaller then 20 % and the half width of the maximum has been a few meV.

Recently Mezei [8] has observed similar conductance maxima on aluminium diodes containing chromium impurities at low impurity concentration and found that the maxima are situated on a slightly asymmetric, wide background curve with the resistivity maximum around zero bias.

On the basis of Appelbaum's theory [4] Rowell and Shen [2] interpreted their results as follows. The background curve is caused by non-magnetic effects and the conductance maximum is due to an antiferromagnetic coupling between the impurity and electron spins. Supposing local processes only, which in the case of an exchange interaction is rather well justified, in the third order of perturbation theory we have got a conductance maximum only for ferromagnetic coupling. Furthermore Mezei's measurements suggest that the background curve is partly caused by the impurities. Three possible interpretations are mentioned here, the second and third ones being suggested by Mezei's experiments.

1. The background curve has no connection with the magnetic moments of the transition metal atoms. The conductance maximum might be due to the ferromagnetic coupling between the electrons and localized magnetic levels. According to the results obtained in Sec. 9. these maxima may have an amplitude of about 15-20 %. The shape of the conductance maximum can be fitted by the result of the perturbation theory, eq. /68/, provided the values of the parameters are changed according to eq. /82/. It is worth mentioning that our results concerning the voltage and temperature dependence of the conductance are the same as those obtained by Appelbaum [4] on the basis of a non-local type mechanism, but the coupling constant

and the overall sign of the effect are different in the two cases. Fitting Wyatt's results measured on Ta-TaO-Al junctions by formulas /68/ and /70/ we get the following values for parameters

$$\frac{J_{eff}}{N}\rho_o = 0{,}105 \sqrt[3]{\frac{N_s}{N_{i,eff}} \frac{Z}{S(S+1)}} \qquad /96/$$

and

$$E_{c,eff} = 9{,}4 \text{ meV} \qquad /97/$$

The first result depends only slightly on the uncertain quantities under the cubic root and using eq. /82/ the following estimate of the real coupling constant can be obtained

$$\frac{J\rho_o}{N} = \frac{1}{\frac{N}{J_{eff}\rho_o} + 2\log\frac{E_c}{E_{c,eff}}} \sim 0{,}1 - 0{,}03 \qquad /98/$$

where the value $E_c = 10^4 - 10^5$ kT is used. In the above fitting we were able to avoid what has been a difficulty in Appelbaum's fitting [6] , namely the use of an unreasonably small cutoff energy of 10 meV.

The effect of an external magnetic field on the tunneling characteristics has been investigated by Shen and Rowell [30] . The observed splitting of the maximum into two peaks is in qualitative agreement with the explanation proposed by Appelbaum [4] and described in Sec. 10. A quantitative agreement with the result obtained in perturbation theory can not be expected as it has already been discussed.

2. A part of the background curve can be understood by considering Abrikosov's scattering amplitude for antiferromagnetic coupling. For $E_0 > 3$ kT the calculated characteristics as shown on Fig. 8. have similar energy dependence to the experimental results. No quantitative comparison is possible, however, because the part of the background curve which is not due to impurities cannot be separated. A further difficulty arises from the need of a selfconsistent solution in certain cases.

3. In principle it might be possible that the superimposed maximum and minimum would be the effect of two different zero bias anomalies corresponding e.g. to two different types of impurities, or the same impurity oxidized and without oxidization.

b./ Giant resistivity maximum.

First Rowell and Shen [2] observed giant resistivity maxima measuring Cr-CrO-Ag diodes, where the relative increase of the resistivity has been about 50. Recently Wyatt and Lythall [9] have studied Al-AlO-Ag diodes containing titanium and copper ions, and Mezei [8] Al-AlO-Al diodes containing Cr impurities and in both cases giant resistivity maxima have been observed with a relative increase of resistivity of 25-200. In magnetic field no splitting has been observed. In Mezei's experiment the amount of the chronium has been controlled and the thickness of the chromium layer was less than ten atomic diameters. Mezei has found a qualitative correlation between the amplitude of the giant resistivity maximum and its sharpness, namely that the maximum becomes sharper and the amplitude higher as the concentration is increased.

Now we shall restrict ourselves to the discussion of the results of the experiments in which the paramagnetic impurity atoms were at one side the barrier. Some information can be obtained for the possible maximal value of the resistivity peak at zero bias from the eqs. /84/ and /92/ assuming Abrikosov's and Nagaoka's scattering amplitudes, resp. For the sake of simplicity we discuss only the T=0 case. First of all an estimation of the effective thickness of the impurity layer is needed. Using the value E=20 meV, the coherence length calculated from eq. /21/ is $\xi = 80$ Å. Therefore the impurities distributed within a thickness 10-20 atomic diameters are inside the coherence length. The parameter a^2 introduced by eq. /75/ may be estimated by taking S=2 and z=3 with the result $a^2=5\frac{N_i}{N_S}$. In the case of Abrikosov's scattering amplitude the value of the maximum according to eq. /84/ is

$$\frac{Max\ R(v)}{R(v\approx\infty)} = \frac{5}{\varkappa^2}\,\frac{N_i}{N_S} \qquad /99/$$

which with $k^2=2$ is of the same order of magnitude as the observed relative resistivity increase.

In the case of Nagaoka's scattering amplitude the estimated maximum is smaller, namely, using eq. /92/ it is
Thus a possible decision between different scattering amplitudes might be made on the basis of the amplitudes of the maximum, for which, however, very well controlled impurity layers would be needet.

Unfortunately the logarithmic voltage dependence, which has been observed in some range of the applied bias is according to the eqs. /89/ and /95/ quite independent of the used scattering amplitudes.

12. Conclusions

In this paper we have developed a theory of zero bias anomalies due to paramagnetic impurities. First the local density of states appearing in the expression of the tunneling current has been expressed in terms of the life-time of the conduction electrons. It has been shown, that the effect of the impurities is to diminish the local density of states. Moreover as the Kondo scattering is very sensitive to the energy of the scattered electrons, the local density of states will be energy dependent and this causes the anomaly in the current-voltage characteristics of diodes containing paramagnetic impurities. On the basis of the general theory we have shown which types of characteristics can be expected assuming different scattering amplitudes for the electron- paramagnetic impurity scattering /e.g. the resonant state or quasi-bound state solutions/. Now we want to compare these results with those of other theories.

As it has been duscussed in the "Introduction" zero bias anomalies can be caused by the excitation of quasiparticles or by the scattering of conduction electrons on magnetic impurities. The former case cannot be treated in the framework of the present theory thus we will restrict ourselves to the discussion of the latter one. Appelbaum, Phillips and Tzouras [17] have used the tunneling Hamiltonian method in calculating the tunneling current and the conductance. They have introduced two new, anomalous tunneling Hamiltonian terms /H_2 and H_3 in their notation/ which are due to impurity assisted nonmagnetic tunneling and tunneling with spin flip, respectively. The latter term is due to the nonlocal nature of the exhange interaction while the former one is present in a local theory as well. They have found the two terms lead to different consequences in the current-voltage characteristics, thus e.g. in the local case the conductance maximum appears for ferromagnetic coupling, while in the case of nonlocal effect for antiferromagnetic coupling. Moreover the nonlocal term can only lead to a relatively small increase or decrease of the conductance and thus is incapalbe of explaining the giant resistivity maxima.

Camparing their results with ours, there are three essential differences. The first is due to the fact that they have started from a nonlocal interaction while we have used a local s-d exchange interaction. As it has been shown this theory can explain at least qualitatively all the experimental results /e.g. the giant resistivity maxima/. As to the cases in which there is only a small change of the conductance, experiments would be necessary to decide whether nonlocal effects give important contribution or not.

The other two differences are connected with the use of the tunneling Hamiltonian method. The tunneling current contribution coming from the impurity assisted tunneling /H_2 and H_3/ increases the current of the pure junction. In the present theory the local density of states decreases as compared with the unperturbed density of states and this leads to a decrease of the tunneling current. The other problem connected with the tunneling Hamiltonian method is that the coupling constants T, T_a, T_J are undetermined phenomenological parameters and thus the magnitudes of the contributions coming from the different parts of the Hamiltonian cannot be compared while in the Green function approach such problem does not arise. Appelbaum et al.'s result can explain the observed large increase of the resistivity only in a very special and unprobable case when T_a is much bigger than T.

The advantage of the present theory lies in the direct relationship between the life-time of the electrons scattered on the paramagnetic impurities and the diode characteristics. It seems to us that as the problem of Kondo scattering has not been solved yet the measurement of characteristics can prove to be a very suitable tool for investigating this problem experimentally. Measurements at low enough impurity concentrations and at very low temperatures could give valuable information about the impurity-conduction electron bound state, if it exists at all. The other problem worth investigating experimentally is the role played by the impurities at different positions. Thus the investigation of diodes with evaporated impurity layers of different thicknesses can be useful to decide, whether the impurities outside the coherence length give contribution to the tunneling current or not.

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Appendix I.

The explicit form of the wave functions e.g. of the right hand side problem is given here. For the sake of simplicity we consider the case of a square potential well

$$V(x) = \begin{cases} V & x < 0 \\ 0 & x > 0 \end{cases} \qquad /AI,1/$$

The eigenfunctions of the Schrödinger equation are given by

$$f(x) = \begin{cases} \sqrt{\dfrac{2\varkappa_\perp^2}{k_\perp^2 + \varkappa_\perp^2}} \left\{ \sin k_\perp x + \dfrac{k_\perp}{\varkappa_\perp} \cos k_\perp x \right\} & x > 0 \\ \sqrt{\dfrac{2\varkappa_\perp^2}{k_\perp^2 + \varkappa_\perp^2}} \, e^{-\varkappa_\perp |x|} & x < 0 \end{cases} \qquad /AI,2/$$

where the notations given by eqs. /11/ and /12/b/ are used.

The product of two wave functions occuring in the matrix element /19/ using /AI,2/ for $x > 0$ is

$$f_{k_\parallel,\nu}(x) f_{k_\parallel,\nu'}(x) =$$

$$= \sqrt{\frac{2\varkappa_\perp'^2}{k_\perp'^2 + \varkappa_\perp'^2}} \sqrt{\frac{2\varkappa_\perp^2}{k_\perp^2 + \varkappa_\perp^2}} \left\{ \sin k_\perp x + \frac{k_\perp}{\varkappa_\perp} \cos k_\perp x \right\} \left\{ \sin k_\perp' x + \frac{k_\perp'}{\varkappa_\perp'} \cos k_\perp' x \right\} \qquad /AI,3/$$

Supposing a homogeneous impurity distribution in a region of the metal at the barrier with distance from the barrier not larger than d, in the matrix element given by eq. /19/ the following integral occurs

$$\int_0^d \Big\{ \cos(k_\perp - k_\perp')x + \frac{k_\perp k_\perp'}{\varkappa_\perp \varkappa_\perp'} \cos(k_\perp - k_\perp')x - \frac{k_\perp'}{\varkappa_\perp'} \sin(k_\perp - k_\perp')x + \frac{k_\perp}{\varkappa_\perp} \sin(k_\perp - k_\perp')x \Big\} \, dx \qquad /AI,4/$$

$$= \frac{1}{k_\perp - k_\perp'} \left(1 + \frac{k_\perp k_\perp'}{\varkappa_\perp \varkappa_\perp'} \right) \sin(k_\perp - k_\perp') d + \frac{\dfrac{k_\perp}{\varkappa_\perp} - \dfrac{k_\perp'}{\varkappa_\perp'}}{k_\perp - k_\perp'} \left(1 - \cos(k_\perp - k_\perp') d \right)$$

where the inequality $(k_\perp + k_\perp')d \gg 1$ is made use of.
For $(k_\perp - k_\perp')d \ll 1$ the matrix element /AI,4/ simplifies to the following one

$$\sqrt{\frac{2\varkappa_\perp^2}{k_\perp^2 + \varkappa_\perp^2}} \sqrt{\frac{2\varkappa_\perp'^2}{k_\perp'^2 + \varkappa_\perp'^2}} \left(1 + \frac{k_\perp k_\perp'}{\varkappa_\perp \varkappa_\perp'} \right) d \qquad /AI,5/$$

The integrand in eq. /AI,4/ is given by eq. /2o/ as a function of the difference of the wave numbers $k_\perp$ and $k_\perp'$.

Appendix II.

The current formula /4/ derived by one of the authors [20] in a Green function approach of tunneling may be written in matrix notation as

$$j = 2 \lim_{E \to 0} (C \to R) e \int \frac{dE'}{2\pi} \sum_{\lambda, \lambda', \lambda'', \lambda'''}$$

$$\left\{ T_{\substack{\lambda''', \lambda \\ l, r}} G_{\lambda, \lambda'; r} (E' + E) T_{\substack{\lambda', \lambda'' \\ r, l}} G_{\lambda'', \lambda'''; l} (E') - (r \leftrightarrow l) \right\} \qquad /AII,1/$$

where the tunneling matrix elements are

$$T_{\substack{\lambda, \lambda' \\ l, r}} = \int \chi^{x}_{\lambda'; l} (\vec{x}) \left(\frac{\overrightarrow{\nabla}_{\vec{x}} - \overleftarrow{\nabla}_{\vec{x}}}{2m} \right)_i \chi_{\lambda, r} (x) df_{x, i} \qquad /AII,2/$$

Inserting the spectral representation of the Green function and following the straightforward calculation of the original paper [20] the following is obtained

$$j = 4\pi e \int dE \sum_{\lambda, \lambda', \lambda'', \lambda'''} T_{\substack{\lambda''', \lambda \\ l, r}} \varrho_{\lambda, \lambda'; r} (E + eV)$$

$$T_{\substack{\lambda', \lambda'' \\ r, l}} \varrho_{\lambda'', \lambda'''} (E) (n_F (E) - n_F (E + eV)) \qquad /AII,3/$$

The tunneling matrix element T depends very weakly on quantum numbers ν and ν', therefore it may be written as

$$T_{\lambda, \lambda'} \sim \frac{1}{\sqrt{\Omega_l \Omega_r}} T_{\vec{k}_{\parallel}} \delta_{\vec{k}_{\parallel}, \vec{k}_{\parallel}'} \qquad /AII,4/$$

where the form /11/ of the wave function χ is used.

The final result may be obtained by using /AII,4/ and the definiton /29/ of the averaged spectral function

$$j = 4\pi e \sum_{\vec{k}_{\parallel}} \int dE \, | T_{\vec{k}_{\parallel}} |^2 \, \bar{\varrho}_r (\vec{k}_{\parallel} ; E + eV) .$$

$$\bar{\varrho}_l (\vec{k}_{\parallel} ; E) \{ n_F (E) - n_F (E + eV) \} \qquad /AII,5/$$

which is just the formula /35/.

The averaged density of states $\bar{\varrho}_{\alpha}(k_{\parallel}; E)$ given by eq. /29/ can have a much simpler form, if the Green functions are diagonal in the indeces ν and ν',

$$\varrho_{(k_{\parallel}; \nu)} \varrho_{(k_{\parallel}, \nu')} (E) = \varrho(k_{\parallel}, \nu; E) \delta_{\nu, \nu} \qquad /AII,6/$$

and then we have

$$\bar{\rho}(k_{\parallel};E)=\sum_{r}\rho(k_{\parallel},r;E) \qquad /AII,7/$$

The obtained effective density of states is equal to the one derived by Schrieffer, Scalapino and Wilkins [27], given in Table I, if the index r is the wave vector perpendicular to the barrier surface, $\vec{k}_{\perp}$.

Appendix III.

The effect of multiple scattering on the life-time of the electrons.

Yosida and Okiji [29] have shown that using Nagaoka's equations [24] the following expression can be obtained for the life-time of the electrons for energies higher than kT$_C$

$$\frac{1}{\tau}=\frac{1}{\tau_0}\left\{\left[1+\frac{2J\rho_0}{N}\ln\frac{E_c}{|E|}\right]^2+\left(\frac{J\rho_0}{N}\right)^2\pi^2 s(s+1)\right\}^{-1} \qquad /AIII,1/$$

where

$$\frac{1}{\tau_0}=2N_i\left(\frac{J}{N}\right)^2\pi\rho_0\, s(s+1) \qquad /AIII,2/$$

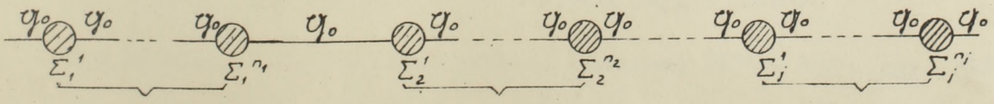
Abrikosov has derived a similar expression but failed in obtaining the term $\left(\frac{J\rho_0}{N}\right)^2\pi^2 s(s+1)$ in eq. /AIII,1/, denoted by $\left(\frac{2J\rho_0}{N}\right)^2 k^2$ in eq. /56/. Abrikosov's expression of the self-energy is divergent at some energy and he argued that the imaginary part of the vertex function would be needed to avoid this divergency. It will be shown here how to obtain this term is Abrikosov's approach. We do not want to claim that the imaginary part of the vertex function is not important, only to show that the divergency can be removed by taking into account multiple scattering.

When calculating the self-energy Abrikosov has neglected scattering processes in which the electrons scatter many times on the same impurity.

The corresponding self-energy is given by

$$\Sigma(E)=-i\left(\frac{J}{N}\right)^2\pi\rho_0\, s(s+1)\left\{1+\frac{2J\rho_0}{N}\ln\frac{E_c}{|E|}\right\}^{-2} \qquad /AIII,3/$$

Considering multiple scattering on the same impurity a typical Green function correction can be represented by the following diagram



where the subscript i at the self-energy diagrams denotes scattering on the i^{th} impurities. Calculating this type of diagrams first we have to sum up the scatterings on the same impurity. The momentum variable of the unperturbed electron Green functions connecting self-energy corrections corresponding to the same impurity is free and after integration their contributions is $-i\pi\rho_0$. Taking into account this multiple scattering the self-energy obtained by Abrikosov, given by eq. /AIII,3/, has to be replaced by the following one

$$\Sigma_{multiple\,;\,i} = \Sigma_i + \Sigma_i \mathcal{G}_0 \Sigma_i + \Sigma_i \mathcal{G}_i \Sigma \mathcal{G}_i \Sigma_i + \cdots = \frac{\Sigma_i}{1 + i\pi\rho_0 \Sigma_i} \qquad /AIII,4/$$

Inserting /AIII,3/ into eq. /AIII,4/ we get for the lifetime the same expression as in eq. /AIII,1/.

The multiple scattering on the same impurity has to be investigated in more detail.

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Figure captions

1. Tunneling of electron assisted by emission and reabsorption of a quasiparticle.
2. /a/ Metal - metal oxide - metal junction with paramagnetic impurities on one side of the barrier within the coherence length ξ .
   /b/ Depression of the density of states within the coherence length.
3. Diagrams of the current in the second order of the tunneling rate.
4. Potentials of the /a/ left hand side, /b/ right hand side and /c/ original problems.
5. Energy dependence of the life-time of electrons according to /a/ Abrikosov, /b/ Suhl and Wong, /c/ Nagaoka.
6. Self-energy diagrams in /a/second and /b/ third order.
7. The energy dependence of the renormalization factor Z/E/ for /a/ ferromagnetic and /b/ antiferromagnetic coupling.
8. Voltage dependence of the conductance for ferromagnetic coupling if there are impurities /a/ only on one side of the barrier, /b/ on both sides of the barrier.
9. Voltage dependence of the conductance on logarithmic scale /see Fig. 8.a/.
10. Temperature dependence of zero bias conductance in the case of ferromagnetic coupling if there are impurities only on one side of the barrier.
11. Voltage dependence of resistivity for antiferromagnetic coupling if there are impurities only on one side of the barrier.
12. Voltage dependence of resistivity on logarithmic scale /see Fig.11./
13. Schematic plot of the renormalization factor Z/E/ taking into account the self-consistency /solid line/.
14. The decrease of the height of the resistivity maximum due to the thermal smearing.

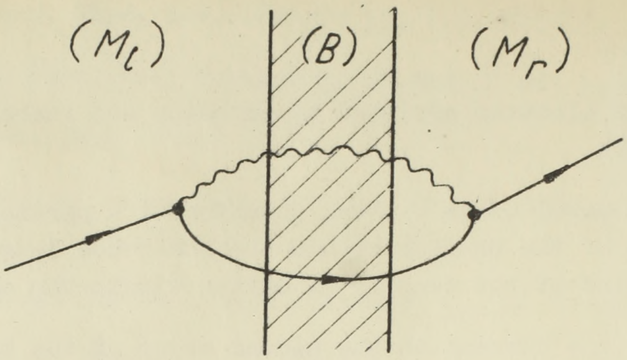
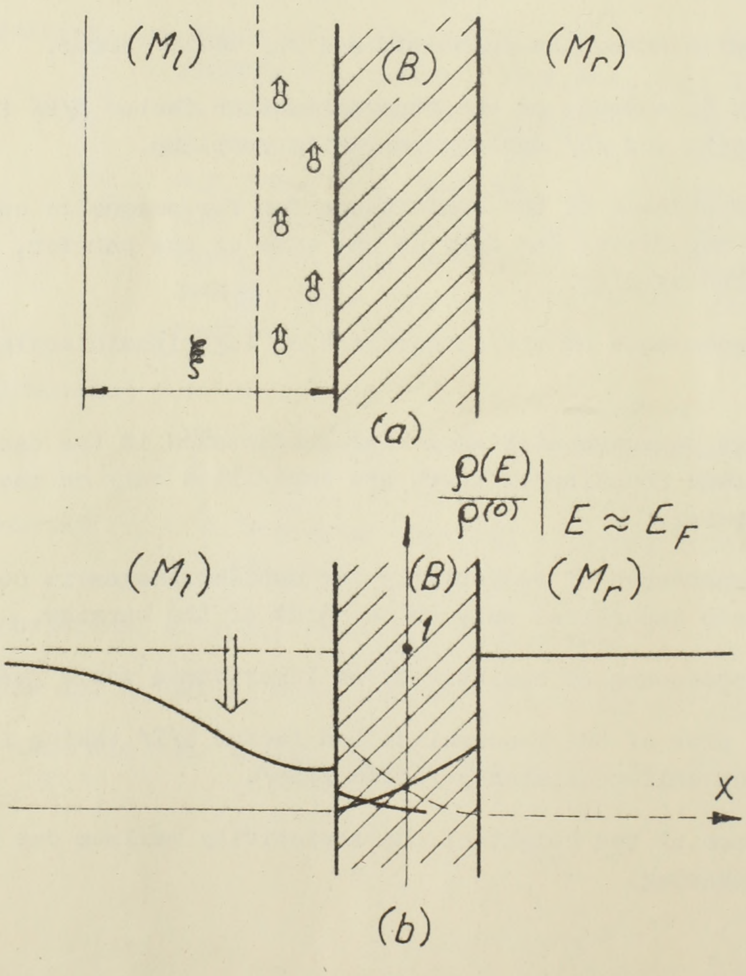


Fig. 1.



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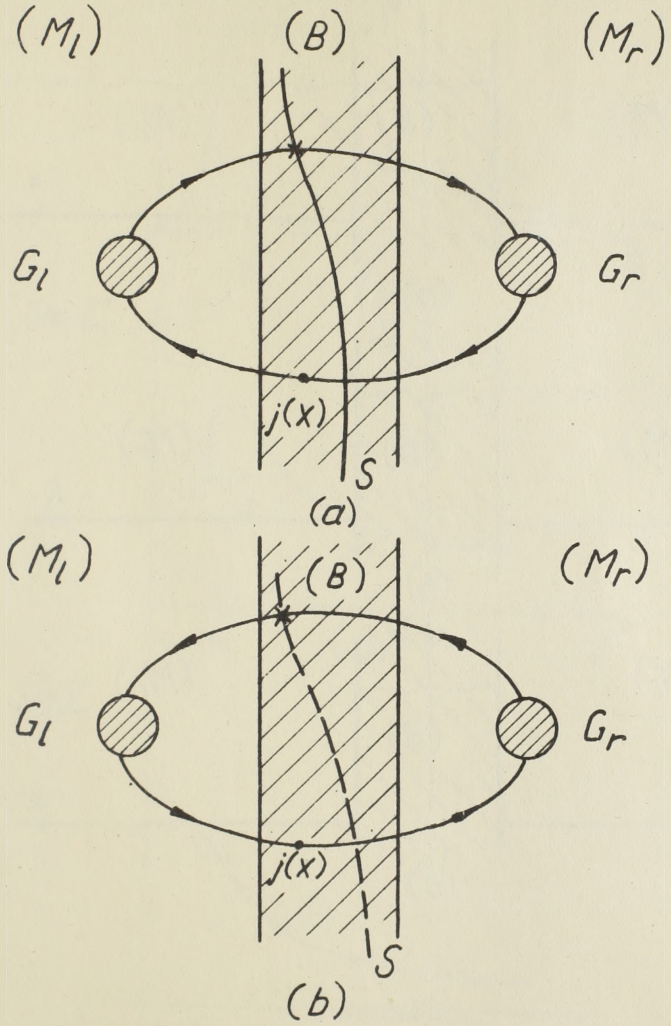

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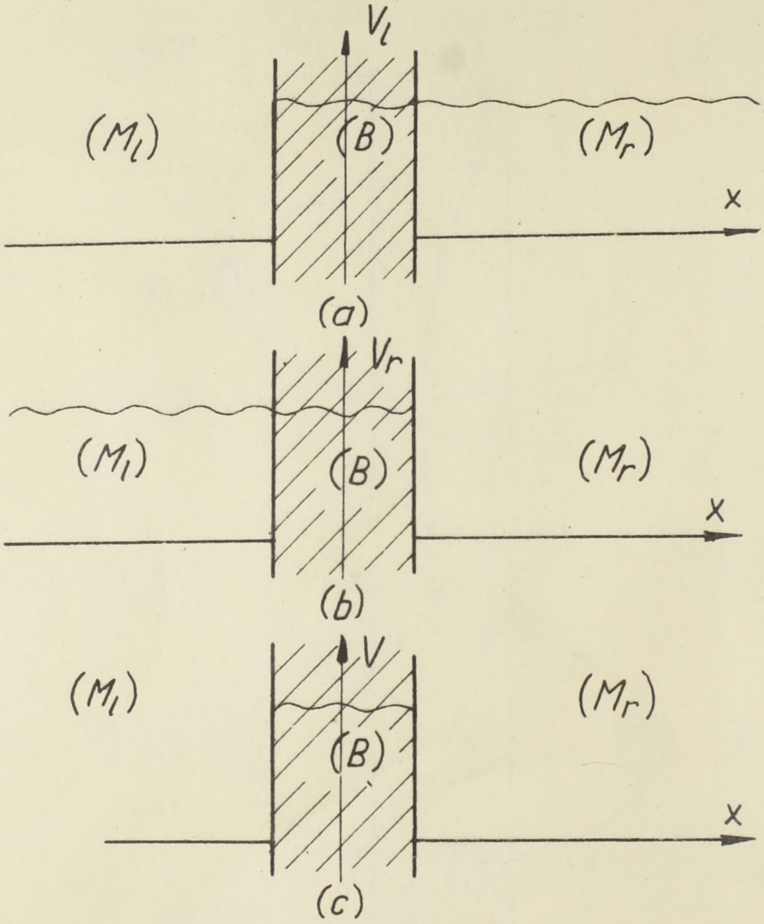

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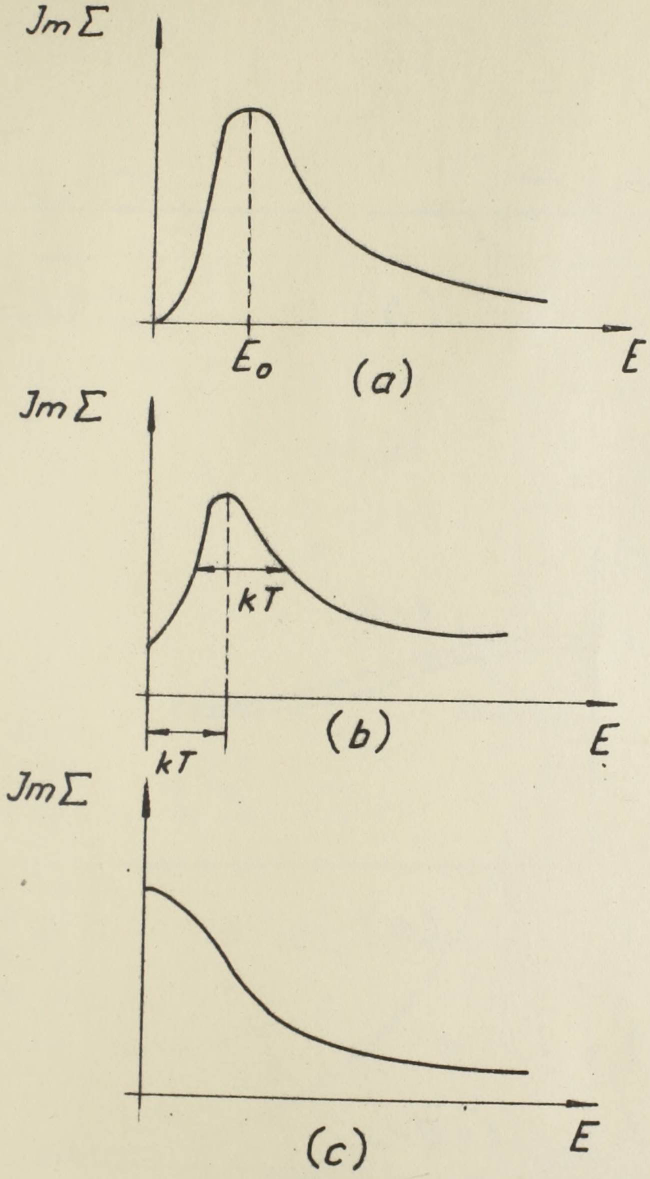

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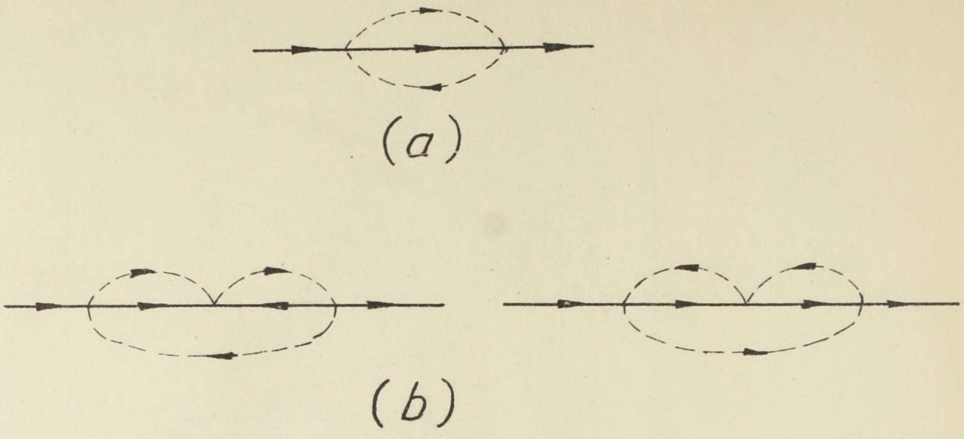

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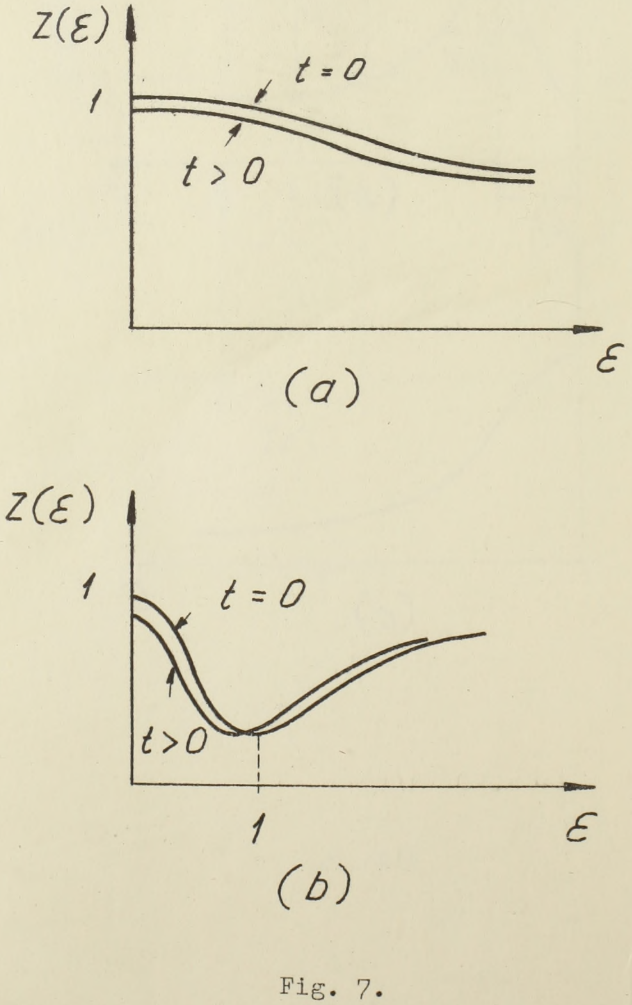

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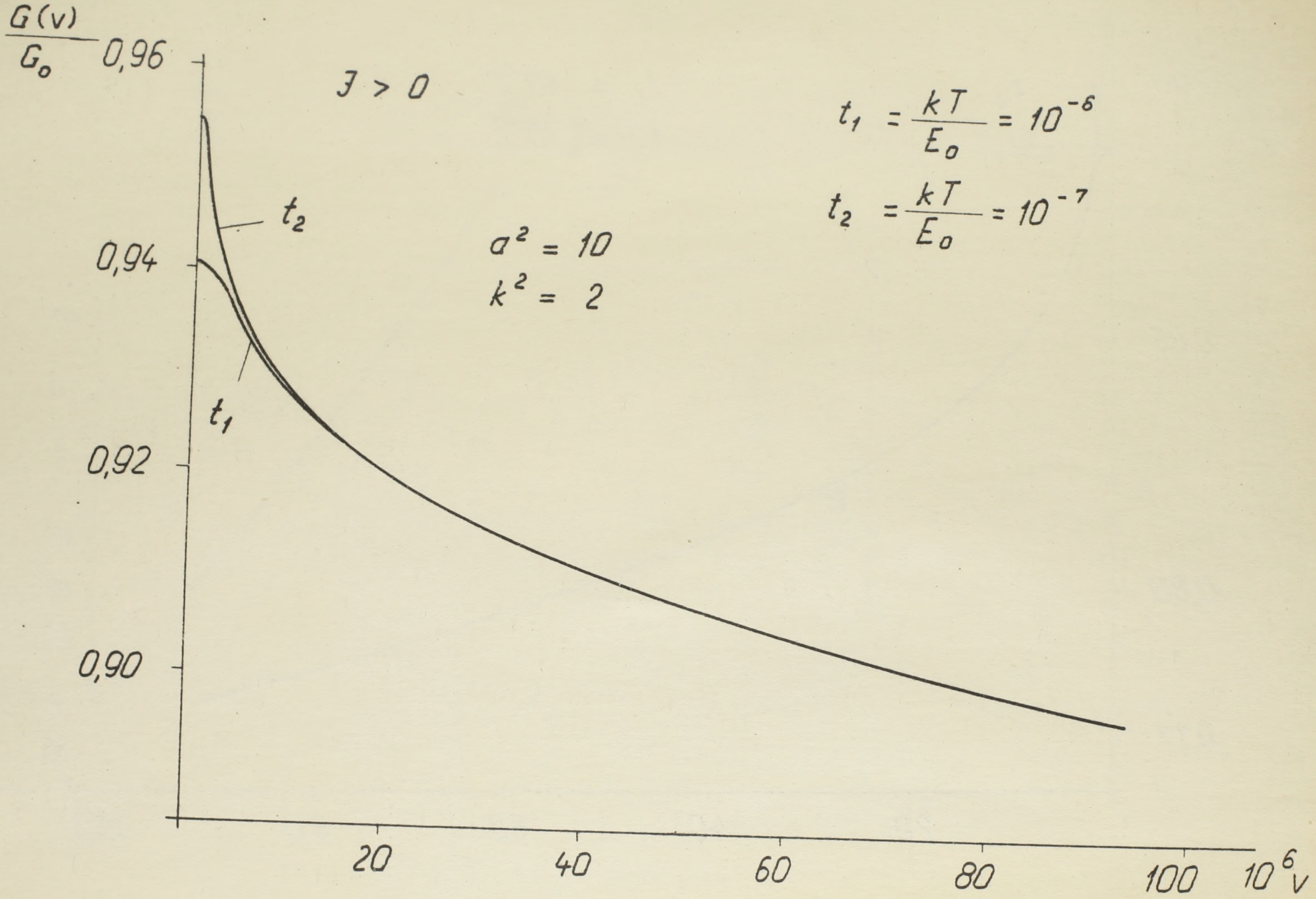

$\frac{G(v)}{G_o}$
0,96
0,94
0,92
0,90
$J > 0$
$t_1 = \frac{kT}{E_o} = 10^{-6}$
$t_2 = \frac{kT}{E_o} = 10^{-7}$
t_2
t_1
$a^2 = 10$
$k^2 = 2$
20
40
60
80
100
$10^6 v$

Fig. 8a

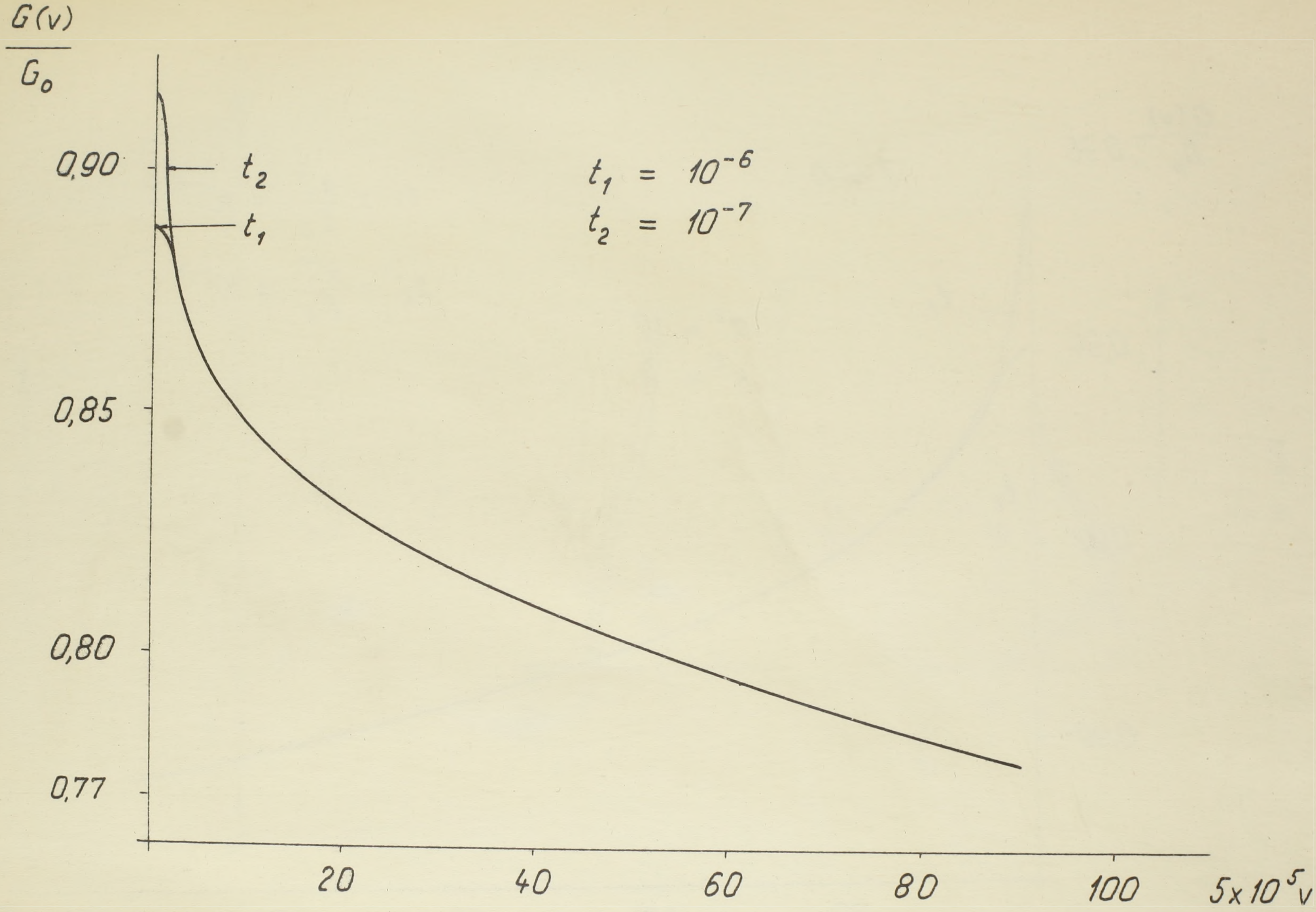
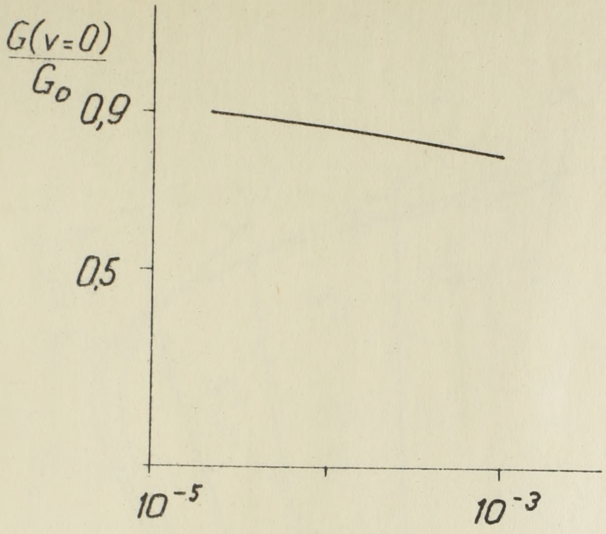


Fig. 8b.



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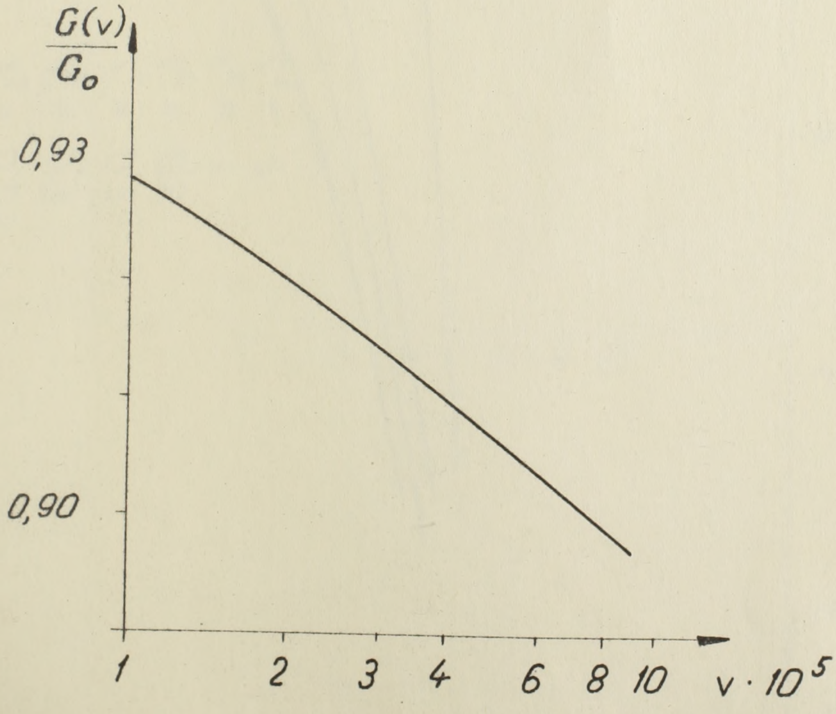

Fig. 10.

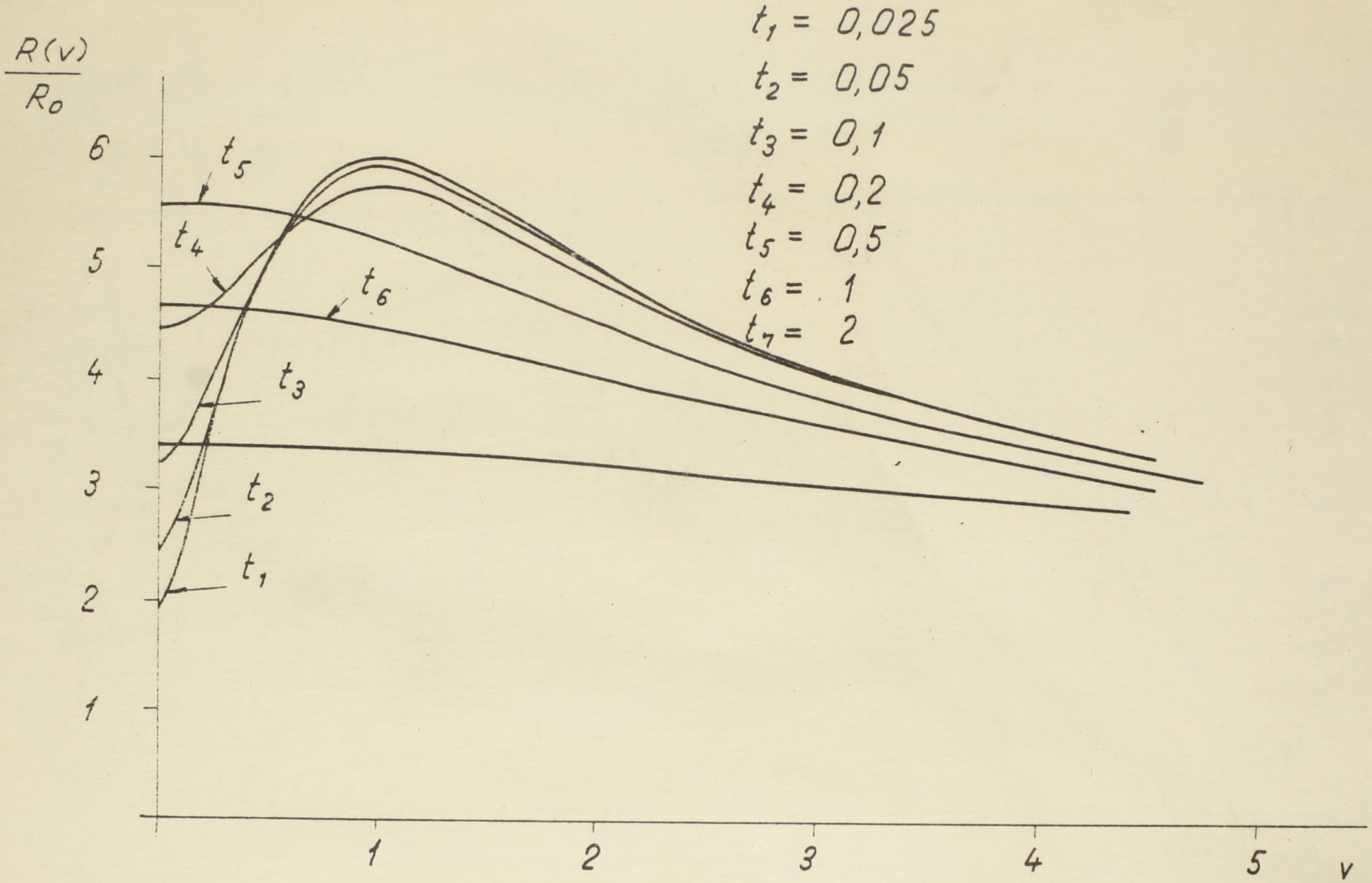
$\frac{R(v)}{R_o}$
6
5
4
3
2
1
1
2
3
4
5
v
t_1
t_2
t_3
t_4
t_5
t_6
t_1 = 0,025
t_2 = 0,05
t_3 = 0,1
t_4 = 0,2
t_5 = 0,5
t_6 = 1
t_7 = 2

Fig. 11.

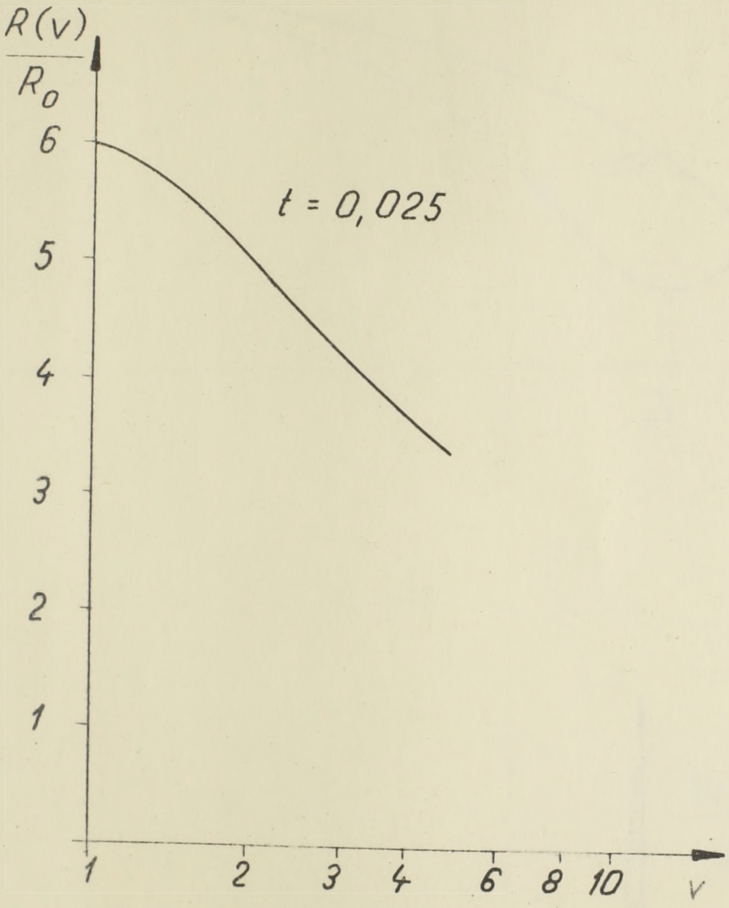

Fig. 12.

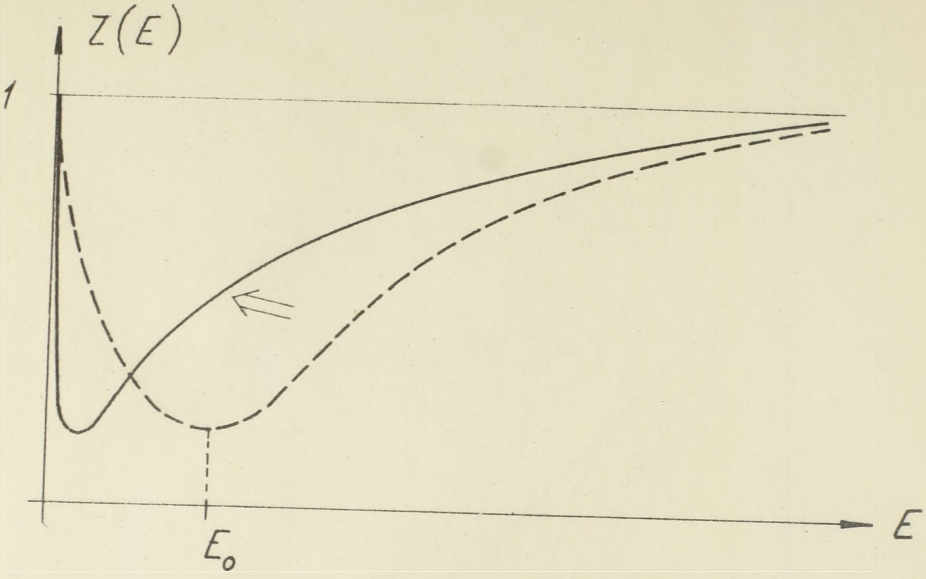

Fig. 13

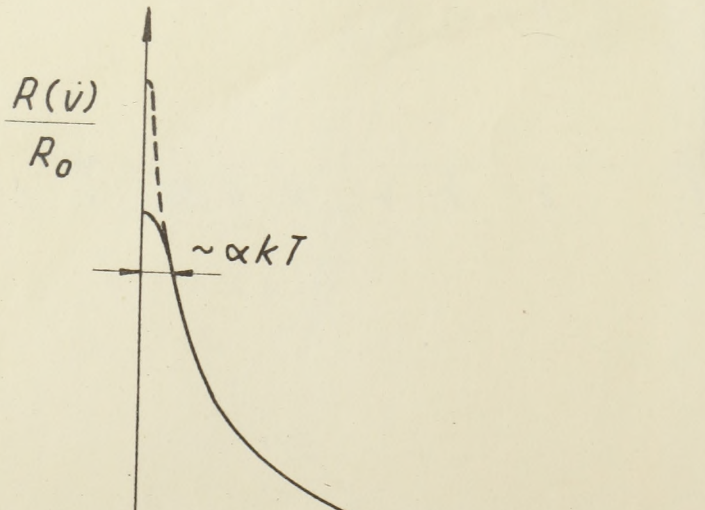

Fig. 14.