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AND TUNNELING ANOMALIES

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CHANGE IN THE ELECTRON DENSITY OF STATES DUE TO KONDO SCATTERING II.:
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The change of the conduction electron density of states due to arbitrary electron-impurity scattering is investigated for a layer like distribution of impurities, extending the calculations of the preceding paper. It is shown, that due to the coherent effect of several impurities the changes in the local electronic density of states depend on the distance measured from the impurities in a much smoother manner than for a single impurity, and therefore this gives a better chance for the experimental observations. Theoretical aspects of adequate tunneling experiments proposed are presented in detail with special emphasis on the determination of the coherence length ξ_A characterising the spatial extent of the perturbations caused by impurity scattering, which is at the present of primary interest in the case of the Kondo effect. Some particular features concerning the Kondo scattering and possible connections with giant zero bias tunneling anomalies are discussed as well.

I. Introduction.

In the previous paper [referred to as I/ we have shown, that resonant electron-impurity scattering may cause crude change in the local conduction electron density of states [e.d.s.] around the impurities. By experimental observation of this change one could gain detailed information on the energy and momentum dependence of non-spin-flip scattering amplitude. This information would be particularly interesting for the case of Kondo scattering. In the present paper we are going to point out, that tunneling could be a very adequate and powerful method to investigate the e.d.s. anomalies in details. We mention at this point, that there are several experimental data on tunneling, which can be interpreted along the lines we are discussing in the present paper. The experimental situation, however, is not clear enough to make a detailed

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comparison between a particular theory and experiments. Therefore our purpose is now to discuss the subject from theoretical point of view only, without considering the available experimental data of interest in any details.

If we consider the result /I.3.28/ and Fig. 2. of the previous paper, we may realize, that in an adequate experiment we have to measure the local e.d.s. as a function of energy at different distances from the impurities. Measuring quantities sensitive to some energy-averaged property of the impurity scattering only, e.g. macroscopic behavior of dilute alloys, NMR studies on host or impurity nuclei etc. we lose all direct information on the energy dependence of scattering, and the spatial structure studies of the impurity scattering state is made more tedious as well. Namely, e.g. as it can be seen in Fig.2. of I, the energy-averaged change of the e.d.s. would fall off much more rapidly with distance measured from the impurity than that for energies near to the resonance. Thus the possibility of measuring e.d.s. as a function of energy given in tunneling seems to be very advantageous in the investigation of resonant impurity scattering. The proposed experimental set-up is illustrated in Fig. 1. The impurities have to be displaced in a layer-like distribution parallel to the junction surface at a distance D within one of the electrodes of the tunnel junction. Provided, that the bulk e.d.s. of the other electrode is a constant, the dynamical conductance of this arrangement at a given voltage V is, roughly speaking, proportional to the e.d.s. of the impure electrode at its barrier surface and at the energy eV , where e is the electronic charge. Thus measuring the anomalies of the conductance vs. voltage characteristics for different values of D , and using some suitable normalization to the non-anomalous, background part of the conductance proportional to the bulk e.d.s., we can obtain directly the e.d.s. function of primary interest, $\rho(r, \omega)$ introduced in /I.3.5./. In the detailed calculation we shall point out that the spatial dependence of the e.d.s. anomaly around the impurity layer is similar to that around a single impurity given in /I.3.28./ except for the lack of the r^{-2} term. This has the important consequence, that the change in the e.d.s. falls off less rapidly for the impurity layer, which may make the investigation of the spatial structure considerable easier.

In sum, if Kondo type impurity scattering with a resonance at the Fermi energy is concerned for a tunnel junction of the structure shown in Fig.1. we may expect the following behaviour: if the impurities are not farther apart from the junction surface than a critical distance ξ_{Δ} , which we call coherence length, the dynamical conductance vs. voltage characteristics of the junction has to show up anomalies around zero bias. The form of the voltage dependence of the anomaly would give detailed information on the energy dependence of the scattering amplitude, while the value of ξ_{Δ} is connected with its momentum dependence.

As far as the conductance vs. voltage characteristics is concerned such type of tunneling anomalies have been observed a few years ago, and rather extensive experimental and theoretical efforts have been devoted to understand these so called "zero bias anomalies". In spite of considerable progress, for the time being there are plenty of problems left in this field. Therefore at the present we do not see worthwhile to discuss in detail these studies in looking for experimental confirmation of the foregoing considerations. For this further experiments with better controllable conditions are needed. At this time we shall only very briefly review this field for sake of completeness. In the course of this review we are not going to account for details of the particular studies, the general tendencies are to be sketched only.

Essentially two kinds of anomalies centered around zero bias have been discovered up to now in the dynamical conductance vs. voltage characteristics of particular metal-oxide-metal tunnel junctions. The first one discovered by Wyatt¹ in 1964 consists of a conductance maximum at zero bias not greater than about 10 % and typically a few mV's wide. /Hereafter referred to as "conductance peak"./ The second one first observed by Rowell and Shen² in 1966 reveals a broad minimum of the conductance at zero voltage having a width typically of the order of 100 mV's, and the reduction of the conductance at zero bias compared to that at a few hundred mV's is almost 100 %, i.e. the conductance at zero voltage can be by orders of magnitude smaller than that at voltages above 100 mV's./ Hereafter referred to as "giant resistance peak"./ After preliminary suggestions of Anderson and Kim, Appelbaum³ proposed an explanation for the "conductance peak" based on impurity assisted tunneling theory supposing magnetic impurities present in the barrier. The theory was worked out in details, and good quantitative agreement was obtained in several aspects with experiments too⁴, particularly for the magnetic field dependence. Thus it can be regarded as fairly well established that the "conductance peak" is due to magnetic impurities displaced in the tunneling barrier and coupled to the tunneling electrons via an exchange interaction.

The situation concerning the "giant resistance peak" is much more confused. Sólyom and Zawadowski⁵ have raised an explanation based on the reduction of the e.d.s. around magnetic impurities near to the junction surface, as mentioned in the paper I. The magnetic origin of this type anomaly is supported by the experimental fact first observed by Mezei⁶ that both types of zero bias anomalies can be produced by doping the barrier region with the same dopant, changing purely its amount. This situation has been found to apply for a wide variety of tunnel junctions made from different materials and containing different dopants⁷. Finally we mention a recent work of Mezei⁸ which was an attempt to realize the experimental arrangement just described in connection with Fig.1. His results can be well interpreted along the lines

discussed in the present paper: i.e. the suppression of the local e.d.s. around an impurity layer displaced at a distance from the barrier surface not greater than a coherence length of a few ten \bar{A} 's is supposed to be responsible for the observed "giant resistance peak". However, there is a basic experimental difficulty present in all of these works: the insufficient knowledge of the structure of the barrier region. In some cases the impurities had their origin in some unknown contamination. The doping procedures used up to now introduce the "impurities" entirely uncontrollably in the sense that one can not know whether single atoms or oxide molecules, metallic particles, oxidized layers etc. are produced. Thus it is also possible that "giant resistance peaks" are due to some crude macroscopic changes in the structure of the junction region rather than to impurities of atomic size. Such theories proposed up to now^{9,10} are based on different assumptions concerning the junction structure. At the present stage none of these explanations or that relying on impurity scattering can be regarded to be valid for each cases known or to be inapplicable at all.

Thus we conclude that a direct, well established tunneling observation of the local suppression of the e.d.s. around impurities is not yet available even if this was the possible origin of zero bias anomalies observed in a group of tunneling experiments. However, tunneling seems to be a possible powerful method in investigation of the impurity scattering of conduction electrons. So we feel that further experimental efforts in this direction are tempting and worthwhile. The purpose of this paper is just to work out the theoretical aspects of such experiments. In sections II. - IV. we shall calculate the change of the e.d.s. and its spatial dependence in the case of an arbitrary electron-impurity scattering amplitude for a layer-like distribution of impurity atoms. In Sec. V. the results are applied to tunnel junctions containing an impurity layer as shown in Fig. 1. Finally in the Sec. VI. we discuss the particular features expected if Kondo scattering is concerned, with special emphasis on some aspects of the impurity-impurity interaction within the impurity layer.

II. The formulation of the problem.

In order to determine the e.d.s. around a paramagnetic impurity layer we calculate the thermodynamical one-particle Green's functions. Supposing that the average over the impurity site is carried out, all of the physical quantities show translational invariance in those directions which are parallel to the plane of the impurity layer. Introducing the parallel and perpendicular components of the vectors with respect to the plane of the

impurity layer, e.g. r_{\parallel} and r_{\perp} for r , the oneparticle Green's function can be written as a function of the new variables as

$$G(r, r'; i\omega_n) = G(r_{\perp}, r'_{\perp}, r_{\parallel} - r'_{\parallel}; i\omega_n) \quad /2,1/$$

The definition of the Fourier transform with respect to the parallel variable is:

$$G(r, r'; i\omega_n) = \frac{1}{(2\pi)^2} \int dk_{\parallel} e^{ik_{\parallel}(r_{\parallel} - r'_{\parallel})} G_{k_{\parallel}}(r_{\perp}, r'_{\perp}; i\omega_k) \quad /2,2/$$

The partial e.d.s. in a distance x measured from the impurity layer for a definite value of the parallel wave vector k_{\parallel} can be obtained by making use of the spectral theorem as

$$\rho_{k_{\parallel}}(x, \omega) = \frac{1}{\pi} \text{Im} \left\{ G_{k_{\parallel}}(x, x; \omega - i\delta) \right\} \quad /2,3/$$

It will be assumed that the kinetic energy of the conduction electrons can be written as

$$\epsilon_k = \frac{k^2}{2m} = \epsilon_{\parallel} + \epsilon_{\perp} = \frac{k_{\parallel}^2}{2m} + \frac{k_{\perp}^2}{2m} \quad /2,4/$$

where ϵ_{\parallel} and ϵ_{\perp} denote the parallel and perpendicular contributions to the kinetic energy. Similarly to /2,2/ the Fourier transform of the free electron Green's functions is the following

$$G_{k_{\parallel}}^{(0)}(r_{\perp} - r'_{\perp}; i\omega_n) = \frac{1}{2\pi} \int dk_{\perp} e^{ik_{\perp}(r_{\perp} - r'_{\perp})} G^{(0)}(k; i\omega_n) \quad /2,5/$$

where

$$G^{(0)}(k, i\omega_n) = \frac{1}{i\omega_n - \xi_k}$$

and the notation $\xi_k = \epsilon_k - \mu$ is introduced. In the neighbourhood of the resonance energy ϵ_0 the kinetic energy can be given as

$$\epsilon_k = \epsilon_{\parallel} + v_{k_{\parallel}} \left[|k_{\perp}| - k_{0\perp}(k_{\parallel}) \right] + \epsilon_0(k_{\parallel}) \quad /2,6/$$

where $v_{k_{\parallel}}$ is the velocity corresponding to the energy $\epsilon_0(k_{\parallel}) = \frac{k_{0\perp}^2(k_{\parallel})}{2m} =$

$\approx \varepsilon_0 - \frac{k_{\parallel}^2}{2m}$ in the one-dimensional problem for a fixed k_{\parallel} .

Furthermore, the unperturbed e.d.s. is

$$\rho_{k_{\parallel}}^{(0)}(\omega) = \frac{1}{\pi} \operatorname{Im} \psi_{k_{\parallel}}^{(0)}(0, \omega - i\delta) = 2 \frac{1}{v_{k_{\parallel}}} \quad /2,7/$$

for $\omega \sim \varepsilon_0 - \mu$, where the factor two arises from the two regions in the momentum space centered at $\pm k_{0\perp}(k_{\parallel})$. In the following we assume that the bulk e.d.s. is independent of the energy in both momentum regions.

One can take into account the effect of the impurity layer by a T-matrix which is related to the Green's functions via the Dyson equation

$$\psi(k, k'; i\omega_n) = \psi^{(0)}(k; i\omega_n) \delta(k - k') + \psi^{(0)}(k; i\omega_n) T_{kk'}(i\omega_n) \psi^{(0)}(k'; i\omega_n) \quad /2,8/$$

which is similar to /I.3,3/. The T-matrix is defined for a given distribution of the impurities. The average over the impurity sites will be performed in the next Sec.

III. T-matrix and average over the impurity distribution.

In paper I we have dealt only with one impurity located at $R = 0$ and the conduction-electron-impurity scattering has been represented by the non-spin-flip scattering amplitude $t_{kk'}^{(i)}(\omega)$. This scattering amplitude for the i 'th impurity located at the point $R^{(i)}$ can be given as

$$t_{kk'}^{(i)}(\omega) = e^{-i(k-k')R^{(i)}} t_{kk'}^{(i)}(\omega) \quad /3,1/$$

The T-matrix defined in /2,8/ corresponding to an impurity layer is a result of subsequent scatterings on different impurities and one can write it as a series of the scattering amplitudes

$$T_{kk'}(\omega) = \sum_i t_{kk'}^{(i)}(\omega) + \frac{1}{(2\pi)^3} \int d^3k \sum_{i,j}' t_{kk''}^{(i)}(\omega) \psi(k''; \omega) t_{k''k'}^{(j)}(\omega) + \dots \quad /3,2/$$

where the prime over the symbol of summation denotes that two subsequent scatterings must correspond to different impurities.

Assuming that the impurity distribution is translational invariant in the plane representing the impurity layer, one can take the density of the impurities as a function of the distance x measured from this plane and it will be denoted by $c(x)$. In this way instead of /3,2/ one gets the averaged T-matrix.

$$\overline{T_{kk'}(i\omega_n)} = \int dR^{(i)} c(R^{(i)}) t_{kk'}^{(i)}(i\omega_n) + \\ + \sum_{ij} \int dR^{(i)} c(R^{(i)}) \int dR^{(j)} c(R^{(j)}) \int \frac{d^3 k''}{(2\pi)^3} t_{kk''}^{(i)}(i\omega_k) y^{(0)}(k'', i\omega_n) t_{k''k'}^{(j)}(i\omega_n) \quad /3,3/$$

where the integrals with respect to $R_{||}^{(i)}$ can be performed and one obtains considering /3,1/, that

$$\frac{1}{(2\pi)^2} \overline{T_{kk'}(i\omega_n)} = t_{kk'}(i\omega_n) \delta(k_{||} - k'_{||}) c(k_{\perp} - k'_{\perp}) + \\ + \frac{1}{2\pi} \int dk'' t_{kk''}(i\omega_n) \delta(k_{||} - k''_{||}) c(k_{\perp} - k'_{\perp}) y^{(0)}(k'', i\omega_n) t_{k''k'}(i\omega_n) \delta(k'' - k'_n) c(k''_{\perp} - k'_{\perp}) + \dots \quad /3,4/$$

where

$$c(k) = \int dx e^{-ikx} c(x) \quad /3,5/$$

The momentum dependence of the scattering amplitude has been given in /I.3,4/ as

$$t_{kk'}(i\omega_n) = (2\ell+1) F(k) F(k') P_{\ell}(\cos \theta_{kk'}) t(i\omega_n) \quad /3,6/$$

However, this momentum dependence can be taken into account in a simple way, if we are interested only in the case $k_{||} \sim 0$, which is the important one calculating the tunneling current. For $k_{||}, k'_{||} = 0$ the angle $\theta_{kk'}$ between k and k' is roughly zero or π , because k and k' are near the energy surface due to the occurrence of the cut-off functions $F(k)$ given by /I.2,4/. Therefore, $P_{\ell}(\cos \theta_{kk'}) = 1$ for even angular momentum ℓ . In this way we get instead of /3,6/

$$t_{kk'}(i\omega_n) \approx (2\ell+1) F(k) F(k') t_\ell(i\omega_n) \quad /3,7/$$

Furthermore, in the case $k_{||} = 0$ one has $k_{\perp}, k'_{\perp} \sim \pm k_0$, where $k_0^2/2m = \epsilon_0$ and only two values of the Fourier transform occur in /3,4/ namely,

$$c(k \approx 0) = c \quad /3,8/$$

which is the surface concentration of the impurities and

$$c(k \approx \pm 2k_0) \quad /3,9/$$

where the latter one is very sensitive to the impurity distribution. Especially, when the impurities can be found in the mathematical surface given by equation $x = 0$, i.e. $c(x) = \delta(x)$ one gets

$$c(\pm 2k_0) = c \quad /3,9a/$$

while for an experimentally available smooth distribution

$$c(\pm 2k_0) = 0, \quad |c(\pm 2k_0)| \ll c \quad /3,9b/$$

if the thickness of the impurity layer, d , satisfies the inequality $dk_0 \gg 1$. This condition is roughly fulfilled if the impurity distribution spreads over more than one or two atomic layers.

These two cases, further referred to as (a) and (b) will be treated separately. The intermediate situations might be understood considering these two limits. In case (a) the transversal momentum k_{\perp} may conserve or change its sign due to the scattering, while in case (b) the sign can not be altered by scattering as it can be easily seen from /3,4/, /3,8/, /3,9a/ and /3,9b/.

It is useful to introduce the modified Green's functions

$$R_{\ell k_{||}}^{(+)}(i\omega_n) = \frac{1}{2\pi} \int_0^{\infty} dk_{\perp} F^2(k) \frac{1}{i\omega_n - \xi_k} = \frac{1}{2} R_{\ell k_{||}}(i\omega_n) \quad /3,10a/$$

and

$$R_{\ell k}^{(-)}(i\omega_n) = \frac{1}{2\pi} \int_{-\infty}^0 dk_{\perp} F^2(k) \frac{1}{i\omega_k - \xi_k} = \frac{1}{2} R_{\ell k_{||}}(i\omega_n) \quad /3,10b/$$

where

$$R_{\ell k_{\parallel}}(i\omega_n) = R_{\ell k}^{(+)}(i\omega_n) + R_{\ell k_{\parallel}}^{(-)}(i\omega_n) \quad /3,11/$$

Let us turn to the solution of /3,4/ for sharp impurity distribution, case (a). Considering /3,4/, /3,7/, /3,8/, /3,9/, /3,11/ and /3,10a-b/ one gets

$$\overline{T_{kk'}}(i\omega_n) = (2\pi)^2 \delta(k - k') F(k) F(k') T_{\ell k_{\parallel}}(i\omega_n) \quad /3,12/$$

where

$$\begin{aligned} T_{\ell k_{\parallel}=0}(i\omega_n) &= c(2\ell+1) t_{\ell}(i\omega_n) + \\ &+ c^2(2\ell+1)^2 t_{\ell}(i\omega_n) R_{\ell k_{\parallel}=0}(i\omega_n) t_{\ell}(i\omega_n) + \dots \end{aligned} \quad /3,13/$$

The series can be summed up with the result

$$T_{\ell k_{\parallel}=0}(i\omega_n) = \frac{c(2\ell+1) t_{\ell}(i\omega_n)}{1 - c(2\ell+1) t_{\ell}(i\omega_n) R_{\ell k_{\parallel}=0}(i\omega_n)} \quad /3,14/$$

Similarly to /I.3,6/, /I.3,7/ we introduce

$$y_{k_{\parallel}, \text{cutoff}}^{(+)}(x; i\omega_n) = \int_{-\infty}^{+\infty} \frac{dk_{\perp}}{2\pi} e^{ik_{\perp}x} y_{k_{\parallel}, \text{cutoff}}^{(+)}(k_{\perp}; i\omega_n) = \int_0^{\infty} \frac{dk_{\perp}}{2\pi} F(k) \frac{1}{i\omega_n - \xi_k} e^{ik_{\perp}x} \quad /3,15a/$$

and

$$y_{k_{\parallel}, \text{cutoff}}^{(-)}(x; i\omega_n) = \int_{-\infty}^{+\infty} \frac{dk_{\perp}}{2\pi} e^{ik_{\perp}x} y_{k_{\parallel}, \text{cutoff}}^{(-)}(k_{\perp}; i\omega_n) = \int_{-\infty}^0 \frac{dk_{\perp}}{2\pi} F(k) \frac{1}{i\omega_n - \xi_k} e^{ik_{\perp}x} \quad /3,15b/$$

furthermore

$$y_{k_{\parallel}, \text{cutoff}}(x; i\omega_n) = y_{k_{\parallel}, \text{cutoff}}^{(+)}(x; i\omega_n) + y_{k_{\parallel}, \text{cutoff}}^{(-)}(x; i\omega_n) \quad /3,16/$$

Considering /3,12/, /3,15a-b/ and /3,16/ the Dyson equation /2,8/ can be written in the form

$$\begin{aligned} y_{\mathbf{k}, \mathbf{k}'; i\omega_n}^{(a)} &= y_{\mathbf{k}; i\omega_n}^{(0)} \delta(\mathbf{k} - \mathbf{k}') + \\ &+ y_{\mathbf{k}_{\perp}; i\omega_n}^{(0)} (2\pi)^2 T_{\ell \mathbf{k}_{\parallel}}(i\omega_n) y_{\mathbf{k}_{\perp}'; i\omega_n}^{(0)} \delta(\mathbf{k}_{\parallel} - \mathbf{k}_{\parallel}') F(\mathbf{k}) F(\mathbf{k}') \end{aligned} \quad /3,17/$$

and, finally, applying the Fourier transformation given by /2,2/ one gets /3,17/ in coordinate space as

$$\begin{aligned} y_{\mathbf{k}_{\parallel}}^{(a)}(\mathbf{r}_{\perp}, \mathbf{r}'; i\omega_n) &= y_{\mathbf{k}_{\parallel}}^{(0)}(\mathbf{r}_{\perp} - \mathbf{r}_{\perp}'; i\omega_n) + \\ &+ y_{\mathbf{k}_{\parallel}, \text{cutoff}}(i\omega_n) (2\pi)^2 T_{\ell \mathbf{k}_{\parallel}}(i\omega_n) y_{\mathbf{k}_{\parallel}, \text{cutoff}}(-\mathbf{r}_{\perp}; i\omega_n) \end{aligned} \quad /3,18/$$

The e.d.s. can be obtained by inserting /3,18/ into /2,3/ and considering /2,7/

$$\begin{aligned} \rho_{\mathbf{k}_{\parallel}=0}^{(a)}(\mathbf{x}, \omega) &= \rho_{\mathbf{k}_{\parallel}=0}^{(0)} + 4\pi \operatorname{Im} \left\{ T_{\ell \mathbf{k}_{\parallel}}(\omega - i\delta) y_{\mathbf{k}_{\parallel}, \text{cutoff}}(\mathbf{x}, \omega - i\delta) y_{\mathbf{k}_{\parallel}, \text{cutoff}}(-\mathbf{x}, \omega - i\delta) \right\} \\ &\quad \mathbf{k}_{\parallel}=0 \end{aligned} \quad /3,19/$$

where $T_{\ell \mathbf{k}_{\parallel}}(i\omega_n)$ is given by /3,14/. This result is the generalization of /I.3,13/ for an impurity layer.

In the case of the smooth impurity distribution the calculation goes in a similar way, but the positive and negative momentum values must be treated separately. The Green's function can be expressed by the scattering amplitudes similarly to /3,18/ and one obtains

$$\begin{aligned} y_{\mathbf{k}_{\parallel}}^{(b)}(\mathbf{r}_{\perp}, \mathbf{r}_{\perp}'; i\omega_n) &= y_{\mathbf{k}_{\parallel}}^{(0)}(\mathbf{r}_{\perp} - \mathbf{r}_{\perp}'; i\omega_n) + \\ &+ (2\pi)^2 y_{\mathbf{k}_{\parallel}, \text{cutoff}}^{(+)}(\mathbf{r}_{\perp}; i\omega_n) T_{\ell \mathbf{k}_{\parallel}}^{(+)}(i\omega_n) y_{\mathbf{k}_{\parallel}, \text{cutoff}}^{(-)}(-\mathbf{r}_{\perp}'; i\omega_n) + \\ &+ (2\pi)^2 y_{\mathbf{k}_{\parallel}, \text{cutoff}}^{(-)}(\mathbf{r}_{\perp}; i\omega_n) T_{\ell \mathbf{k}_{\parallel}}^{(-)}(i\omega_n) y_{\mathbf{k}_{\parallel}, \text{cutoff}}^{(+)}(-\mathbf{r}_{\perp}'; i\omega_n) \end{aligned} \quad /3,20/$$

where the scattering amplitudes are the following

$$T_{\ell k_{\parallel}}^{(\pm)}(i\omega_n) = \frac{c(2\ell+1) t_{\ell}(i\omega_n)}{1 - c(2\ell+1) t_{\ell}(i\omega_n) R_{\ell k_{\parallel}}^{(\pm)}(i\omega_n)} \quad /3,21/$$

By comparing /3,10a-b/ and /3,11/ we get

$$T_{\ell k_{\parallel}}^{(+)}(i\omega_n) = T_{\ell k_{\parallel}}^{(-)}(i\omega_n) = \frac{c(2\ell+1) t_{\ell}(i\omega_n)}{1 - \frac{1}{2}c(2\ell+1) t_{\ell}(i\omega_n) R_{\ell k_{\parallel}}(i\omega_n)} \quad /3,22/$$

Inserting /3,20/ into /2,3/ and considering /3,22/ the final expression of the e.d.s. is obtained

$$\begin{aligned} \rho_{k_{\parallel}=0}^{(b)}(x, \omega) &= \rho_{k_{\parallel}=0}^{(o)} + \\ &+ 4\pi \operatorname{Im} \left\{ T_{\ell k_{\parallel}}^{+}(\omega-i\delta) \left[y_{k_{\parallel}, \text{cutoff}}^{(+)}(x; \omega-i\delta) y_{k_{\parallel}, \text{cutoff}}^{(+)}(-x, \omega-i\delta) + \right. \right. \\ &\left. \left. + y_{k_{\parallel}, \text{cutoff}}^{(-)}(x; \omega-i\delta) y_{k_{\parallel}, \text{cutoff}}^{(-)}(-x; \omega-i\delta) \right] \right\}_{k_{\parallel}=0} \quad /3,23/ \end{aligned}$$

Furthermore, the following identity can be seen from the comparison of /3,15a/ and /3,15b/

$$y_{k_{\parallel}, \text{cutoff}}^{(\pm)}(-x; i\omega_n) = y_{k_{\parallel}, \text{cutoff}}^{(\mp)}(x; i\omega_n) \quad /3,24/$$

Making use of this identity the expressions of the e.d.s., /3,19/ and /3,23/ can be further simplified as

$$\rho_{k_{\parallel}=0}^{(a)}(x, \omega) = \rho_{k_{\parallel}=0}^{(o)} + 4\pi \operatorname{Im} \left\{ T_{\ell k_{\parallel}}(\omega-i\delta) y_{k_{\parallel}, \text{cutoff}}^2(x; \omega-i\delta) \right\}_{k_{\parallel}=0} \quad /3,25/$$

for sharp impurity distribution and

$$\rho_{k_{\parallel}=0}^{(b)}(x, \omega) = \rho_{k_{\parallel}=0}^{(o)} + 4\pi \operatorname{Im} \left\{ T_{\ell k_{\parallel}}^{(+)}(\omega-i\delta) y_{k_{\parallel}, \text{cutoff}}^{(+)}(x; \omega-i\delta) y_{k_{\parallel}, \text{cutoff}}^{(-)}(x; \omega-i\delta) \right\}_{k_{\parallel}=0} \quad /3,26/$$

for smooth impurity distribution, where the definitions of the scattering amplitudes are given by /3,9/ and /3,22/. The equations, /3,25/ and /3,26/ are similar to /I.3,8/. i.e. $|\omega$

The modified Green's function $R_{\ell k_{\parallel}}(\omega - i\delta)$ can be easily evaluated for $|\tilde{\omega}| \ll \Delta$ i.e. $|\omega - \epsilon_0 + \mu| \ll \Delta$ and then one has

$$R_{\ell k_{\parallel}}(\omega \pm i\delta) = \mp i\pi \rho_{k_{\parallel}}^{(0)}$$

which can be inserted into /3,14/ and /3,22/.

IV. Spatial dependence of the electron density of states.

In order to determine the spatial dependence of the e.d.s. the modified Green's functions $y_{k_{\parallel}, \text{cutoff}}^{(+)}$ and $y_{k_{\parallel}, \text{cutoff}}^{(-)}$ will be calculated. One can prove using the definitions /3,15a/ and /3,15b/ that

$$y_{k_{\parallel}, \text{cutoff}}^{(-)}(x, \omega) = \left(y_{k_{\parallel}, \text{cutoff}}^{(+)}(x, \tilde{\omega}) \right)^* \quad /4,1/$$

The calculation will closely follow the previous one given in the Appendix of paper I. The integral with respect to the positive momentum values can be transformed to an integral with respect to the energy as

$$\int_0^{\infty} \frac{dk_{\perp}}{2\pi} \rightarrow \frac{\rho_{k_{\parallel}}^{(0)}}{2} \int d\epsilon$$

Making use of /I.2,4/, /I.2,5/ and /2,6/ the modified Green's function $y_{k_{\parallel}, \text{cutoff}}^{(+)}$ given by /3,15a/ may be written as

$$y_{k_{\parallel}, \text{cutoff}}^{(+)}(x, \omega \pm i\delta) = \frac{\rho_{k_{\parallel}}^{(0)}}{2} \int d\tilde{\epsilon} \frac{\Delta^2}{\Delta^2 + \tilde{\epsilon}^2} \frac{1}{\tilde{\omega} - \tilde{\epsilon} \pm i\delta} e^{i(k_{0\perp} + v_{k_{\parallel}}^{-1} \tilde{\epsilon})x} \quad /4,3/$$

This integration can be easily performed by the contour integration method and it yields the result

$$y_{k_{\parallel}=0, \text{cutoff}}^{(+)}(x, \omega \pm i\delta) =$$

$$= \frac{1}{4} \rho_{k_{\parallel}=0}^{(0)} \frac{\Delta^2}{\Delta^2 + \omega^2} \left\{ e^{-\frac{x\Delta}{v}} e^{ik_0 x} (\tilde{\omega} + i\Delta) - i\Delta (1 + \text{sg}\delta) e^{i(k_0 + \frac{\tilde{\omega}}{v})x} \right\} \quad /4,4/$$

for $x > 0$, where $v = v_{k_{\parallel}=0}$

In the case (a) of sharp energy distribution /4,4/ has to be inserted into /3,25/. The change in the e.d.s. consists of two parts, namely, the oscillating and the nonoscillating one, $\Delta \rho_{k_{\parallel}=0,0}^{(a)}$ and $\Delta \rho_{k_{\parallel}=0,n.o.}^{(a)}$ resp., i.e.

$$\rho_{k_{\parallel}=0}^{(a)}(x, \omega) = \rho_{k_{\parallel}=0}^{(0)} + \Delta \rho_{k_{\parallel}=0,0}^{(a)}(x, \omega) + \Delta \rho_{k_{\parallel}=0,n.o.}^{(a)}(x, \omega) \quad /4,5/$$

The final result can be obtained after doing some algebra and it can be expressed with the aid of different coherence lengths ξ_{Δ} and $\xi_{\tilde{\omega}}$ introduced in paper I by the equations /I.3,16/ and /I.3,17/. In this way one gets

$$\begin{aligned} \Delta \rho_{k_{\parallel}=0,0}^{(a)}(x, \omega) = & -\frac{\pi}{2} \left(\rho_{k_{\parallel}=0}^{(0)} \frac{\Delta^2}{\Delta^2 + \omega^2} \right)^2 \left\{ \text{Im} \left(T_{\ell k_{\parallel}=0}(\omega - i\delta) \right) \left[2 \cos 2 \left(k_0 + \frac{1}{\xi_{\tilde{\omega}}} \right) x - \right. \right. \\ & - 2e^{-\frac{|x|}{\xi_{\Delta}}} \left(\cos \left(2k_0 + \frac{1}{\xi_{\tilde{\omega}}} \right) x - \frac{\tilde{\omega}}{\Delta} \sin \left(2k_0 + \frac{1}{\xi_{\tilde{\omega}}} \right) |x| \right) + \\ & + e^{-\frac{2|x|}{\xi_{\Delta}}} \left(\left(1 - \frac{\tilde{\omega}^2}{\Delta^2} \right) \cos 2k_0 x + 2 \frac{\tilde{\omega}}{\Delta} \sin 2k_0 |x| \right) \Big] + \\ & + \text{Re} \left(T_{\ell k_{\parallel}=0}(\omega - i\delta) \right) \left[-2 \sin 2 \left(k_0 + \frac{1}{\xi_{\tilde{\omega}}} \right) |x| + 2e^{-\frac{x}{\xi_{\Delta}}} \left(\sin \left(2k_0 + \frac{1}{\xi_{\tilde{\omega}}} \right) |x| - \right. \right. \\ & \left. \left. - \frac{\tilde{\omega}}{\Delta} \cos \left(2k_0 + \frac{1}{\xi_{\tilde{\omega}}} \right) x \right) \right] \Big\} \quad /4,6/ \end{aligned}$$

and

$$\begin{aligned} \Delta \rho_{k_{\parallel}=0,n.o.}^{(a)}(x, \omega) = & -\frac{\pi}{2} \left(\rho_{k_{\parallel}=0}^{(0)} \frac{\Delta^2}{\Delta^2 + \omega^2} \right)^2 \\ & \times \left[\text{Im} \left(T_{\ell k_{\parallel}=0}(\omega - i\delta) \right) \left[2e^{-\frac{|x|}{\xi_{\Delta}}} \left(\cos \frac{x}{\xi_{\tilde{\omega}}} - \frac{\tilde{\omega}}{\Delta} \sin \frac{|x|}{\xi_{\tilde{\omega}}} \right) - e^{-\frac{2|x|}{\xi_{\Delta}}} \left(1 + \frac{\tilde{\omega}^2}{\Delta^2} \right) \right] + \right. \end{aligned}$$

$$+ \operatorname{Re} \left(T_{\ell k_{\parallel}=0}(\omega - i\delta) \right) \left[2e^{-\frac{x}{\xi_{\Delta}}} \left(\sin \frac{|x|}{\xi_{\omega}} + \frac{\tilde{\omega}}{\Delta} \cos \frac{|x|}{\xi_{\omega}} \right) \right] \quad /4,7/$$

where it is taken into account that the e.d.s. is an even function of the variable x .

The results /4,6/ and /4,7/ show that the e.d.s. perturbation around a single impurity is coherently enhanced in the neighbourhood of an impurity layer regarding the oscillating, as well, as the nonoscillating part.

This situation is somewhat changed in the case of smooth impurity distribution, where the change in the e.d.s. is definitely nonoscillating,

$$\rho_{k_{\parallel}=0}^{(b)}(x, \omega) = \rho_{k_{\parallel}=0}^{(o)} + \Delta \rho_{k_{\parallel}=0, n.o.}^{(b)}(x, \omega) \quad /4,8/$$

where $\Delta \rho_{k_{\parallel}=0, n.o.}^{(b)}$ can be evaluated similarly as /4,7/ has been done, considering /3,26/ and /4,17/, furthermore, comparing with /4,7/ one finds that

$$\Delta \rho_{k_{\parallel}=0, n.o.}^{(b)}(x, \omega) = \left\{ \Delta \rho_{k_{\parallel}=0, n.o.}^{(a)}(x, \omega) \right\}_{T \rightarrow T^{(+)}} \quad /4,9/$$

where $T \rightarrow T^{(+)}$ means that T has to be replaced by $T^{(+)}$ in /4,7/. This result shows that the spatial dependence of the nonoscillating part is not sensitive to the distribution of the impurities. On the other hand, the oscillating terms appearing in /3,26/ from $y_{k_{\parallel}, \text{cutoff}}^{(+)}$ and $y_{k_{\parallel}, \text{cutoff}}^{(-)}$ cancel each other. It is worth mentioning that the oscillating terms are absent due to the different distances of the impurities measured from the point at which the e.d.s. is asked.

The discussion of the results derived here is left to the succeeding sections. However, we have seen in the paper I that the most pronounced effects appear in the so called "unitarity limit", when the change in the e.d.s. reaches its maximal amplitude. The unitarity limit has been introduced as the case of a phase shift equal to $\pi/2$. In our actual case the scattering amplitudes given by /3,14/ and /3,22/ can not be expressed by a single phase shift in general. However, we may call as unitarity limit the limit when $t(\omega \pm i\delta) \rightarrow \mp i\infty$. The real possibility of approaching this unitarity limit will be discussed in Sec. VI. The scattering amplitudes have simple limiting values, especially

$$T_{\ell k_{\parallel}=0}(\omega \pm i\delta) \rightarrow - \frac{1}{R_{\ell k_{\parallel}=0}(\omega \pm i\delta)} \approx \mp i \frac{1}{\pi \rho_{k_{\parallel}=0}^{(0)}} \quad /4,10/$$

and

$$T_{\ell k_{\parallel}=0}^{(+)}(\omega \pm i\delta) \rightarrow - \frac{1}{\frac{1}{2} R_{\ell k_{\parallel}=0}(\omega \pm i\delta)} \approx \mp i \frac{2}{\pi \rho_{k_{\parallel}=0}^{(0)}} \quad /4,11/$$

where /3,29/ is taken into account.

Let us start the discussion with the case of sharp impurity distributions, where the results /4,6/ and /4,7/ have the following simple forms

$$\begin{aligned} \Delta \rho_{k_{\parallel}=0,0}^{(a)}(x, \omega) \rightarrow - \frac{1}{2} \rho_{k_{\parallel}=0}^{(0)} \left(\frac{\Delta^2}{\Delta^2 + \tilde{\omega}^2} \right)^2 \cdot \\ \cdot \left[2 \cos 2 \left(k_0 + \frac{1}{\xi \tilde{\omega}} x \right) - 2e^{-\frac{|x|}{\xi \Delta}} \left(\cos \left(2k_0 + \frac{1}{\xi \tilde{\omega}} x \right) - \frac{\tilde{\omega}}{\Delta} \sin \left(2k_0 + \frac{1}{\xi \tilde{\omega}} x \right) |x| \right) + \right. \\ \left. + e^{-2 \frac{|x|}{\xi \Delta}} \left(\left(1 - \frac{\tilde{\omega}^2}{\Delta^2} \right) \cos 2k_0 x + 2 \frac{\tilde{\omega}}{\Delta} \sin 2k_0 |x| \right) \right] \quad /4,12/ \end{aligned}$$

and

$$\begin{aligned} \Delta \rho_{k_{\parallel}=0,n.o.}^{(a)}(x, \omega) \rightarrow - \frac{1}{2} \rho_{k_{\parallel}=0}^{(0)} \left(\frac{\Delta^2}{\Delta^2 + \tilde{\omega}^2} \right)^2 \cdot \\ \cdot \left[2e^{-\frac{|x|}{\xi \Delta}} \left(\cos \frac{x}{\xi \tilde{\omega}} - \frac{\tilde{\omega}}{\Delta} \sin \frac{|x|}{\xi \tilde{\omega}} \right) - e^{-2 \frac{|x|}{\xi \Delta}} \left(1 + \frac{\tilde{\omega}^2}{\Delta^2} \right) \right] \quad /4,13/ \end{aligned}$$

which are represented in Fig 2. and 3.

Similarly to the single impurity problem for s-type scattering [see /1.4,2/] the e.d.s. vanishes at the impurity layer. It is interesting to notice that half of the depression of the density of states is provided by the oscillating part and the other half by the nonoscillating part, as it can be seen in Fig. 2 and 3. The derivative of the e.d.s. is zero at the impurity layer. In the case of a single impurity we have a factor r^{-2} in the change

of the e.d.s., in the present case the distance x does not appear in the form of a power function, therefore the damping is smoother for an impurity layer than for a single impurity. The nonoscillating part is damped out beyond the coherence length and on the other hand, it is strongly reduced with changing sign beyond the cutoff energy Δ . This energy dependence is more rapid for larger distances $|x|$.

The change in the e.d.s for a smooth impurity distribution can be obtained by inserting /4,11/ into /4,9/. The final result may be compared with /4,13/ and then one obtains

$$\Delta \rho_{k_{\parallel}=0, n.o.}^{(b)}(x, \omega) = 2 \Delta \rho_{k_{\parallel}=0, n.o.}^{(a)}(x, \omega) \quad /4,14/$$

In this case the nonoscillating part of the e.d.s. at $x = 0$ has the same amplitude as the unperturbed e.d.s. $\rho_{k_{\parallel}=0}^{(0)}$. Thus the e.d.s. at the impurity layer, $|x = 0|$ vanishes for the unitarity limit in both cases.

V. Tunneling anomalies.

Now we turn to the discussion how these e.d.s. anomalies are shown up in the characteristics of a metal-insulator-metal /M-I-M/ tunnel junction containing a layer of impurities in a distance D measured from the barrier surface as shown in Fig. 1. Some of the basic points of this problem was investigated earlier by one of the authors¹¹.

For the sake of simplicity let us treat the case of zero temperature. As it is well known, the dynamical conductance and resistance vs. voltage can be given by the following formulas for junctions containing impurities⁵.

$$\frac{G(D, V)}{G^{(0)}} = Z(D, eV) \quad /5,1/$$

and

$$\frac{R(D, V)}{R^{(0)}} = Z^{-1}(D, eV) \quad /5,2/$$

where the renormalization function of the e.d.s. is

$$Z(x, \omega) = \frac{\rho_{k_{\parallel}=0}(x, \omega)}{\rho_{k_{\parallel}=0}^{(0)}} \quad /5,3/$$

It has been supposed that the e.d.s. of the metal on the left hand-side and on the right hand-side without impurities are independent of the energy, furthermore, $G^{(0)}$ and $R^{(0)}$ denote the conductance and resistance of the pure junction. The parallel momentum component is chosen to be zero, because the tunneling rate of the electrons is the largest in this case.

In the first step of our investigations it is supposed that the impurities can be found on the surface of the barrier; $D = 0$. The expressions of the e.d.s. are given by /4,5/, /4,6/, /4,7/ and /4,8/, /4,9/ for the case (a) and (b), respectively, which can be inserted into /5,3/ and then one obtains

$$Z^{(a)}(0, \omega) = \left(1 - \pi \rho_{k_{\parallel}=0}^{(0)} \operatorname{Im} T_{\ell k_{\parallel}=0}(\omega) \right) \quad /5,4a/$$

and

$$Z^{(b)}(0, \omega) = \left(1 - \frac{\pi}{2} \rho_{k_{\parallel}=0}^{(0)} \operatorname{Im} T_{\ell k_{\parallel}=0}^{(+)}(\omega) \right) \quad /5,4b/$$

where the assumption $eV \ll \Delta$ has been made use of. It is worth mentioning that in the unitarity limit introduced in Sec. IV. by the formulas /4,10/ and /4,11/ the renormalization function $Z(0, \omega)$ vanishes: the conductance becomes zero and the resistance diverges.

Considering /3,14/ and /3,22/ the renormalization function can be expressed by the electron-impurity scattering amplitude $t_{\ell}(\omega)$ in both cases (a) and (b) as

$$Z^{(a,b)}(0, \omega) = \operatorname{Re} \left\{ \frac{1}{1 - i k^{(a,b)} c (2\ell+1) t_{\ell}(\omega - i\delta) \pi \rho_{k_{\parallel}=0}^{(0)}} \right\} \quad /5,5/$$

where $k^{(a)} = 1$ and $k^{(b)} = 1/2$. To compare the theory with experiments it is useful to introduce the number of the monoatomic impurity layers N_1 instead of the surface concentration c . N_1 can be smaller than one. In this way one gets

$$c \rho_{k_{\parallel}=0}^{(0)} = \gamma N_1 \rho^{(0)} \quad /5,6/$$

where γ is a proportionality factor of the order of unity.

The renormalization factor $Z(0, \omega)$ has a rather simpler form if $t_{\ell}(\omega)$ is pure imaginary, namely

$$\kappa^{(a,b)}(0, \omega) = \frac{1}{1 + N_i \pi \rho^{(0)} \gamma \kappa^{(a,b)}(2\ell+1) t_\ell(\omega - i\delta)} \quad /5,7/$$

This formula has been first derived by Sólyom and Zawadowski⁵ for the case (a). Making use of /5,2/ and /5,7/ one gets for the resistance

$$\begin{aligned} \frac{R^{(a,b)}(0, V)}{R^{(0)}} &= 1 + N_i \pi \rho^{(0)} \gamma \kappa^{(a,b)}(2\ell+1) \operatorname{Im} t_\ell(eV - i\delta) + \\ &+ \frac{[N_i \pi \rho^{(0)} \gamma \kappa^{(a,b)}(2\ell+1) \operatorname{Re} t_\ell(eV - i\delta)]^2}{1 + N_i \pi \rho^{(0)} \gamma \kappa^{(a,b)}(2\ell+1) \operatorname{Im} t_\ell(eV - i\delta)} \end{aligned} \quad /5,8/$$

The consequences of the above derived results will be presented in the next Sec. However, let us turn to the case, where the impurity layer is in distance D measured with respect to the barrier surface. Experimentally the preparation of surfaces is never perfect, therefore the real situation may be described by the case (b). Assuming that $|\tilde{\omega}| \ll \Delta$, the dynamical conductance can be obtained up to linear terms in $\tilde{\omega}/\Delta$ by making use of /4,7/ and /4,9/:

$$\begin{aligned} \frac{G(D, V) - G^{(0)}}{G^{(0)}} &= -\frac{\pi}{2} \rho_{k_{\parallel}=0}^{(0)} \left\{ \operatorname{Im} \left(T_{\ell k_{\parallel}=0}^{(+)}(\omega - i\delta) \right) \left[2e^{-\frac{D}{\xi_{\Delta}}} - e^{-\frac{2D}{\xi_{\Delta}}} \right] - \right. \\ &\left. - \operatorname{Re} \left(T_{\ell k_{\parallel}=0}^{+}(\omega - i\delta) \right) 2e^{-\frac{D}{\xi_{\Delta}}} \left(\sin \frac{D}{\xi_{\tilde{\omega}}} + \frac{\tilde{\omega}}{\Delta} \cos \frac{D}{\xi_{\tilde{\omega}}} \right) \right\} \end{aligned} \quad /5,9/$$

ω being equal to eV , and $T^{+}(\omega)$ is given by /3,22/. Furthermore, if $t_\ell(\omega)$ is pure imaginary then $\operatorname{Re} T^{(+)}(\omega) = 0$ and one obtains

$$\frac{G(D, V) - G^{(0)}}{G^{(0)}} = -\frac{\pi}{2} \rho_{k_{\parallel}=0}^{(0)} \operatorname{Im} \left(T_{\ell k_{\parallel}=0}^{(+)}(eV - i\delta) \right) \left[2e^{-\frac{D}{\xi_{\Delta}}} - e^{-\frac{2D}{\xi_{\Delta}}} \right] \quad /5,10/$$

or

$$\frac{G(D, V) - G^{(0)}}{G(0, V) - G^{(0)}} = e^{-\frac{D}{\xi_{\Delta}}} \left(2 - e^{-\frac{D}{\xi_{\Delta}}} - \sigma \left(\frac{\tilde{\omega}^2}{\Delta^2} \right) \right)$$

where by virtue of /4,7/

$$\sigma\left(\frac{\omega}{\Delta}\right) = \left(2 \frac{D}{\xi_{\Delta}} + \frac{D^2}{2} + 2e^{-\frac{D}{\xi_{\Delta}}} - 2\right) \frac{\omega^2}{\Delta^2}$$

gives the lowest order corrections for energies not very close to the resonance ie. $\epsilon - \epsilon_0 \equiv \tilde{\omega} \lesssim \Delta$ which shows a decay with the distance D characterized by the coherence length ξ_{Δ} . This function is shown in Fig. 3. as the curve with the parameter $y = 0$ if we consider only absolute values of the numbers on the left hand vertical scale.

It can be mentioned, that independently of the assumption $\text{Re } T^{(+)}(\omega)=0$ /5,11/ is valid for the voltage $V_0 = (\epsilon_0 - \epsilon_F)/e$ corresponding to the resonance energy.

VI. Discussion of the tunneling anomalies.

The most striking application of the theory is to the Kondo effect, where the scattering amplitude $t_{\ell}(\omega)$ shows a resonant behaviour at the Fermi energy. Something similar may happen when the scattering amplitude is due to the conduction electron scattering on the spinfluctuations at the d-level of the nonmagnetic impurity, as it is pointed out by Hamann¹². However, recently it has been shown by Wang, Evenson and Schrieffer¹³ that the two mentioned possibilities are two opposite limiting cases of the same physical phenomenon. Nevertheless, only the Kondo effect is discussed here as an example.

There are a few general features of the problem which can be applied to the Kondo effect in a straightforward way.

1/ If the resonance takes place at the Fermi energy $\omega = 0$ the characteristics anomalies are found around the zero bias.

2/ If the band structure of the conduction electrons in the neighbourhood of the Fermi energy is approximately symmetrical to the Fermi energy, there exists the electron-hole symmetry in the scattering amplitude, which has the form

$$t^*(\omega - i\delta) = -t(-\omega - i\delta) \quad /6,1/$$

Similar symmetry properties can be proved for the scattering amplitude corresponding to the impurity layer, namely

$$\left(T^{(+)}(\omega - i\delta)\right)^* = -T^{(+)}(-\omega - i\delta)$$

/6,2/

$$T^*(\omega - i\delta) = -T(-\omega - i\delta)$$

where /3,14/ /3,22/ and /3,29/ have been considered.

Inserting this relation into /5,9/ one obtains for $D = 0$

$$G(V) - G^{(0)} = G(-V) - G^{(0)}$$

Thus the electron-hole symmetry of the scattering problem is shown up in the symmetrical characteristics of the junction.*

It is worth mentioning, that if $\varepsilon_0 = \varepsilon_F$ the relation $\omega \rightarrow -\omega$ corresponds to $\tilde{\omega} \rightarrow -\tilde{\omega}$, and by this it can be seen from /4,7/ that the characteristics remains symmetrical for $D \neq 0$ too, since the even function $\text{Im } T(\omega - i\delta)$ and the odd function $\text{Re } T(\omega - i\delta)$ are multiplied in /4,7/ by even and odd functions of $\tilde{\omega}$, respectively.

3/ We have constructed the scattering amplitude for the impurity layer from that for a single impurity. As a first approximation we may take the single impurity scattering amplitude from the one impurity problem. This way entirely neglecting the impurity-impurity interactions we may expect to obtain results valid for low impurity concentrations. In this case in the unitarity limit $t_{\ell}(\omega_0 - i\delta) = i/\pi\rho^{(0)}/\omega_0$ being the resonant energy/ we get for the relative amplitude of the resistance anomaly from /5,8/ if $D = 0$, that

$$\frac{R(V_0) - R^{(0)}}{R^{(0)}} = \gamma N_1(2\ell + 1) \quad /6,3/$$

We mention that in the low concentration limit the one dimensional impurity-concentration function $c(x)$ introduced in Sec. III. makes good sense if the average separation of neighbouring impurities in the layer is much smaller than the electronic mean free path due to scatterings of other origin. Namely, we are interested in the number of impurities in the plane characterized by a particular value of x sensed coherently by an electron.

* Eq./3,29/ is valid for $\tilde{\omega} \ll \Delta$ only. However, if the cut-off function shows electron-hole symmetry itself i.e. it is symmetrical with respect to the Fermi energy, $R_{\ell k \parallel}^*(\omega) = -R_{\ell k \parallel}(-\omega)$ follows, and /6,2/ can be obtained again.

On the other hand, as it was pointed out by Sólyom and Zawadowski¹¹, for larger impurity concentrations we have to take into account the effect of the other impurities in the single impurity scattering amplitude itself. First of all we would have to calculate this quantity for the drastically depressed, energy dependent e.d.s. at the impurity layer rather than for the constant bulk e.d.s. This would mean a self-consistent treatment. Due to mathematical difficulties, however, the solution of the single Kondo-impurity problem is not available for an arbitrary energy dependent e.d.s., not even in an approximation, thus we can make some qualitative considerations only to explore the effects of this selfconsistency.

The maximum possible value of $|t_\ell(\omega - i\delta)|$ is given by the unitarity limit $1/\pi\rho^{(0)}$. If the actual value of the e.d.s. around the Fermi energy is considerably reduced at the impurities, the value of the unitarity limit has to be enhanced. An increase of $|t_\ell(\omega)|$ in turn leads to a further decrease of the e.d.s., so as a result it is possible that for high impurity concentrations

$$\text{Max } |t_\ell(\omega - i\delta)| \gg \frac{1}{\pi\rho^{(0)}} \sim \frac{1}{\pi\rho_{k_{\parallel}=0}^{(0)}} \quad /6,4/$$

In this case from /3,14/ using /3,29/ and /5,6/ with $N_1 \sim 1$ we arrive to the corresponding limit for scattering amplitude of the impurity layer given by /4,10/ and /4,11/ which we have called unitarity limit. In this limit for $D = 0$ the junction conductance approximately vanishes for the resonant energy i.e. at zero bias, as mentioned before.

On the basis of the foregoing considerations we may expect that with increasing amount of impurities the unitarity limit for $t_\ell(\omega)$ increases as well as the maximum actual value of its imaginary part $\text{Im } t_\ell(\omega - i\delta)$. In this case the maximum of the dynamical resistance given by eq. /5,8/ as

$$\text{Max } \left| \frac{R(V)}{R^{(0)}} \right| = 1 + N_1 \pi\rho^{(0)} \gamma_{K^{(a,b)}} (2\ell+1) \text{Max } \left\{ \text{Im } t_\ell(eV - i\delta) \right\}$$

depends on the impurity concentration nonlinearly. Beside the explicit dependence expressed by the term N_1 we have a further variation implicit in $t_\ell(eV - i\delta)$. Order of magnitude changes of the resistance i.e. "giant resistance peaks" can be understood only if we take into account this self-consistent modification of $\text{Max}|t_\ell(\omega)|$ too.

Nevertheless there is another important consequence which is to be seen from the selfconsistent treatment in the case of Kondo scattering. width of the resonance can be characterised by the Kondo energy

$$E_K = E_0 e^{-\frac{N}{2J\rho^{(0)}}}$$

where $\frac{J}{N}$ and E_0 are the electron-impurity exchange coupling constant and the band width, respectively. Taking into account also in this equation the reduction of the e.d.s. at the impurity layer, we may expect a drastic narrowing of the resistance anomaly given by /5,8/ with increasing impurity concentration. The actual value of E_K has to be determined by some average of the actual e.d.s. certainly smaller than $\rho^{(0)}$.

As a qualitative illustration of the behaviour discussed in this point, we reproduce two experimental $R(V)$ characteristics of Ref.6. obtained for different amounts of dopants introduced into the barrier. /Solid line in Fig.4./ The characteristics a and b corresponds to junctions containing the total amount of Cr dopant equivalent to about one half and two mono-atomic layer, respectively, introduced into the barrier region of an Al-Al₂O₃-Al tunnel diode. As another illustration we have plotted in Fig.4. a theoretical characteristics too /dashed line/, calculated for the approximate scattering amplitude proposed by Hamman¹⁴:

$$t(\omega) = \frac{1}{2\pi\rho^{(0)}} \left(1 + \frac{X}{\sqrt{X^2 + s(s+1)\pi^2}} \right)$$

where X is connected with the energy ω in a rather complicated way. The calculation was made using /5,8/ with the reasonable $N_1\gamma_K(2l+1) = 3$. To obtain qualitative agreement with the experimental curve a in Fig.4. we have chosen $T_K = 2000 K^\circ$. /In the computation of the scattering amplitude the impurity spin s was taken to be equal to $1/2$, however, the final numerical results are not very sensitive to the value of s ./ This value of the Kondo temperature on the other hand, would not be unreasonable for the Al/Cr/ system concerned. We should like to emphasize, however, that this demonstration of the adequacy of the present theory to explain experimental data was intended only to show the possibility of such explanation of "giant resistance peaks". As discussed before, a firm experimental evidence for the observation of this type e.d.s. changes by tunneling is not yet achieved.

We see the major interest of the present theory in pointing out an adequate method of determining the characteristic coherence length in the Kondo problem presently very often investigated. As mentioned in the introduction of paper I. the problem of the coherence length is far from being settled. The present method has the advantage that from the measured $G(D,V)$ curves one could easily determine the value of ξ_Δ considering the expected simple

functional form given in /5,11/. It is of interest that the negative definite part of the e.d.s. change has the largest spatial extent for zero energy, and falls off rapidly beyond $|\tilde{\omega}| > \Delta$, see Fig.3. In the coherence length studies just this may give substantial importance to a method appropriate to investigate the perturbations of the electron wave functions due to scattering at different energies separately. Finally let us recall, that any experimental finding concerning the "old" problem of the functional form of the Kondo scattering amplitude $t(\omega)$ would be of interest even now. As we have pointed out, tunneling seems to be, in principle, a unique tool in these problems.

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Figure Captions

- Fig. 1. Schematic diagram of the tunnel junctions containing an impurity layer.
- Fig. 2. The oscillating part of the change in the e.d.s. in the unitarity limit as a function of the distance measured from the impurity layer, for sharp impurity distribution, in the case $\tilde{\omega} = 0$.
- Fig. 3. The nonoscillating part of the change in the e.d.s. in the unitarity limit as a function of the distance measured from the impurity layer for different values of the energy parameter $y = \tilde{\omega}/\Delta$. The curves apply for sharp and smooth impurity distribution as well, if the vertical scales at the right and at the left are considered, respectively.
- Fig. 4. Experimental dynamical resistance vs. voltage characteristics of Cr doped Al-I-Al tunnel junctions normalized to the characteristics of a pure junction having the same resistance at -200 mV /from Ref.6/ as compared to the theoretical curve /see the text./.

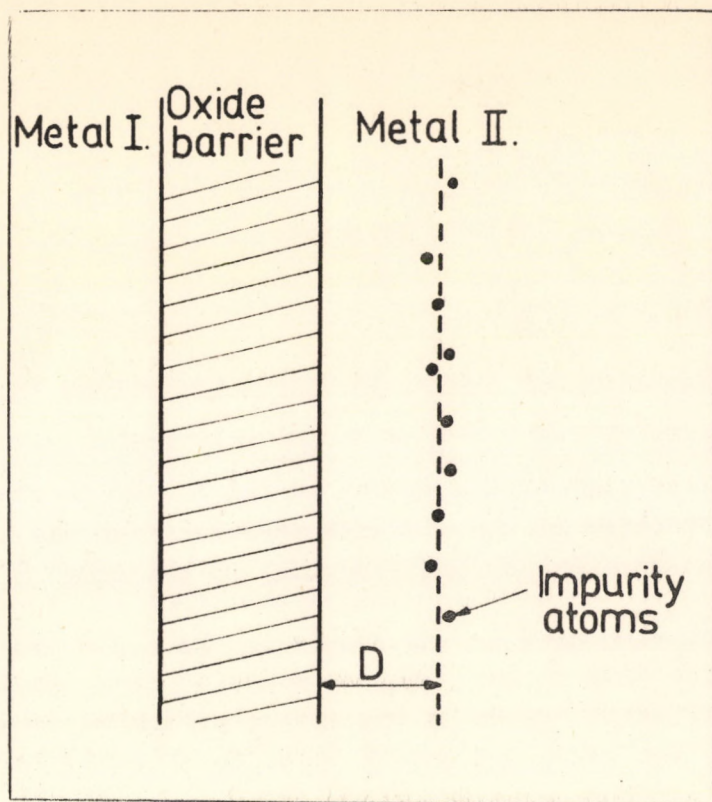


Fig. 1.

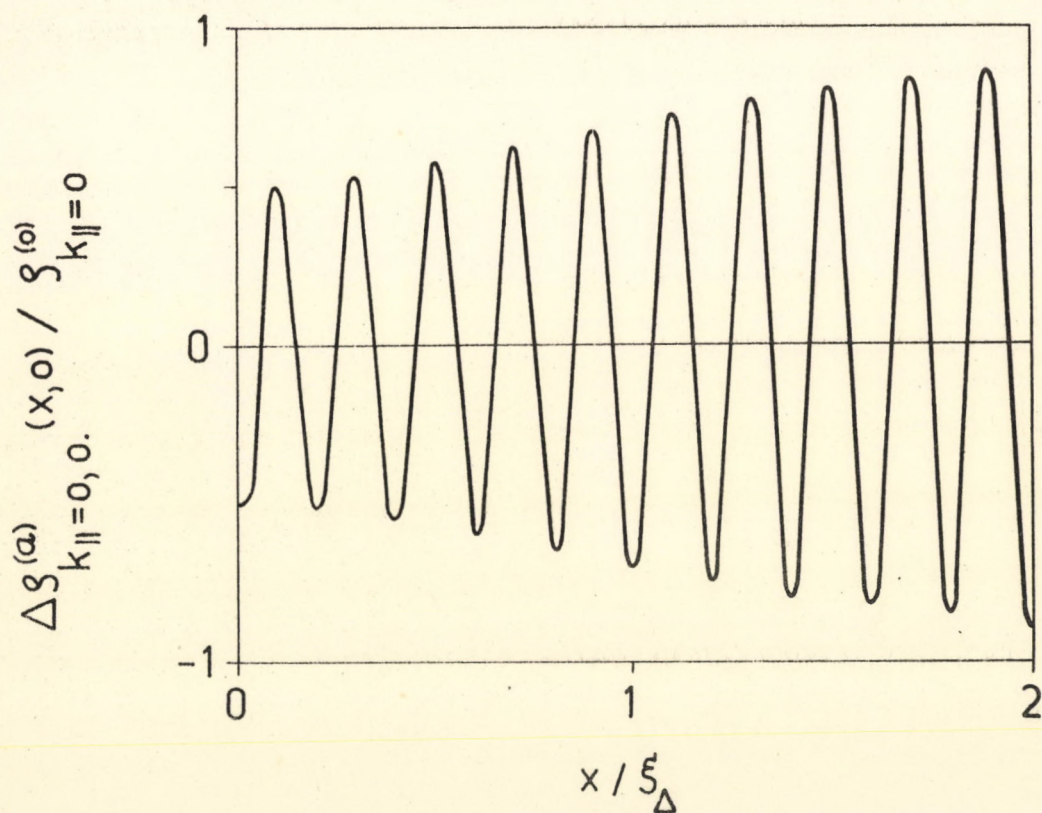


Fig. 2.

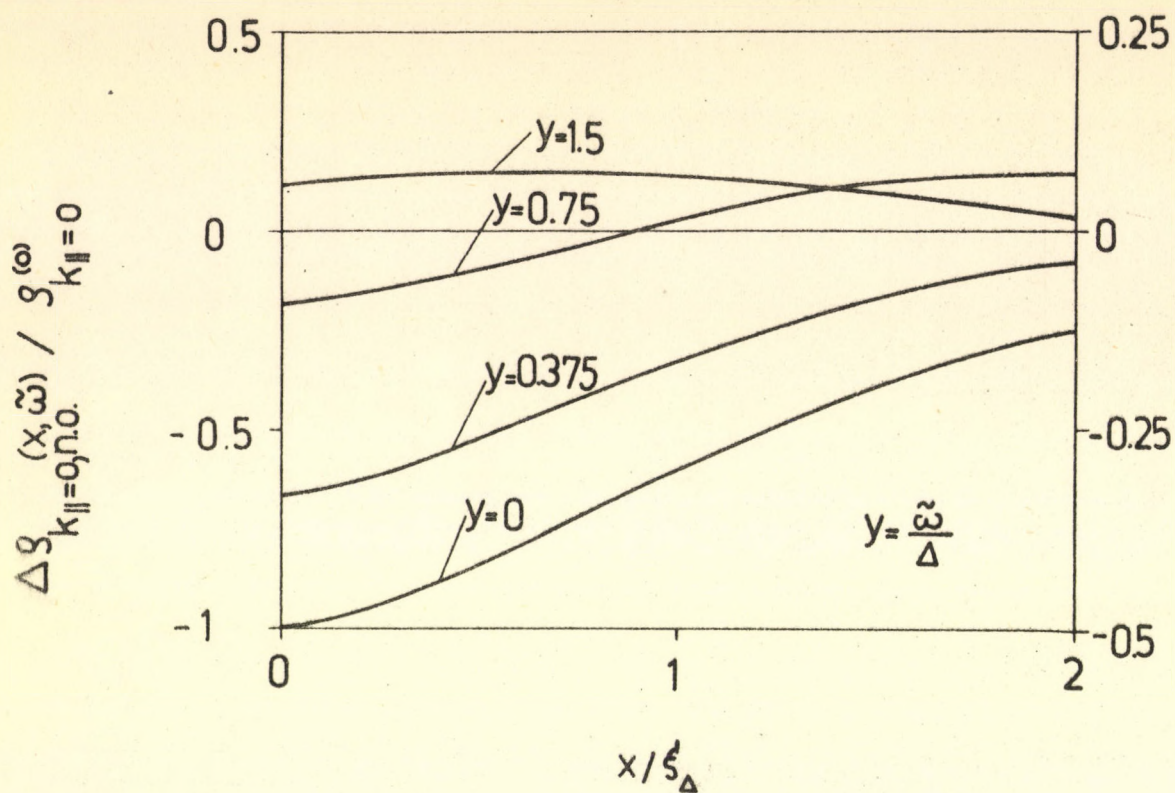


Fig. 3.

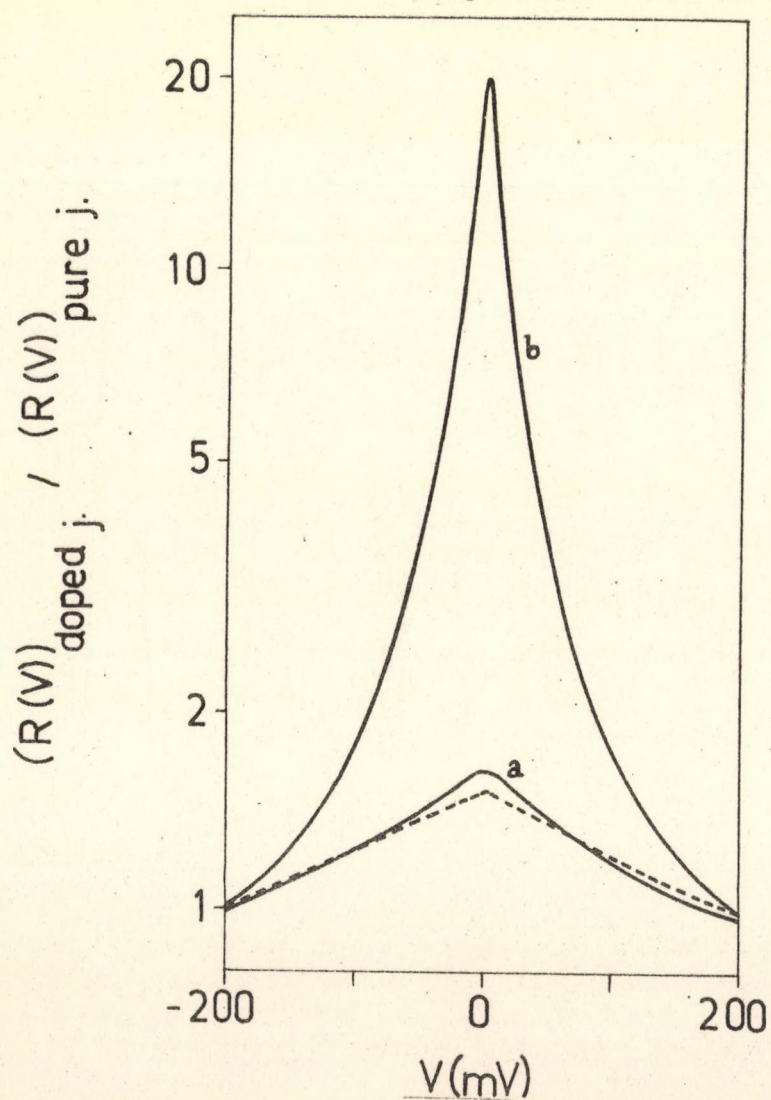


Fig. 4.

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