Kinematic Change in Conduction-Electron Density of States due to Impurity Scattering. II. Problem of an Impurity Layer and Tunneling Anomalies

F. Mezei
Central Research Institute for Physics, Budapest, Hungary

and

A. Zawadowski*†
Department of Physics, University of Virginia, Charlottesville, Virginia 22901
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The change of the conduction-electron density of states due to electron-impurity scattering has been investigated in a previous paper for one impurity; that calculation is extended now to the case of an impurity layer. A strong momentum dependence of the electron-impurity scattering is assumed, but no restrictions are placed on its energy dependence. Particular attention is paid to the spatial structure of the conduction-electron density of states around the impurity layer, which can be characterized by the same coherence length ξ_Δ introduced in the case of one impurity. The amplitude of this change shows a smoother dependence on distance measured from the impurity layer than in the case of one impurity, because of some coherent enhancement due to the scattering of different impurities. Therefore, this improves the chances for experimental observations. Theoretical aspects of adequate tunneling experiments on junctions doped by impurities are presented in detail with special emphasis on the determination of the coherence length ξ_Δ. The perturbations caused by magnetic-impurity scattering is at present of primary interest. Some particular features concerning Kondo scattering and possible connections with giant zero-bias tunneling anomalies are discussed as well. In the case of resonant scattering, the most striking feature is that the conduction-electron–impurity scattering amplitude may be strongly enhanced in the unitarity limit due to the cooperative reduction in the conduction-electron density of states inside the impurity layer at the Fermi energy.

I. INTRODUCTION

In a previous paper[1] (hereafter referred to as I) we showed that resonant electron-impurity scattering may cause crude changes in the local conduction-electron density of states (EDS) around the impurities. By experimental observation of this change, one could obtain detailed information on the energy and momentum dependence of the non-spin-flip scattering amplitude. This information is particularly interesting for the case of Kondo scattering. In the present paper we discuss in detail the tunneling experiments on junctions doped with magnetic impurities. These experiments could be a very adequate and powerful method for investigating the EDS anomalies. Although there are several sets of experimental data on tunneling which can be interpreted on the basis discussed in the present paper, the experimental situation is not clear enough to make a detailed comparison between a particular theory and experiments. Therefore our purpose is now to discuss the subject only from the theoretical point of view, without considering the available experimental data of interest in detail.

In Paper I we have shown that if the conduction-electron–impurity scattering amplitude is separable in momenta and energy variables, the spatial structure of the change in the EDS is independent of the energy dependence of the scattering amplitude. Thus, it is determined by the momentum dependence only. In this way, measuring the EDS as a function of energy at a fixed distance from the single impurity or impurity layer, we get information on the energy dependence of the scattering amplitude, which in one particular case includes the Kondo effect. On the other hand, investigating the EDS at a fixed value of the energy but at different distances measured from the single impurity or impurity layer, we may get some insight into the momentum dependence of the scattering amplitude. One may realize that these kinds of measurements could be made in dilute alloys with homogeneously distributed impurities only with considerable difficulty. Namely, in measuring quantities sensitive only to some energy-averaged property of the impurity scattering, e.g., macroscopic behavior of dilute alloys, nuclear-magnetic-resonance (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 are made more tedious as well. Considering the layerlike distribution of the impurities, we may measure the EDS by building up a metal–metal-oxide–metal junction near the impurity layer. The discussed experimental setup 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

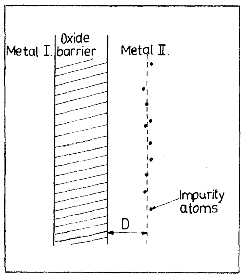

FIG. 1. Schematic diagram of the tunnel junctions containing an impurity layer.

tunnel junction. Provided that the bulk EDS of the other electrode is constant, the dynamical conductance of this arrangement at a given voltage V is, roughly speaking, proportional to the EDS 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-versus-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 EDS, we can directly obtain the EDS. In the detailed calculation we point out that the spatial dependence of the EDS anomaly around the impurity layer is similar to that around a single impurity given by (I3.28), except for the lack of the r^{-2} term, where the distance r is measured from the impurity or impurity layer, respectively. This has the important consequence that the change in the EDS falls off less rapidly for the impurity layer, which may make the investigation of the spatial structure considerably easier.

Furthermore, if Kondo-type impurity scattering with a resonance at the Fermi energy is considered for a tunnel junction of the structure shown in Fig. 1, we may expect the following behavior: If the impurities are not farther apart from the junction surface than a critical distance ξ_Δ, which we call the coherence length, the dynamical-conductance-versus-voltage characteristics of the junction have to show up anomalies around zero bias. The coherence length ξ_Δ has been introduced in Paper I assuming that the momentum region contributing to the conduction-electron–impurity scattering amplitude can be found around the Fermi momentum with a width characterized by the energy Δ and that it is given as $\xi_\Delta = V_F/\Delta$, where V_F stands for the Fermi velocity. 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 discussed in detail in I, this momentum dependence of the scattering amplitude is connected with the k and k' dependence of the exchange coupling $J_{kk'}$, and thus ξ_Δ is related to the size of the spin-polarization cloud in the Kondo state.

As far as the conductance-vs-voltage characteristics are concerned, such types of tunneling anomalies were 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 present, we do not consider it 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 experimental field for the sake of completeness. In the course of this review we are not going to account for details of the particular studies; the general tendencies only are to be sketched. From the theoretical point of view we are going to give a more detailed summary, however.

Essentially two kinds of anomalies centered around zero bias have been discovered up to now in the dynamical-conductance-vs-voltage characteristics of several metal-oxide–metal tunnel junctions. The first one discovered by Wyatt[2] in 1964 consists of a conductance maximum at zero bias not greater than about 10% and typically a few mV wide (hereafter referred to as "conductance peak"). The second one, first observed by Rowell and Shen[3] in 1966, reveals a broad minimum of the conductance at zero voltage having a width typically of the order of 100 mV; the reduction of the conductance at zero bias compared to that at a few hundred mV is almost 100%; i.e., the conductance at zero voltage can be by orders of magnitude smaller than that at voltages above 100 mV (hereafter referred to as "giant resistance peak").

The possibility that the conductance peak is due to magnetic impurities and is based on Kondo scattering has been suggested by Anderson,[4] Appelbaum,[5] Kim,[6] and Suhl.[7] These explanations concerning, at least, the magnetic origin of the anomalies, have been confirmed particularly by the magnetic field dependence of the conductance peak, first observed by Shen and Rowell.[8]

The situation concerning the giant resistance peak is much more confused. Sólyom and Zawadowski[9–11] offered an explanation based on the reduction of the EDS around magnetic impurities near the junction surface. The first experiments with junctions doped by magnetic impurities were carried out by Wyatt and Lythall,[12] and Mezei,[13] who found giant zero-bias anomalies. The magnetic origin of this type of anomaly is especially supported by the experimental fact first observed by Mezei,[13] that both types of zero-bias anomalies can be produced by doping the barrier region with the same dopant, only changing its amount. This situation has been found to apply to a wide variety of tunnel junctions made from different materials and containing different dopants.[14] Finally, we mention a recent work of Mezei[15] 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 EDS around an impurity layer displaced at a distance from the barrier surface not greater than a coherence length of a few tens of Å 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 cannot know whether single atoms or oxide molecules, metallic particles, oxidized layers, etc., are produced.

Another explanation of the giant zero-bias anomalies was proposed by Giaever and Zeller,[16] considering crude macroscopic changes in the structure of the junction region rather than impurities of atomic size. At the present time none of these explanations (magnetic impurities and structure of the barrier region) can be regarded as either valid or inapplicable to all of the experimental cases.

The theory of the effect of magnetic impurities on tunneling characteristics has been worked out following two different directions. According to the first direction,[4-7] the magnetic impurities in the barrier provide an easy way for the electron tunneling through the barrier. This tunneling due to the magnetic impurities has been considered a "new tunneling channel" which has been described by adding a phenomenological term to the conventional tunneling Hamiltonian. This new term represents a tunneling through the barrier associated with an exchange interaction process. A microscopic foundation of this idea has been suggested by Anderson,[4] and the consequences of the new tunneling channel have been derived by Appelbaum.[5,17,18] The extra term of the current due to tunneling assisted by magnetic impurities shows logarithmic voltage dependence in the third order of the perturbation theory, which is a particular case of the Kondo effect. In the case of antiferromagnetic interaction, that the current is always increased supports the idea of a "new channel." In this way the conductance peak, but not the giant resistivity anomaly, could be explained.

The other theoretical works have aimed at understanding the tunneling process when different interactions are taking place inside the barrier or near the barrier, without introducing any further phenomenological parameters. Thus, Zawadowski[19] derived an expression for the current, supposing that the electron interaction with impurities shows a local character (electron self-energy contains a Dirac δ function, considering the two space variables); in this, Sólyom and Zawadowski[11] found that the amplitude of the tunneling current is determined by the local EDS inside the barrier. According to the latter results, the local EDS should be calculated neglecting the tunneling, and then the current should be derived from the EDS.[20] Recently these results have been confirmed by Appelbaum and Brinkman[21] and Davis.[22] Appelbaum and Brinkman[21] gave a very simple elegant derivation of the results derived previously,[11,19] while Davis paid particular attention to the self-energy effects caused by phonons inside the barrier.[22,23]

Thus, in order to calculate the current, considering the effect of paramagnetic impurities, one needs to determine the EDS around the impurities. Here two cases should be distinguished, where the impurities are (i) inside the barrier or (ii) in one of the metal electrodes. The first case has been considered by Sólyom and Zawadowski[9-11] and recently by Appelbaum and Brinkman[24] in two different limits. Sólyom and Zawadowski[9-11] supposed that the exchange interaction coupling constant[25] shows a strong dependence on the momenta of incoming and outgoing electrons; i.e., the most essential contribution arises from the region of Fermi momentum. This momentum dependence has been taken into account by introducing an energy-cutoff parameter which has been assumed to be small compared to the Fermi energy.[26] In other words, it was assumed that the conduction-electron wave functions for a fixed momentum component parallel to the barrier surface are approximately the same inside the barrier. In this case, we get a depression in the EDS due to the magnetic impurities, and the result is an enhancement in the resistivity, just the opposite of what the "new channel" theory[5] predicted.

However, in a recent work, Appelbaum and Brinkman[24] pointed out that the existence of a depression or an enhancement of tunneling current depends on introducing the cutoff parameter. They showed that not introducing any cutoff for the interaction depresses the current if the impurity is found in the first atomic layer of the barrier, but, on the other hand, enhances the current if the impurities are more deeply inside the barrier. These results can be derived from the previous ones[9-11] by calculating some of the integrals without cutoff parameters.

The situation is very different in the other case, when the impurities are inside the bulk electrode but near the barrier surface. As we have shown in I, the EDS may be depressed around one impurity; it will be shown in the present paper that this depression can be enhanced, considering an impurity layer. The impurity layer should be found not further than the coherence length to get a large effect which always results in a resistivity maximum. As a special case, without introducing a cutoff energy Δ (corresponding to the limit, coherence length approaching the atomic distance), we get an oscillating result as a function of the distance of the impurity layer measured from the barrier, in agreement with Appelbaum and Brinkman's recent results.[21]

Concerning the giant zero-bias anomalies, the amplitude of the depression of the EDS is of particular importance. In the case of any kind of resonant scattering, the maximum value of the cross section is the so-called unitarity limit, which is independent of the density of the final states, in the present case, of the conduction EDS. On the other hand, the cross section is proportional to the scattering amplitude and the final density of states; thus the scattering amplitude is inversely proportional to the conduction EDS in the unitarity limit. However, inside an impurity layer the EDS at the Fermi energy may be strongly depressed by the impurities; thus the upper limit for the single-electron scattering amplitude is determined by the essentially reduced conduction EDS. In this way the scattering amplitude should be enhanced in a layer of high-impurity concentration. This cooperative increase in the unitarity limit was first suggested by Zawadowski and Sólyom[27] and will be discussed in detail throughout the present paper.

The aim of the present paper is the extension of the results of I for an impurity layer inside a metal, making use of the momentum-dependent exchange interaction corresponding to the energy-cutoff parameter discussed above. This case is closely related to the tunneling experiments. In Secs. II–IV we shall calculate the change of the EDS and its spatial dependence in the case of an arbitrary electron-impurity scattering amplitude for a layerlike distribution of impurity atoms. In Sec. V, the results are applied to tunnel junctions containing an impurity layer, as shown in Fig. 1. Furthermore, in Sec. VI we discuss the particular features associated with Kondo scattering, with special emphasis on some aspects of the impurity-impurity interaction within the impurity layer. Finally, in Sec. VII we give a brief summary of our conclusions.

II. FORMULATION OF PROBLEM

In order to determine the EDS 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 one-particle Green's function can be written as a function of the new variables as

$$\mathfrak{G}(r, r'; i\omega_n) = \mathfrak{G}(r_\perp, r'_\perp, r_\parallel - r'_\parallel; i\omega_n) \quad . \tag{2.1}$$

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

$$\mathfrak{G}(r, r'; i\omega_n) = (2\pi)^{-2} \int dk_\parallel \exp\left[ik_\parallel(r_\parallel - r'_\parallel)\right] \times \mathfrak{G}_{k_\parallel}(r_\perp, r'_\perp; i\omega_n) \quad . \tag{2.2}$$

The partial EDS 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

$$\rho_{k_\parallel}(x, \omega) = (1/\pi)\,\mathrm{Im}\left[\mathfrak{G}_{k_\parallel}(x, x; \omega - i\delta)\right] \quad . \tag{2.3}$$

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

$$\epsilon_k = \frac{k^2}{2m} = \epsilon_\parallel + \epsilon_\perp = \frac{k_\parallel^2}{2m} + \frac{k_\perp^2}{2m} \quad , \tag{2.4}$$

where $\epsilon_\parallel$ and $\epsilon_\perp$ denote the parallel and perpendicular contributions to the kinetic energy. Similar to (2.2), the Fourier transform of the free-electron Green's functions is

$$\mathfrak{G}^{(0)}_{k_\parallel}(r_\perp - r'_\perp; i\omega_n) = (1/2\pi) \int dk_\perp \exp[ik_\perp(r_\perp - r'_\perp)] \times \mathfrak{G}^{(0)}(k; i\omega_n) \quad , \tag{2.5}$$

where

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

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

$$\epsilon_k = \epsilon_\parallel + v_{k_\parallel}\left[\,|k_\perp| - k_{0\perp}(k_\parallel)\right] + \epsilon_0(k_\parallel) \quad , \tag{2.6}$$

where $v_{k_\parallel}$ is the velocity corresponding to the energy

$$\epsilon_0(k_\parallel) = k_{0\perp}^2(k_\parallel)/2m = \epsilon_0 - k_\parallel^2/2m$$

in the one-dimensional problem for a fixed $k_\parallel$.

Furthermore, the unperturbed EDS is

$$\rho^{(0)}_{k_\parallel}(\omega) = (1/\pi)\,\mathrm{Im}\,\mathfrak{G}^{(0)}_{k_\parallel}(0, \omega - i\delta) = 2(1/v_{k_\parallel}) \tag{2.7}$$

for $\omega \sim \epsilon_0 - \mu$, where the factor of 2 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 EDS 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

$$\mathfrak{G}(k, k'; i\omega_n) = \mathfrak{G}^{(0)}(k; i\omega_n)\,\delta(k - k') + \mathfrak{G}^{(0)}(k, i\omega_n) T_{kk'}(i\omega_n)\, \mathfrak{G}^{(0)}(k'; i\omega_n), \tag{2.8}$$

which is similar to (I3.3). The T matrix is defined for a given distribution of the impurities. The average over the impurity sites will be performed in Sec. III.

III. T MATRIX AND AVERAGE OVER IMPURITY DISTRIBUTION

In I we 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 $t_{kk'}(\omega)$. This scattering amplitude for the j'th impurity located at the point $R^{(j)}$ can be given as

$$t_{kk'}^{(j)}(i\omega_n)=e^{-i(k-k')R(j)}\,t_{kk'}(i\omega_n)\ . \qquad (3.1)$$

The T matrix defined in (2.8) corresponding to an impurity layer is a result of subsequent scatterings on different impurities. One can write it as a series of the scattering amplitudes:

$$T_{kk'}(i\omega_n)=\sum_j t_{kk'}^{(j)}(i\omega_n)+\frac{1}{(2\pi)^3}\int d^3k''\sum_{j,l}{}' t_{kk''}^{(j)}(i\omega_n)\times\mathfrak{G}^{(0)}(k'';i\omega_n)\,t_{k''k'}^{(l)}(i\omega_n)+\cdots\ , \qquad (3.2)$$

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:

$$\langle T_{kk'}(i\omega_n)\rangle_{\rm av}=\int dR^{(j)}\,c(R^{(j)})\,t_{kk'}^{(j)}(i\omega_n)+\sum_{j,l}{}'\int dR^{(j)}\,c(R^{(j)})\int dR^{(l)}\,c(R^{(l)})\times\int\frac{d^3k''}{(2\pi)^3}\,t_{kk''}^{(j)}(i\omega_n)\mathfrak{G}^{(0)}(k'';i\omega_n)t_{k''k'}^{(l)}(i\omega_n)\ , \qquad (3.3)$$

where the integrals with respect to $R^{(j)}$ can be performed, and considering (3.1), one obtains

$$[1/(2\pi)^2]\,\langle T_{kk'}(i\omega_n)\rangle_{\rm av}=t_{kk'}(i\omega_n)\delta(k_\parallel-k'_\parallel)\,c(k_\perp-k'_\perp)+(1/2\pi)\int dk''\,t_{kk''}(i\omega_n)\delta(k_\parallel-k''_\parallel)c(k_\perp-k''_\perp)\times\mathfrak{G}^{(0)}(k'';i\omega_n)\,t_{k''k'}(i\omega_n)\delta(k''_\parallel-k'_\parallel)c(k''_\perp-k'_\perp)+\cdots\ , \qquad (3.4)$$

where

$$c(k_\perp)=\int dx\,e^{-ik_\perp x}c(x)\ . \qquad (3.5)$$

The momentum dependence of the scattering amplitude has been given by (I3.4) for l-type scattering as

$$t_{kk'}(i\omega_n)=(2l+1)F(k)F(k')\,P_l(\cos\theta_{kk'})\,t_l(i\omega_n)\ , \qquad (3.6)$$

where $F(k)$ describes the momentum dependence of the scattering amplitudes, and it is assumed that $F(k)$ exhibits a peak at momentum k_0 corresponding to energy ϵ_0.

However, this momentum dependence can be taken into account in a simple way, if we are interested only in that case, where $k_\parallel\sim 0$, which is the important one for calculating the tunneling current. For $k_\parallel$, $k'_\parallel\approx 0$, the angle $\theta_{kk'}$ between k and k' is roughly zero or π, because k and k' are near the energy surface ϵ_0 due to the occurrence of the cutoff functions $F(k)$ given by (I2.4). Therefore, $P_l(\cos\theta_{kk'})=1$ for even angular momentum l. In this way we get, instead of (3.6),

$$t_{kk'}(i\omega_n)\approx(2l+1)F(k)F(k')\,t_l(i\omega_n)\ . \qquad (3.7)$$

Furthermore, in that case, where $k_\parallel\sim 0$, 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,

$$c(k\approx 0)=c\ , \qquad (3.8)$$

which is the surface concentration of the impurities, and

$$c(k\approx\pm 2k_0)\ , \qquad (3.9)$$

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

$$c(\pm 2k_0)=c\ , \qquad (3.9')$$

while for an experimentally available smooth distribution, one has

$$c(\pm 2k_0)\approx 0,\quad |c(\pm 2k_0)|\ll c\ , \qquad (3.9'')$$

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, hereafter 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 cannot be altered by scattering, as can be easily seen from (3.4), (3.8), (3.9′), and (3.9″).

It is useful to introduce the modified Green's functions

$$R_{lk_\parallel}^{(+)}(i\omega_n)=\frac{1}{2\pi}\int_0^\infty dk_\perp\, F^2(k)\frac{1}{i\omega_n-\xi_k}=\tfrac{1}{2}R_{lk_\parallel}(i\omega_n)\ , \qquad (3.10a)$$

$$R_{lk_\parallel}^{(-)}(i\omega_n)=\frac{1}{2\pi}\int_{-\infty}^0 dk_\perp F^2(k)\frac{1}{i\omega_n-\xi_k}=\tfrac{1}{2}R_{lk_\parallel}(i\omega_n)\ , \qquad (3.10b)$$

where

$$R_{lk_\parallel}(i\omega_n)=R_{lk_\parallel}^{(+)}(i\omega_n)+R_{lk_\parallel}^{(-)}(i\omega_n)\ . \qquad (3.11)$$

Let us turn to the solution of (3.4) for sharp impurity distribution, case (a). Considering (3.4) and (3.7)–(3.11), one gets

$$\langle T_{kk'}(i\omega_n)\rangle_{\rm av}=(2\pi)^2\delta(k_\parallel-k_\parallel')\,F(k)F(k')T_{lk_\parallel}(i\omega_n)\ , \qquad (3.12)$$

where

$$T_{lk_\parallel=0}(i\omega_n)=c(2l+1)\,t_l(i\omega_n)+c^2(2l+1)^2t_l(i\omega_n)\,R_{lk_\parallel=0}(i\omega_n)\,t_l(i\omega_n)+\cdots\ . \qquad (3.13)$$

The series can be summed up with the result

$$T_{lk_\parallel=0}(i\omega_n)=\frac{c(2l+1)\,t_l(i\omega_n)}{1-c(2l+1)\,t_l(i\omega_n)\,R_{lk_\parallel=0}(i\omega_n)}\ . \qquad (3.14)$$

As in (I3.6) and (I3.7), we introduce

$$\mathfrak{G}_{k_\parallel\rm cutoff}^{(+)}(x;i\omega_n)=\int_{-\infty}^\infty\frac{dk_\perp}{2\pi}\,e^{ik_\perp x}\mathfrak{G}_{k_\parallel\rm cutoff}^{(+)}(k_\perp;i\omega_n)=\int_0^\infty\frac{dk_\perp}{2\pi}\,F(k)\frac{1}{i\omega_n-\xi_k}\,e^{ik_\perp x}\ , \qquad (3.15a)$$

$$\mathfrak{G}_{k_\parallel\rm cutoff}^{(-)}(x;i\omega_n)=\int_{-\infty}^\infty\frac{dk_\perp}{2\pi}\,e^{ik_\perp x}\mathfrak{G}_{k_\parallel\rm cutoff}^{(-)}(k_\perp;i\omega_n)=\int_{-\infty}^0\frac{dk_\perp}{2\pi}\,F(k)\frac{1}{i\omega_n-\xi_k}\,e^{ik_\perp x}\ , \qquad (3.15b)$$

and, furthermore,

$$\mathfrak{G}_{k_\parallel\rm cutoff}(x;i\omega_n)=\mathfrak{G}_{k_\parallel\rm cutoff}^{(+)}(x;i\omega_n)+\mathfrak{G}_{k_\parallel\rm cutoff}^{(-)}(x;i\omega_n). \qquad (3.16)$$

Considering (3.12), (3.15a), (3.15b), and (3.16), the Dyson equation (2.8) can be written in the form

$$\mathfrak{G}^{(a)}(k,k';i\omega_n)=\mathfrak{G}^{(0)}(k;i\omega_n)\delta(k-k')+\mathfrak{G}_{k_\parallel}^{(0)}(k_\perp;i\omega_n)(2\pi)^2T_{lk_\parallel}(i\omega_n)\delta(k_\parallel-k_\parallel')F(k)F(k')\mathfrak{G}_{k_\parallel'}^{(0)}(k';i\omega_n), \qquad (3.17)$$

and, finally, applying the Fourier transformation given by (2.2), one gets (3.17) in coordinate space as

$$\mathfrak{G}_{k_\parallel}^{(a)}(r_\perp,r_\perp';i\omega_n)=\mathfrak{G}_{k_\parallel}^{(0)}(r_\perp-r_\perp';i\omega_n)+\mathfrak{G}_{k_\parallel\rm cutoff}(r_\perp;i\omega_n)(2\pi)^2\mathfrak{G}T_{lk_\parallel}(i\omega_n)\mathfrak{G}_{k_\parallel\,\rm cutoff}(-r_\perp;i\omega_n). \qquad (3.18)$$

The EDS can be obtained by inserting (3.18) into (2.3) and considering (2.7):

$$\rho_{k_\parallel=0}^{(a)}(x,\omega)=\rho_{k_\parallel=0}^{(0)}+4\pi\ \mathrm{Im}[T_{lk_\parallel}(\omega-i\delta)\mathfrak{G}_{k_\parallel\rm cutoff}(x,\omega-i\delta)\mathfrak{G}_{k_\parallel\rm cutoff}(-x,\omega-i\delta)]_{k_\parallel=0}\ , \qquad (3.19)$$

where $T_{lk}(i\omega_n)$ is given by (3.14). This result is the generalization of (I3.13) for an impurity layer.

In the case of the smooth impurity distribution, the calculation proceeds 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

$$\mathfrak{G}_{k_\parallel}^{(b)}(r_\perp,r_\perp';i\omega_n)=\mathfrak{G}_{k_\parallel}^{(0)}(r_\perp,r_\perp';i\omega_n)+(2\pi)^2\mathfrak{G}_{k_\parallel\rm cutoff}^{(+)}(r_\perp;i\omega_n)T_{lk_\parallel}^{(+)}(i\omega_n)\mathfrak{G}_{k_\parallel\rm cutoff}^{(+)}(-r_\perp';i\omega_n)+(2\pi)^2\mathfrak{G}_{k_\parallel\rm cutoff}^{(-)}(r_\perp;i\omega_n)T_{lk_\parallel}^{(-)}(i\omega_n)\mathfrak{G}_{k_\parallel\rm cutoff}^{(-)}(-r_\perp';i\omega_n)\ , \qquad (3.20)$$

where the scattering amplitudes are the following:

$$T_{lk_\parallel}^{(\pm)}(i\omega_n)=\frac{c(2l+1)t_l(i\omega_n)}{1-c(2l+1)t_l(i\omega_n)R_{lk_\parallel}^{(\pm)}(i\omega_n)}\ . \qquad (3.21)$$

By comparing (3.10a) and (3.11), we get

$$T_{lk_\parallel}^{(+)}(i\omega_n)=T_{lk_\parallel}^{(-)}(i\omega_n)=\frac{c(2l+1)t_l(i\omega_n)}{1-\frac{1}{2}c(2l+1)t_l(i\omega_n)R_{lk_\parallel}(i\omega_n)}\ . \qquad (3.22)$$

Inserting (3.20) into (2.3) and considering (3.22), the final expression of the EDS is obtained:

$$\rho^{(b)}_{k_\parallel=0}(x,\omega)=\rho^{(0)}_{k_\parallel=0}+4\pi\,\mathrm{Im}\{T^{(+)}_{lk_\parallel}(\omega-i\delta)\times[\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}(x;\omega-i\delta)\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}(-x;\omega-i\delta)+\mathfrak{G}^{(-)}_{k_\parallel\mathrm{cutoff}}(x;\omega-i\delta)\mathfrak{G}^{(-)}_{k_\parallel\mathrm{cutoff}}(-x;\omega-i\delta)]\}_{k_\parallel=0}\,. \tag{3.23}$$

Furthermore, the following identity can be seen from the comparison of (3.15a) and (3.15b):

$$\mathfrak{G}^{(\mp)}_{k_\parallel\mathrm{cutoff}}(-x;i\omega_n)=\mathfrak{G}^{(\mp)}_{k_\parallel\mathrm{cutoff}}(+x;i\omega_n). \tag{3.24}$$

Making use of this identity, the expressions of the EDS [(3.19) and (3.23)] can be further simplified:

$$\rho^{(a)}_{k_\parallel=0}(x,\omega)=\rho^{(0)}_{k_\parallel=0}+4\pi\,\mathrm{Im}[T_{lk_\parallel}(\omega-i\delta)\mathfrak{G}^{2}_{k_\parallel\mathrm{cutoff}}(x;\omega-i\delta)]_{k_\parallel=0} \tag{3.25}$$

for a sharp impurity distribution and

$$\rho^{(b)}_{k_\parallel=0}(x,\omega)=\rho^{(0)}_{k_\parallel=0}+4\pi\,\mathrm{Im}[T^{(+)}_{lk_\parallel}(\omega-i\delta)\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}(x;\omega-i\delta)\times\mathfrak{G}^{(-)}_{k_\parallel\mathrm{cutoff}}(x;\omega-i\delta)]_{k_\parallel=0} \tag{3.26}$$

for a smooth impurity distribution, where the definitions of the scattering amplitudes are given by (3.9) and (3.22). These equations, (3.25) and (3.26), are similar to (I3.8).

The modified Green's function $R_{lk_\parallel}(\omega-i\delta)$ given by (3.10a), (3.10b), and (3.11) can be easily evaluated for $|\tilde{\omega}|\ll\Delta$, i.e., $|\omega+\epsilon_0-\mu|\ll\Delta$, and by then considering that in this interval $F(k)\sim 1$,[28] one has

$$R_{lk_\parallel}(\omega\pm i\delta)=\mp i\pi\rho^{(0)}_{k_\parallel}\,, \tag{3.27}$$

which can be inserted into (3.14) and (3.22). In (3.10a) and (3.10b) the integrals have been evaluated making use of the approximation leading to (4.2).

IV. SPATIAL DEPENDENCE OF EDS

In order to determine the spatial dependence of the EDS, the modified Green's functions $\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}$ and $\mathfrak{G}^{(-)}_{k_\parallel\mathrm{cutoff}}$ will be calculated. One can prove, using the definitions (3.15a) and (3.15b), that

$$\mathfrak{G}^{(-)}_{k_\parallel\mathrm{cutoff}}(x;\omega)=[\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}(x;\omega^*)]^*\,. \tag{4.1}$$

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

$$\int_0^\infty \frac{dk_\perp}{2\pi}\to\int\frac{\rho^{(0)}_{k_\parallel}}{2}\,d\epsilon\,. \tag{4.2}$$

Making use of (I2.4), (I2.5), and (2.6), the modified Green's function $\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}$ given by (3.15a) may be written as

$$\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}(x,\omega\pm i\delta)=\frac{\rho^{(0)}_{k_\parallel}}{2}\int d\tilde{\epsilon}\,\frac{\Delta^2}{\Delta^2+\tilde{\epsilon}^2}\,\frac{1}{\tilde{\omega}-\tilde{\epsilon}\pm i\delta}\times\exp[i(k_{0\perp}+v^{-1}_{k_\parallel}\tilde{\epsilon})x]\,. \tag{4.3}$$

This integration can be easily performed by the contour integration method to yield the result

$$\mathfrak{G}^{(+)}_{k_\parallel=0,\,\mathrm{cutoff}}(x,\omega\pm i\delta)=\tfrac{1}{4}\rho^{(0)}_{k_\parallel=0}\,\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2}\times[e^{-x\Delta/v}\,e^{ik_0x}\,(\tilde{\omega}+i\Delta)-i\Delta(1+sg\delta)e^{i(k_0+\tilde{\omega}/v)x}]\quad\text{for } x>0, \tag{4.4}$$

where

$$v=v_{k_\parallel=0}\,.$$

In the case (a) of sharp impurity distribution, Eq. (4.4) has to be inserted into (3.25). The change in the EDS consists of two parts, the oscillating and the nonoscillating one, $\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{o}}$ and $\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{no}}$, respectively, i.e.,

$$\rho^{(a)}_{k_\parallel=0}(x,\omega)=\rho^{(0)}_{k_\parallel=0}+\Delta\rho^{(a)}_{k_\parallel=0,\,\mathrm{o}}(x,\omega)+\Delta\rho^{(a)}_{k_\parallel=0,\,\mathrm{no}}(x,\omega)\,. \tag{4.5}$$

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 I by the Eqs. (I3.16) and (I3.17) as, respectively,

$$\xi_\Delta=v/\Delta\,,\quad \xi_{\tilde{\omega}}=v/\tilde{\omega}\,.$$

In this way one gets

$$\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{o}}(x,\omega)=-\frac{\pi}{2}\left(\rho^{(0)}_{k_\parallel=0}\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2}\right)^2\Bigg(\mathrm{Im}[T_{lk_\parallel=0}(\omega-i\delta)]\Bigg\{2\cos2\left(k_0+\frac{1}{\xi_{\tilde{\omega}}}\right)x-2e^{-|x|/\xi_\Delta}\left[\cos\left(2k_0+\frac{1}{\xi_{\tilde{\omega}}}\right)x-\frac{\tilde{\omega}}{\Delta}\sin\left(2k_0+\frac{1}{\xi_{\tilde{\omega}}}\right)x\right]+e^{-2|x|/\xi_\Delta}\left[\left(1-\frac{\tilde{\omega}^2}{\Delta^2}\right)\cos2k_0x+2\frac{\tilde{\omega}}{\Delta}\sin2k_0|x|\right]\Bigg\}+\mathrm{Re}[T_{lk_\parallel=0}(\omega-i\delta)]\Bigg\{-2\sin2\left(k_0+\frac{1}{\xi_{\tilde{\omega}}}\right)|x|+2e^{-x/\xi_\Delta}\left[\sin\left(2k_0+\frac{1}{\xi_{\tilde{\omega}}}\right)|x|-\frac{\tilde{\omega}}{\Delta}\cos\left(2k_0+\frac{1}{\xi_{\tilde{\omega}}}\right)x\right]\Bigg\}\Bigg)\,, \tag{4.6}$$

$$\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{no}}(x,\omega)=-\frac{\pi}{2}\left(\rho^{(0)}_{k_\parallel=0}\frac{\Delta^2}{\Delta^2+\tilde\omega^2}\right)^2\left\{\mathrm{Im}\,[T_{lk_\parallel=0}(\omega-i\delta)]\left[2e^{-|x|/\xi_\Delta}\left(\cos\frac{x}{\xi_{\tilde\omega}}-\frac{\tilde\omega}{\Delta}\sin\frac{|x|}{\xi_{\tilde\omega}}\right)-e^{-2|x|/\xi_\Delta}\left(1+\frac{\tilde\omega^2}{\Delta^2}\right)\right]\right.$$
$$\left.+\mathrm{Re}\,[T_{lk_\parallel=0}(\omega-i\delta)]\left[2e^{-x/\xi_\Delta}\left(\sin\frac{|x|}{\xi_{\tilde\omega}}+\frac{\tilde\omega}{\Delta}\cos\frac{|x|}{\xi_{\tilde\omega}}\right)\right]\right\}, \qquad (4.7)$$

where it is taken into account that the EDS is an even function of the variable x.

This situation is somewhat changed in the case of a smooth impurity distribution, where the change in the EDS is definitely nonoscillating:

$$\rho^{(b)}_{k_\parallel=0}(x,\ \omega)=\rho^{(0)}_{k_\parallel=0}+\Delta\rho^{(b)}_{k_\parallel=0,\mathrm{no}}(x,\ \omega)\ , \qquad (4.8)$$

where $\Delta\rho^{(b)}_{k_\parallel=0,\mathrm{no}}(x,\ \omega)$ can be evaluated as (4.7) was, considering (3.26) and (4.17). Furthermore, comparison with (4.7) yields

$$\Delta\rho^{(b)}_{k_\parallel=0,\mathrm{no}}(x,\ \omega)=[\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{no}}(x,\ \omega)]_{T\to T^{(+)}}\ , \qquad (4.9)$$

where $T\to T^{(+)}$ 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 $\mathfrak{G}^{(+)}_{k_\parallel\mathrm{cutoff}}$ and $\mathfrak{G}^{(-)}_{k_\parallel\mathrm{cutoff}}$ 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 EDS is questioned.

The discussion of the results derived here is left to the succeeding sections. However, we have seen in Paper I that the most pronounced effects appear in the so-called "unitarity limit," when the change in the EDS reaches its maximal amplitude. The unitarity limit has been introduced as the case of a phase shift equal to $\frac{1}{2}\pi$. In our actual case the scattering amplitudes given by (3.14) and (3.22) cannot be expressed by a single phase shift in general. However, we may call the unitarity limit the limit when $t(\omega\pm i\delta)\to\pm i\infty$ or $c\to\infty$. The real possibility of approaching this unitarity limit will be discussed in Sec. VI. The scattering amplitudes have simple limiting values, especially

$$T_{lk_\parallel=0}(\omega\pm i\delta)\to-[R_{lk_\parallel=0}(\omega\pm i\delta)]^{-1}\approx\mp i(\pi\rho^{(0)}_{k_\parallel=0})^{-1}\ , \qquad (4.10)$$

$$T^{(+)}_{lk_\parallel=0}(\omega\pm i\delta)\to-\frac{1}{\frac{1}{2}R_{lk_\parallel=0}(\omega\pm i\delta)}\approx\mp i\frac{2}{\pi\rho^{(0)}_{k_\parallel=0}}\ , \qquad (4.11)$$

where (3.27) 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:

$$\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{o}}(x,\ \omega)\to-\tfrac{1}{2}\rho^{(0)}_{k_\parallel=0}\left(\frac{\Delta^2}{\Delta^2+\tilde\omega^2}\right)^2\left\{2\cos2\left(k_0+\frac{1}{\xi_{\tilde\omega}}\right)x-2e^{-|x|/\xi_\Delta}\left[\cos\left(2k_0+\frac{1}{\xi_{\tilde\omega}}\right)x-\frac{\tilde\omega}{\Delta}\sin\left(2k_0+\frac{1}{\xi_{\tilde\omega}}\right)|x|\right]\right.$$
$$\left.+e^{-2|x|/\xi_\Delta}\left[\left(1-\frac{\tilde\omega^2}{\Delta^2}\right)\cos2k_0x+2\frac{\tilde\omega}{\Delta}\sin2k_0|x|\right]\right\}\ , \qquad (4.12)$$

$$\Delta\rho^{(a)}_{k_\parallel=0,\mathrm{no}}(x,\ \omega)\to-\tfrac{1}{2}\rho^{(0)}_{k_\parallel=0}\left(\frac{\Delta^2}{\Delta^2+\tilde\omega^2}\right)^2\left[2e^{-|x|/\xi_\Delta}\left(\cos\frac{x}{\xi_{\tilde\omega}}-\frac{\tilde\omega}{\Delta}\sin\frac{|x|}{\xi_{\tilde\omega}}\right)-e^{-2|x|/\xi_\Delta}\left(1+\frac{\tilde\omega^2}{\Delta^2}\right)\right]\ , \qquad (4.13)$$

which are represented in Figs. 2 and 3, considering the right-hand vertical scale in the latter one.

In the unitarity limit, similar to the single-impurity problem for s-type scattering [see (I4.2)], the EDS vanishes at the impurity layer. It is interesting that one-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 Figs. 2 and 3. The derivative of the EDS is zero at the impurity layer. It is interesting that at large distances only the oscillating part with a very large amplitude remains.

The results (4.6) and (4.7) show that the EDS perturbation around a single impurity is coherently enhanced in the neighborhood of an impurity layer, with respect to the oscillating, as well as the nonoscillating part. In the case of a single impurity we have a factor r^{-2} in the change of the EDS; 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 as shown in Fig. 3. This energy dependence is more rapid for larger distances $|x|$.

The change in the EDS for a smooth impurity distribution can be obtained by inserting (4.11) into (4.9), and it is illustrated in Fig. 3 using the left-

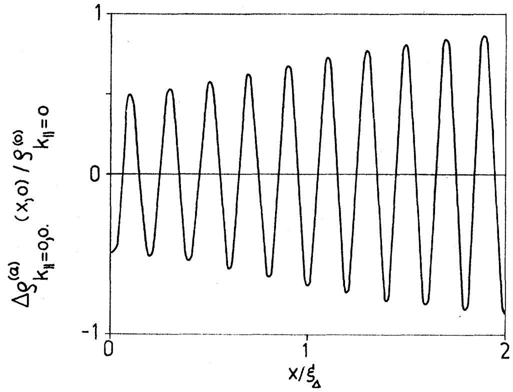

FIG. 2. Oscillating part of the change in the EDS in the unitarity limit as a function of the distance measured from the impurity layer, for sharp impurity distribution [case (a)] for $\tilde{\omega}=0$.

hand vertical scale. The final result may be compared with (4.13), and then one obtains

$$\Delta\rho^{(b)}_{k=0,\mathrm{no}}(x,\ \omega)=2\Delta\rho^{(a)}_{k=0,\mathrm{no}}(x,\ \omega)\ . \qquad (4.14)$$

In this case the nonoscillating part of the EDS at $x=0$ has the same amplitude as the unperturbed EDS $\rho^{(0)}_{k=0}$, but it has opposite sign. Thus the EDS at the impurity layer ($x=0$) vanishes for the unitarity limit in both cases.

V. TUNNELING ANOMALIES

Now we discuss how these EDS anomalies show up in the characteristics of a metal-insulator-metal (MIM) 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 were investigated earlier by Sólyom and one of the present authors.[9–11,27]

For the sake of simplicity we treat the case of zero temperature. As it has been derived earlier,[10,11] the dynamical conductance at voltage V is proportional to the EDS $\rho(D, eV)$ at the barrier surface where the energy variable ω is taken as eV. Let us suppose that the EDS of the metal on the left- and right-hand sides without impurities are independent of the energy; furthermore, $G^{(0)}$ and $R^{(0)}$ denote the conductance and resistance of the pure junction. In this way, the dynamical conductance and resistance versus voltage can be given by the following formulas for junctions containing impurities[11]:

$$G(D,\ V)/G^{(0)}=Z(D,\ eV)\ , \qquad (5.1)$$

$$R(D,\ V)/R^{(0)}=Z^{-1}(D,\ eV)\ , \qquad (5.2)$$

where the renormalization function of the EDS is

$$Z(x,\ \omega)=\rho_{k_\parallel=0}(x,\ \omega)/\rho^{(0)}_{k_\parallel=0}\ . \qquad (5.3)$$

The parallel momentum component is chosen to be zero because the tunneling rate of the electrons is the largest in this case.[29]

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 EDS are given by (4.5)–(4.9) for cases (a) and (b), respectively, which can be inserted into (5.3). Then one obtains

$$Z^{(a)}(0,\ \omega)=1-\pi\rho^{(0)}_{k_\parallel=0}\,\mathrm{Im}\,T_{lk_\parallel=0}(\omega-i\delta)\ , \qquad (5.4a)$$

$$Z^{(b)}(0,\ \omega)=1-\tfrac{1}{2}\pi\rho^{(0)}_{k_\parallel=0}\,\mathrm{Im}\,T^{(+)}_{lk_\parallel=0}(\omega-i\delta)\ , \qquad (5.4b)$$

where the assumption $\tilde{\omega}\ll\Delta$ has been made. 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.

The results (5.4a) and (5.4b) might be slightly changed if one considers the presence of the barrier by assuming some particular surface scattering.

Considering (3.14) and (3.22), the renormalization function can be expressed by the electron-impurity scattering amplitude $t_l(\omega)$ in both cases (a) and (b) as

$$Z^{(a,b)}(0,\ \omega)=\mathrm{Re}\,[1-i\kappa^{(a,b)}c(2l+1)\,t_l(\omega-i\delta)\pi\rho^{(0)}_{k=0}]^{-1}\ , \qquad (5.5)$$

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

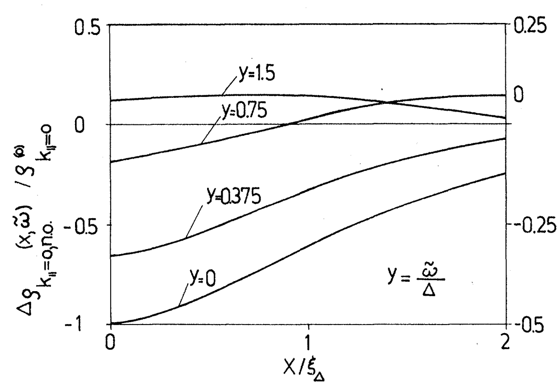

FIG. 3. Nonoscillating part of the change in the EDS in the unitarity limit as a function of the distance measured from the impurity layer for different values of the energy parameter $y=\tilde{\omega}/\tilde{\omega}$. The curves apply for sharp [case (a)] and smooth [case (b)] impurity distribution as well, if the vertical scales at the right and at the left are considered, respectively.

$$c\rho^{(0)}_{k_\parallel=0}=\gamma N_i\,\rho^{(0)}\ , \tag{5.6}$$

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

The renormalization factor $Z(0,\ \omega)$ has a rather simpler form if $t_l(\omega)$ is purely imaginary, namely,

$$Z^{(a,b)}(0,\ \omega)=[1+N_i\pi\rho^{(0)}\gamma\kappa^{(a,b)}(2l+1)\,t_l(\omega-i\delta)]^{-1}\ . \tag{5.7}$$

This formula was first derived by Sólyom and Zawadowski[10,11] for case (a). Making use of (5.2) and (5.7), one obtains for the resistance

$$\frac{R^{(a,b)}(0,\ V)}{R^{(0)}}=1+N_i\pi\rho^{(0)}\gamma\kappa^{(a,b)}(2l+1)\,\mathrm{Im}\,t_l(eV-i\delta)$$
$$+\frac{[N_i\pi\rho^{(0)}\gamma\kappa^{(a,b)}(2l+1)\,\mathrm{Re}\,t_l(eV-i\delta)]^2}{1+N_i\pi\rho^{(0)}\gamma\kappa^{(a,b)}(2l+1)\,\mathrm{Im}\,t_l(eV-i\delta)}\ . \tag{5.8}$$

The consequences of the above-derived results will be presented in Sec. VI.

Let us turn to the case where the impurity layer is at distance D measured with respect to the barrier surface. Experimentally, the preparation of the impurity layer is never perfect. Therefore, the real situation may be described by 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):

$$\frac{G(D,\ V)-G^{(0)}}{G^{(0)}}$$
$$=-\tfrac{1}{2}\pi\rho^{(0)}_{k_\parallel=0}\Big[\mathrm{Im}\,[T^{(+)}_{lk_\parallel=0}(\omega-i\delta)]\,(2e^{-D/\xi_\Delta}-e^{-2D/\xi_\Delta})$$
$$-\mathrm{Re}\,[T^{(+)}_{lk_\parallel=0}(\omega-i\delta)]2e^{-D/\xi_\Delta}$$
$$\times\left(\sin\frac{D}{\xi_{\tilde{\omega}}}+\frac{\tilde{\omega}}{\Delta}\cos\frac{D}{\xi_{\tilde{\omega}}}\right)\Big]_{\omega=eV}\ , \tag{5.9}$$

ω being equal to eV, and $T^{(+)}(\omega)$ given by (3.22). Furthermore, if $t_l(\omega)$ is purely imaginary, then $\mathrm{Re}\,T^{(+)}(\omega)=0$ and one obtains

$$[G(D,\ V)-G^{(0)}]/G^{(0)}$$
$$=-\tfrac{1}{2}\pi\,\rho^{(0)}_{k=0}\,\mathrm{Im}\,[T^{(+)}_{lk=0}(\omega-i\delta)]\,(2e^{-D/\xi_\Delta}-e^{-2D/\xi_\Delta}) \tag{5.10}$$

or

$$\frac{G(D,\ V)-G^{(0)}}{G(0,\ V)-G^{(0)}}=e^{-D/\xi_\Delta}\left[2-e^{-D/\xi_\Delta}-\sigma\left(\frac{\tilde{\omega}^2}{\Delta^2}\right)\right], \tag{5.11}$$

where, by virture of (4.7),

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

gives the lowest-order corrections for energies not very close to the resonance; i.e., $|\omega-\epsilon_0|\equiv|\tilde{\omega}|\ll\Delta$ is not satisfied. The result given by (5.11) 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 independent of the assumption $\mathrm{Re}\,T^{(+)}(\omega)=0$, (5.11) is valid for the voltage $V_0=(\epsilon_0-\mu)/e$ corresponding to the resonance energy.

VI. DISCUSSION OF TUNNELING ANOMALIES

The most striking application of the theory is to the Kondo effect, where the scattering amplitude $t_l(\omega)$ shows a resonant behavior at the Fermi energy.[30] The theory of Kondo scattering can be applied if a magnetic moment is formed on the transition-metal impurity. The alternate case is when there is no moment on the impurity, but the occupation of spin-up and spin-down d (or f) level is fluctuating. This is known as the spin-fluctuation model, where the conduction-electron–impurity scattering amplitude exhibits a peak at the position of the d level,[31] which might accidentally coincide with the Fermi energy. However, recently it has been shown by Wang, Evenson, and Schrieffer[32] that the two mentioned possibilities are two opposite limiting cases of the same physical phenomenon; therefore, the realization of intermediate cases is very likely. 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.

Position of anomaly. If the resonance takes place at the Fermi energy $\omega=0$, the characteristic anomalies are found around the zero bias.

Symmetry of characteristics. If the band structure of the conduction electrons in the neighborhood of the Fermi energy is approximately symmetrical with respect to the Fermi energy, there exists the electron-hole symmetry in the scattering amplitude, which has the form[30,33]

$$t^*(\omega-i\delta)=-t(-\omega-i\delta)\ . \tag{6.1}$$

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

$$[T^{(+)}(\omega-i\delta)]^*=-T^{(+)}(-\omega-i\delta),$$
$$T^*(\omega-i\delta)=-T(-\omega-i\delta), \tag{6.2}$$

where (3.14), (3.22), and (3.27) have been considered. Inserting this relation into (5.9), one obtains for $D=0$:

$$G(V) = G(-V).$$

Thus the electron-hole symmetry of the scattering problem shows up in the symmetrical characteristics of the junction.[34]

It is worth mentioning that if $\epsilon_0 = \mu$, the relation $\omega \to -\omega$ corresponds to $\tilde{\omega} \to -\tilde{\omega}$, and by this it can be seen from (4.7) that the characteristics remain symmetrical for $D \neq 0$ also, since the even function $\mathrm{Im}\,T(\omega - i\delta)$ and the odd function $\mathrm{Re}\,T(\omega - i\delta)$ are multiplied in (4.7) by even and odd functions of $\tilde{\omega}$, respectively.

Effect of impurity-impurity interaction. 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 $t_l(\omega - i\delta) \to i/\pi\rho^{(0)}$ we obtain for the relative amplitude of the resistance anomaly from (5.8), if $D = 0$,

$$[R(V_0) - R^{(0)}]/R_0 = \gamma N_i (2l+1). \qquad (6.3)$$

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 neighboring 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.

On the other hand, for high impurity concentrations we should take into account the interaction between impurities. We mention here two types of interactions: (i) The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is negligible if the corresponding energy is rather small compared to the Kondo energy,[35] which is not necessarily the case in general. (ii) If the impurity can be found in an impurity layer, then the conduction-electron–impurity scattering amplitude is determined not by the bulk EDS, but by the EDS modified by the other impurities in the layer. First of all we would have to calculate the scattering amplitude for the drastically depressed energy-dependent EDS at the impurity layer rather than that for the constant bulk EDS, as has been discussed by Sólyom and Zawadowski.[11,27] 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 EDS, not even in an approximation; thus we can make only some qualitative considerations, to explore the effects of this self-consistency. Two consequences will be discussed.

A. Amplitude of Resistivity Peak

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

$$\max|t_l(\omega - i\delta)| \gg (\pi\rho^{(0)})^{-1}. \qquad (6.4)$$

In this case, as it can be seen from (3.14) using (3.27) and (5.6) with $N_i \sim 1$, $T_{lk_\parallel=0}$ approaches the unitarity limit of the scattering amplitude which has been defined by (4.10) and (4.11). In this limit for $D = 0$, the junction conductance approximately vanishes for the resonant energy, i.e., at zero bias, as mentioned before. It is worth noticing that in the case of s-type scattering, as the scattering amplitude approaches the unitarity limit, the EDS vanishes at the impurity site for single impurity [see (I4.2) for the phase shift $\delta = \frac{1}{2}\pi$], and similarly, the unitarity limit for the case of an impurity layer defined as $\mathrm{Im}\,t \to \infty$ corresponds to zero EDS in the layer.

On the basis of the foregoing considerations we may expect that with increasing impurities, the unitarity limit for $t_l(\omega)$, as well as the maximum actual value of its imaginary part, $\mathrm{Im}\,t_l(\omega - i\delta)$ increases. In this case the maximum of the dynamical resistance given by Eq. (5.8) as

$$\max|R(V)/R_0| = 1 + N_i \pi\rho^{(0)} \gamma \kappa^{(a,b)} (2l+1) \max[\mathrm{Im}\,t_l(eV - i\delta)] \qquad (6.5)$$

depends on the impurity concentration nonlinearly. Thus, beside the explicit dependence expressed by the term N_i, we have a further variation implicit in $t_l(eV - i\delta)$. 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 $\max|t_l(\omega)|$ also.

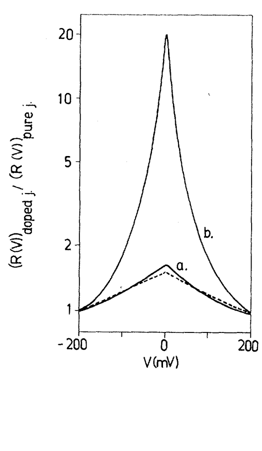

FIG. 4. Experimental dynamical resistance vs voltage characteristics of Cr-doped Al-Al tunnel junctions normalized to the characteristics of a pure junction having the same resistance at − 200 mV (from Ref. 6) as compared to the theoretical curve (see text).

B. Narrowing of Resistance Peak

Nevertheless, there is another important consequence which follows from the self-consistent treatment. The width of the resonance can be characterized by the Kondo energy

$$E_K = \Delta e^{-N/2J\rho^{(0)}} ,$$

where J/N and Δ are the electron-impurity exchange coupling constant and cutoff energy, respectively. Also taking into account in this equation the reduction of the EDS 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 EDS certainly smaller than $\rho^{(0)}$.

As a qualitative illustration of this behavior, we reproduce two experimental $R(V)$ characteristics of Ref. 13 obtained for different amount of dopants introduced into the barrier (solid lines in Fig. 4). The characteristics a and b correspond to junctions containing the total amount of Cr dopant equivalent to about one-half and two monoatomic layers, respectively, introduced into the barrier region of an Al-Al_1O_3-Al tunnel diode. As another illustration we have plotted in Fig. 4 a theoretical characteristic also (dashed line), calculated for the approximate scattering amplitude proposed by Hamman[14]:

$$t(\omega) = \frac{1}{2\pi\rho^{(0)}} \left(1 + \frac{X}{[X^2 + S(S+1)\pi^2]^{1/2}}\right) ,$$

where X is connected with the energy ω in a rather complicated way. The calculation was made using (5.8) with the reasonable value $N_i \gamma \kappa (2l+1) = 3$. To obtain qualitative agreement with the experimental curve a in Fig. 4 we chose $T_K = 2000$ °K. (In the computation of the scattering amplitude the impurity spin S was taken to be equal to $\frac{1}{2}$; 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. We should like to emphasize, however, that this demonstration that the present theory is adequate to explain experimental data was intended only to show the possibility of such explanation of giant resistance peaks. As discussed before, firm experimental evidence for the observation of EDS changes by tunneling is not yet achieved.

VII. CONCLUSIONS

Theoretical investigation of the change in the conduction EDS around one impurity has been extended to the case of an impurity layer. It has been supposed that the conduction-electron–impurity scattering amplitude was a separable function in the variables of the energy and momenta of the incoming and outgoing electrons [see (3.7)]. No particular assumption has been applied to the energy dependence, but the present paper has been aimed at resonant scattering. The spatial structure of the change in the conduction EDS has been characterized by only one characteristic distance, called coherence length, since only one region of the momentum has been assumed to contribute to the scattering amplitude. In the case of s-d exchange interaction without potential scattering, this momentum region should be exhibited by the exchange coupling constant $J_{kk'}$ as has been discussed in Paper I. Furthermore, the present theoretical treatment can be applied to potential scattering also, if the potential is a separable function among the momentum variables. In this case the coherence length is determined by the momentum dependence of the potential. Finally, if the potential scattering and exchange interaction are to be considered simultaneously, then the results presented here should be essentially reinvestigated.

We have seen that the scattering of conduction electrons by transition-metal impurity atoms may cause tunneling anomalies, if the impurities are near the barrier, because the EDS changes around the impurities inside the coherence length. It is worth mentioning that homogeneously distributed impurities in the metal electrode (dilute alloys) do not change the EDS essentially,[11,36] which fact seems to be in agreement with some recent experimental results.[37]

If the anomalous part of the characteristics is symmetrical in the applied voltage, we may conclude that the scattering at least approximately shows the electron-hole invariance. Furthermore, a giant anomaly being centered at zero bias may be due to Kondo scattering which occurs when there is a magnetic moment on the d level of the impurities. On the other hand, if no moment is formed on the d level, but the momentum is fluctuating (local spin-fluctuation model), then the resistivity peak should be around the voltage corresponding to the energy of the d level.

If one assumes that the giant zero-bias anomalies are due to Kondo scattering, it seems to be a good check to measure the concentration dependence of the characteristics. For larger amounts of the impurities the giant resistivity peak should show a nonlinear dependence on the impurity concentration and the peak should narrow as discussed in Sec. VI.

To make use of zero-bias anomalies for studying the Kondo effect, first of all very well-controlled experimental situations should be realized. There are two possible applications.

(i) The first is to determine the coherence length and to get information on the momentum dependence of the exchange coupling. We see that the major interest of the present theory lies in pointing out an adequate method of determining the characteristic coherence length in the Kondo problem currently very often investigated. As mentioned in the Introduction of 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 EDS change has the largest spatial extent for zero energy, and falls off rapidly beyond $|\hat{\omega}| > \Delta$ (see Fig. 3). In the coherence-length studies, just this may give substantial importance to a method appropriate to investigating the perturbations of the electron wave functions due to scattering at different energies separately.

(ii) The second application is to study the energy dependence of the Kondo-scattering amplitude. For this purpose those junctions seem to be the most appropriate in which the impurities are near the barrier ($D \ll \xi_\Delta$), but not in the barrier, and, on the other hand, the concentration of the impurities is small enough not to change the single-impurity scattering amplitude $t_l(\omega)$ (see Sec. VI). Thus considering (5.8) and keeping only the term linear in the impurity concentration, N_i, the change of the resistivity, is proportional to the imaginary part of the scattering amplitude. As we have pointed out in the Introduction, tunneling seems to be, in principle, a unique tool for the study of this problem.

We mention here that the coherence length plays an important role in the formation of the spatial structure of the Kondo spin-compensated state at low temperature. The conduction-electron spin polarization around a paramagnetic impurity contains such a contribution which extends in the range of one atomic distance, if the calculation is performed using a cutoff energy corresponding to the conduction-electron bandwidth.[38] However, the spatial range of this contribution can be enlarged up to the coherence length ξ_Δ when a cutoff procedure is applied in the momentum dependence of the exchange coupling constant.

As we discussed in the Introduction, many experimental results show the giant resistivity and conductance peak simultaneously. We briefly summarize here what could be an explanation of these effects, by supposing that the magnetic impurities are responsible for both anomalies.

Let us suppose that some of the impurities are in the metal electrode and others can be found in the barrier. Those in the metal may be responsible for the giant part of the resistivity peak, as we have discussed in the present paper. Furthermore, making use of the assumption that for the electron-impurity scattering inside of the barrier there is no small cutoff parameter ($\ll E_F$), then according to Appelbaum and Brinkman's recent work[24] the impurities inside the barrier may change the EDS to cause a conductance peak. This conductance peak was formally fitted by Appelbaum[5] by an adequate choice of the impurity-assisted tunneling amplitude. However, we emphasize that this change is the effect of the local self-energy on the EDS and is not connected with a new[39] assisted tunneling channel, which is always based on the nonlocal behavior of the interaction (e.g., contrary to the molecular-vibration-assisted tunneling). At this point it is worth mentioning that the Kondo scattering becomes weaker as the position of the impurity is shifted to the middle of the barrier, because the amplitude of the tail of the conduction-electron wave function falls off very rapidly in the barrier. In other words, the predicted conductance should always be narrower than the resistivity peak. Furthermore, if the density of the electrons depressed at and inside the barrier is due to impurities found in the electrode, the strength of the exchange coupling interaction is reduced, because the coupling strength is proportional to the effective exchange integral and the EDS in the neighborhood of the Fermi energy. Thus the giant resistivity peak and the conductance peak should be narrowed simultaneously by increasing the concentration of the impurities. However, we may mention that we still cannot rule out the possibility, admittedly unlikely, that the conductance peak is a consequence of the impurity-impurity interaction or of some structure in the scattering amplitude.

Finally, we mention another ambiguity in the theory. The main argument against the existence of a new assisted tunneling channel could be the local behavior of the exchange interaction in space, in which case there is no new channel.[11] From first principles it is quite impossible to justify this point.[39] Unfortunately, the experiments also cannot provide this information. Using a Green's-function decoupling scheme first applied by Appelbaum, Phillips, and Tzouras[18] to the theory of zero-bias anomalies, the change in the EDS and a phenomenologically introduced impurity-spin-assisted tunneling channel as that suggested by Appelbaum[5] can be treated at the same time. Such a calculation has been performed by Sz-Nagy,[40] paying particular attention to the averaging over the impurity sites. She found, if both phenomena, i.e., local change in the EDS and assisted tunneling, are present, then these two effects produce an interference cross term which yields asymmetric contributions to the resistivity.[41] Since the experiments show fairly symmetric $R(V)$ characteristics, one of the phenomena should be negligible.

If the change in the EDS can be taken to be well justified, we may conclude that the introduction of the new assisted channel is probably not necessary.

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*Research supported by the Center for Advanced Studies at the University of Virginia.

†Permanent address: Central Research Institute for Physics, Budapest, Hungary.

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