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A. Zawadowski and F. Mezei

HUNGARIAN ACADEMY OF SCIENCES
CENTRAL RESEARCH INSTITUTE FOR PHYSICS

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CHANGE IN THE ELECTRON DENSITY OF STATES DUE TO KONDO SCATTERING I.:

The problem of a single impurity

F. Mezei and A. Zawadowski[+]
Central Research Institute for Physics, Budapest, Hungary

For an arbitrary conduction-electron-impurity scattering the conduction electron density of states is calculated by making use of the thermodynamical Green's function technique with particular respect to its spatial structure. If the interaction depends on the momenta of the scattered waves in such a way that it is important only in the neighbourhood of the Fermi suface /characterized by the corresponding energy width Δ /, a coherence length can be introduced: $\xi_\Delta = v/\Delta$, where v is the Fermi velicity./Present experimental data obtained for different Kondo systems can be interpreted as yielding 5-50 Å for ξ_Δ./The spatial variation of the change in the electron density of states is found to be: in the short-range region, $r << \xi_\Delta$ negative definite due to the interference between the incoming and outgoing scattered waves and in the long-range region, $r >> \xi_\Delta$ showing the Freidel oscillation. The results are expressed by a phase shift, δ and it is found e.g. that the electron density of states at the impurity site is proportional to $\cos^2\delta$ for scattering of s-type, while it does not change for d-type. In the case of the Kondo effect the results are very sensitive to the energy variable and they take the maximal amplitude at the Fermi surface. It is worth mentioning that the spatial dependence of the change in the electron density of states does not depend on the scattering amplitude and, in this way, on the Kondo temperature, or, at least it does not depend explicitly. These results have been derived supposing that the bulk electron density of states is independent of the energy. By dropping this assumption, however, they alter only slightly.

[+]Present address: Department of Physics, University of Virginia Charlottesville, Virginia

I. Introduction

About fifteen years ago Friedel[1] has called the attention to the charge oscillation around an impurity atom in metallic host. This charge oscillation is a result of the change in the electron density of states caused by the perturbing impurity atom, which change shows a similar oscillation. This modification of the electron density of states /e.d.s./ is of particular importance in the case of a resonant conduction-electron-impurity scattering associated with the unfilled d-level. The problem has taken a new striking feature by the discovery of the Kondo[2] effect: it has been shown that the conduction-electron-paramagnetic-impurity scattering exhibits a resonance at the Fermi energy usually called Abrikosov[3]-Shul[4] resonance.

The purpose of the present paper is to investigate the change in the e.d.s. in the vicinity of the impurity for Abrikosov-Suhl resonance. This problem has not been investigated in detail until now. Everts and Ganguly[5] have calculated the conduction e.d.s. around a paramagnetic impurity on the basis of the Kondo exchange model applying perturbation theory of second order. This calculation has not led to Kondo anomaly associated with the appearance of the characteristic logarithmic terms. To our knowledge no calculations of higher order contributions have been reported so far for one impurity problem. However, the effect of a paramagnetic impurity layer on the e.d.s. of the host metal has been investigated in detail by Sólyom and Zawadowski[6-9] with respect to the zero bias anomalies observed in metal-metal-oxide-metal junctions doped by magnetic impurities[10]. The result of these calculations is that the e.d.s. may be depressed by the resonant electron-paramagnetic-impurity scattering in the vicinity of the impurity. This phenomenon can be understood as a strong destructive interference between the incoming and outgoing waves. The extinction occurs always because of the phase shift of the scattered wave.

The Kondo effect has been particularly investigated during the last years[11] and at very low temperature it is interpreted as the resonant scattering of conduction electrons on spin compensated state formed continuously below the characteristic Kondo temperature T_K by an impurity spin and the magnetically polarized conduction electron cloud in the neighbourhood of the impurity. Recently many authors[10-20] have investigated theoretically the spatial stucture of this spin compensated state. According to Nagaoka's paper[12] the electron magnetization is damped out beyond a coherence length. Nagaoka's coherence length is given by the Kondo temperature T_K and the Fermi velocity v_F as $\xi_{T_K} = \frac{v_F}{kT_K}$ or $\xi_{T_K} \sim a \frac{\varepsilon_F}{kT_K}$ where a and ε_F denote the atomic distance and the Fermi energy, respectively. The coherence length must be of the order of

$\xi_{T_K} \sim 10^3$-10^5 Å for $\varepsilon_F \sim 1$-10 eV and $kT_K \sim 10^{-4}$-10^{-2} eV. Similar result has been obtained by Heeger et.al.[16] who have investigated the stucture of the ground state proposed by Appelbaum and Kondo[21]. Unfortunately, the latter ground state is determined by a variational method, where important terms have been omitted[22], furthermore, Nagaoka's approximation[12] has been proved to be very poor[14,20]. However, recently Müller-Hartmann[14] and Bloomfield et.al.[20] have provided a very careful analysis of the problem based on Nagaoka's decoupling scheme of the Green's function equations. These investigations have shown that the electron polarization consists of two parts, namely an oscillating part and a nonoscillating part, where the latter one has a short-range as well as a long-range contribution. The short-range part falls off beyond a coherence length ξ_D which is determined by a cut-off energy D reflecting the band structure /the conduction electron band width/. The coherence length introduced by Bloomfield et.al[20] is approximately $\xi_D \sim a \frac{\varepsilon_F}{D}$ which must be of the order of one atomic distance[23]. The long-range part has the asymptotic form $-r^{-3}S(S+1)\log^{-2}(r/\xi_{T_K})$, where r stands for the distance measured from the impurity and S denotes the value of the spin. The spatial dependence of the change in the e.d.s. for a single impurity has not been investigated until now. However, studying the zero bias tunneling anomalies Sólyom and Zawadowski[8] have calculated the e.d.s. in the vicinity of an impurity layer and found that its expansion in space must be characterized by the same coherence length as in the problem of a single impurity. They have pointed out that the cut-off energy, which gives the coherence length may be determined by the momentum dependence of the exchange coupling constant $J_{kk'}$, which is usually neglected. Since this dependence may be stronger than the energy dependence of the bulk e.d.s. the proposed coherence length ξ_Δ might be much longer than ξ_D. Actually, if the width of the energy region where $J_{kk'}$ changes essentially is denoted by Δ, $\xi_\Delta = \frac{v_F}{\Delta}$ and $\xi_\Delta \sim a \frac{\varepsilon_F}{\Delta}$; hence $\xi_\Delta >> \xi_D$ if $\Delta << D$.

The existence of a coherence length of the order of 5-50 Å may be regarded as confirmed by experiments made on different dilute alloy systems. First of all Golibersuch and Heeger[24] have concluded from the analysis of their NMR data to a conduction electron polarization of the range of 9 Å around the impurities. Recently, Edelstein[25] has studied superconducting dilute alloys by tunneling which show Kondo effect. Conduction electron states have been found inside the superconducting energy gap. This result may be explained by assuming that superconductivity is destroyed inside of the spatial extent of the spincompensated state. This size has been found to be 7 Å. Experiments on tunneling anomalies caused by an impurity layer in the vicinity of the junction surface made by Mezei[26] could be explained by coherence lengths of 15-50 Å. Preliminary neutron scattering measurements of the impurity form factor by Kroó and Mezei[27] yield a spatial extent of

polarization of the order 8 Å. Thus the available experimental results suggest a coherence length being about 5-50 Å, wich a very probably a consequence of the momentum dependence of $J_{kk'}$ - as it has been suggested by Sólyom and Zawadowski[9].

In this paper the e.d.s. will be calculated. We will suppose that the e.d.s. of the bulk host metal is constant at the Fermi energy and it will be denoted by ρ_o for one spin direction. Müller-Hartmann[28] has first pointed out that the spatial structure of the change in the e.d.s. is independent of the conduction-electron-paramagnetic-impurity scattering amplitude and only the amplitude of the effect is determined by this scattering amplitude. Hence, the momentum dependence of $J_{kk'}$ must be in the center of our investigations. It will be assumed that the exchange coupling constant $J_{kk'}$ is essential only if the momenta k and k' correspond to energies in the neighbourhood /characterized by the energy width Δ/ of the Fermi surface. The actual form of this momentum dependence is not known yet, and in the present calculation a Lorentzian shape has been supposed, which has made possible to carry out the calculations in an analytical form. It can be seen, that the final results are not very sensitive to the details of the momentum dependence. It may be mentioned that the momentum dependence of $J_{kk'}$ and the energy dependence of the bulk e.d.s. enter into our calculations in a similar manner and thus the final results will be the same /if only one of these dependences is assumed to be of importance/, the only difference being in the parameters Δ and D.

As it will be seen the e.d.s. at the impurity site depends very much on whether the conduction electron scattering is of s- or d-type, therefore, the calculations will be carried out generally for ℓ-type. In the real case the scattering is of d-type, but usually the simplest case: s-type scattering is developed in the literature.

In Sec.II. the mathematical model will be described. The subject of Sec.III. and the Appendix will be to determine the thermodynamical Green's functions involved in the problem and the oscillating as well as the nonoscillating part of the e.d.s. will be calculated. At low temperature the Abrikosov-Suhl resonance scattering amplitude for energies near the Fermi energy can be expressed by a single phase shift, therefore, in Sec.IV. all of the important results will be expressed by the phase shift. The conclusion concerning the Kondo effect will be presented in Sec.V. The alteration of our results caused by dropping the assumption of constant bulk e.d.s. ρ_o is estimated in Appendix II. In the following paper the change in the e.d.s. caused by an impurity layer is calculated with respect to the zero bias tunneling anomalies.

II. The mathematical model

Let us consider the basic assumptions of the Kondo model which is given by the Hamiltonian $H=H_o+H_1$ where

$$H_o = \sum_{\vec{k}} \varepsilon_{\vec{k}} a^{\dagger}_{\vec{k}\alpha} a_{\vec{k}\alpha} \qquad /2,1/$$

and

$$H_1 = - \sum_{\vec{k}\vec{k}'} \frac{J_{\vec{k}\vec{k}'}}{N} a^{\dagger}_{\vec{k}\alpha} \vec{\sigma}_{\alpha\beta} a_{\vec{k}\beta} \vec{S} \qquad /2,2/$$

where $\varepsilon_{\vec{k}}$ denotes the energy of the conduction electrons, $a^{\dagger}_{\vec{k}}$ creates a conduction electron with momentum $\vec{k}$, $J_{\vec{k}\vec{k}'}/N$ is the s-d coupling constant, $\vec{S}$ is the impurity spin operator and the greek indices stand for the electron spin variables. In the usual treatment $J_{\vec{k}\vec{k}'}$ is taken to be independent of its momentum indices. However, the purpose of the present work is to point out the importance of this dependence on the momenta in the formation of the spin compensated Kondo state. $J_{\vec{k}\vec{k}'}$ is taken to be

$$J_{\vec{k}\vec{k}'} = (2\ell+1) J_\ell P_\ell(\cos\theta_{\vec{k}\vec{k}'}) F(k) F(k') =$$

$$= 4\pi J_\ell F(k) F(k') \sum_{m=-\ell}^{\ell} (-)^m Y_{\ell -m}(\vec{k}) Y_{\ell m}(\vec{k}') \qquad /2,3/$$

where the angular momentum of the scattered states has the value ℓ, P_ℓ is the Legendre polynomial and $\theta_{\vec{k}\vec{k}'}$ denotes the angle between the momenta of the incoming and out going electrons, J_ℓ is the coupling constant. The dependence on the absolute values of the momenta k and k' is written as a product $F(k)F(k')$, where the cut-off function $F(k)$ will be given below. The suppositions made here are in agreement with the Anderson model[29] if the effective Kondo Hamiltonian given by (2,2) and (2,3) is derived by the application of the Schrieffer-Wolff[30] transformation. This transformation yields an actual expression for the function $F(k)$ which exhibits a maximum roughly at the Fermi momentum k_F. The result of the Schrieffer-Wolff transformation, however, can be regarded as rather informative because the effect of the terms neglected at its application have not been estimated until now, furthermore, the momemtum dependence of the s-d mixing amplitude V_{kd} is not known. Therefore, instead, we choose a very simple analytic expression for it given by two parameters Δ and ε_o as follows

$$F(k) = \frac{\Delta^2}{\Delta^2 + (\varepsilon_k - \varepsilon_o)^2} = \frac{\Delta^2}{\Delta^2 + \tilde{\varepsilon}_k^2} \qquad /2,4/$$

where

$$\tilde{\varepsilon}_k = \varepsilon_k - \varepsilon_o \qquad /2,5/$$

This choice has the advantage of being simple and shows a rough similarity to the results of the Schrieffer-Wolff transformation. This similarity occurs if we choose the values ε_o and Δ to be of the order of the Fermi energy and of the energy of the impurity d level, ε_d measured from the Fermi energy, respectively. However, $\frac{\varepsilon_d}{\varepsilon_F} \ll 1$, hence $\frac{\Delta}{\varepsilon_o} \ll 1$ will be assumed.

III. Density of states

The thermodynamical Green's function technique[31] will be applied. The one-particle free electron Green's function is

$$\mathcal{G}^{(o)}(\vec{x}-\vec{x}';i\omega_n) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{x}')} \mathcal{G}^{(o)}(\vec{k},i\omega_n)$$

and

$$\mathcal{G}^{(o)}(\vec{k};i\omega_n) = \frac{1}{i\omega_n - \xi_k} \qquad /3,1/$$

where $\omega_n = \pi(2n+1)\,T$ and $\xi_k = \varepsilon_k - \varepsilon_F$.

Considering the s-d interaction the one-particle Green's function may be expressed by the non-spinflip scattering amplitude $t_{\vec{k}\vec{k}'}(i\omega_n)$, which is, on the other hand, the self-energy contribution due to one impurity in the notation system used by Abrikosov[3]. The behaviour of the scattering ampliutde will be discussed in Sec.V. Making use of the definition of the double Fourier transform

$$\mathcal{G}(\vec{r},\vec{r}';i\omega) = \frac{1}{(2\pi)^3} \int d^3\vec{k}_1 d^3\vec{k}_2\, \mathcal{G}(\vec{k}_1,\vec{k}_2;i\omega_n)\, e^{i\left(\vec{k}_1\vec{r}-\vec{k}_2\vec{r}'\right)} \qquad /3,2/$$

we have

$$\mathcal{G}(\vec{k},\vec{k}';i\omega_n) = \mathcal{G}^{(o)}(\vec{k};i\omega_n)\delta(\vec{k}-\vec{k}') + \mathcal{G}^{(o)}(\vec{k},i\omega_n) t_{\vec{k}\vec{k}'}(i\omega_n)\, \mathcal{G}^{(o)}(\vec{k}';i\omega_n) \qquad /3,3/$$

The scattering amplitude $t_{\vec{k}\vec{k}'}(i\omega_n)$ can be written in the following form

$$t_{\vec{k}\vec{k}'}(i\omega_n) = 4\pi \sum_{m=-\ell}^{m} (-)^m Y_{\ell-m}(\vec{k}) Y_{\ell m}(\vec{k}') t_\ell(i\omega_n) F(k) F(k') \qquad /3,4/$$

which is a consequence of the structure of the Hamiltonian given by (2,2) and (2,3).

The e.d.s at the point $\vec{r}$, $\rho(\vec{r},\omega)$ can be calculated by the analytic continuation of the Green's function $\mathcal{G}(\vec{r},\vec{r};i\omega_n)$ as

$$\rho(\vec{r},\omega) = \frac{1}{\pi}\mathrm{Im}\left\{\mathcal{G}\ (\vec{r},\vec{r};\omega-i\varepsilon\ )\right\} \qquad /3,5/$$

Introducing a modification of the Green's function by the cut-off function $F(k)$ and the spherical harmonics $Y_{\ell m}$

$$\mathcal{G}^{\ell m}_{\text{cut-off}}(\vec{r}) = \frac{1}{(2\pi)^3}\int d^3\vec{k}\, e^{i\vec{k}\vec{r}}\,\mathcal{G}^{\ell m}_{\text{cut-off}}(\vec{k}) \qquad /3,6/$$

where

$$\mathcal{G}^{\ell m}_{\text{cut-off}}(\vec{k}) = \frac{1}{i\omega_n-\xi_k}\,F(k)\,Y_{\ell m}(\vec{k}) \qquad /3,7/$$

and taking into account (3,3-7) the e.d.s. in the point $\vec{r}$ can be written in the simple form

$$\rho(\vec{r},\omega) = \rho_o + 4\mathrm{Im}\left\{\sum_{m=-\ell}^{\ell}(-)^m\,\mathcal{G}^{\ell-m}_{\text{cut-off}}(\vec{r})\,t_\ell(\omega-i\varepsilon)\,\mathcal{G}^{\ell m}_{\text{cut-off}}(-\vec{r})\right\} . \qquad /3,8/$$

The modified Green's function can be calculated by integrating first with respect to the direction of the momentum $\vec{k}$ and making use of the following identity

$$\int d\Omega_{\vec{k}}\, e^{i\vec{k}\vec{r}}\,Y_{\ell m}(\vec{k}) = 4\pi i^\ell j_\ell(kr)\,Y_{\ell m}(\vec{r}) \qquad /3,9/$$

where j_ℓ is the spherical Bessel function of the second kind. In this way we get

$$\mathcal{G}^{\ell m}_{\text{cut-off}}(\vec{r},i\omega_n) = Y_{\ell m}(\vec{r})\,i^\ell\int\frac{dk}{(2\pi)^2}\,k^2 j_\ell(kr)\,\frac{1}{i\omega_n-\xi_k}\,F(k) =$$

$$= i^\ell Y_{\ell m}(\vec{r})\,\mathcal{G}^\ell(\vec{r},i\omega_n) \qquad /3,10/$$

where $\mathcal{G}^\ell$ is independent of the direction of r. The equation (3,8) can be further reduced taking into account the relations

$$Y_{\ell m}(-\vec{r}) = (-)^\ell Y_{\ell m}(\vec{r}) \qquad /3,11/$$

and

$$\sum_{m=-\ell}^{\ell}(-)^m Y_{\ell-m}(\vec{r})\,Y_{\ell m}(\vec{r}) = \frac{2\ell+1}{4\pi} \qquad /3,12/$$

and (3,10).

Thus we obtain

$$\rho(\vec{r},\omega) = \rho_o + \frac{2\ell+1}{\pi} \mathrm{Im}\left\{ t_\ell(\omega-i\varepsilon)\, \mathcal{Y}^{\ell}(\vec{r},\omega-i\varepsilon)^2 \right\} . \qquad /3,13/$$

It is worth mentioning that the change in the electron density of states due to the impurity as a function of the energy ω and of the distance r /measured from the impurity/ can be factorized as it has been first pointed out by Müller-Hartmann[28]. To determine the spatial dependence we calculate the modified Green's function $\mathcal{Y}^{\ell}(\vec{r},\omega\pm i\varepsilon)$ introduced by (3,10) in the Appendix.I. Similarly to (2,5) a new notation for the real part of the energy variable will be used

$$\tilde{\omega} = \omega - (\varepsilon_o - \varepsilon_F) \qquad /3,14/$$

Inserting the result (A,9) derived in the Appendix into the expression (3,13) of $\rho(\vec{r},\varepsilon)$ we obtain

$$\rho(\vec{r},\omega) = \rho_o + (2\ell+1)\pi\rho_o^2 \ \mathrm{Im}\Big\{ t_\ell(\omega-i\delta)$$

$$\left[\mathrm{Re}\left(h_\ell^{(2)}\left((k_o+iv^{-1}\Delta)r\right)\right) \frac{\Delta}{\tilde{\omega}-i\Delta} + ih_\ell^{(1)}\left((k_o+v^{-1}\tilde{\omega})r\right) \frac{\Delta^2}{\Delta^2+\tilde{\omega}^2} + p_\ell(r,\tilde{\omega}) \right]^2 \Big\} \qquad /3,15/$$

where $h_\ell^{(1)}$ and $h_\ell^{(2)}$ are spherical Bessel functions of third kind and the function $p_\ell(r,\tilde{\omega})$ is a small correction given by (A,10) and (A,11), furthermore v is determined by (A,3).

The arguments of the Bessel functions contain three different characteristic dimensionless quantities, which are proportional to the distance r:

1, $k_o r$, which is of the order of unity if r is of a few atomic distances,

2, $(v^{-1}\Delta)r$, which may be rewritten as r/ξ_Δ introducing a characteristic coherence length

$$\xi_\Delta = \frac{v}{\Delta} \qquad /3,16/$$

determined by the momentum dependence of the exchange coupling constant; hence $(v^{-1}\Delta)r \sim 1$, if $r \sim \xi_\Delta$,

3, $(v^{-1}\tilde{\omega})r$, which can be expressed as $r/\xi_{\tilde{\omega}}$, where the energy coherence length is

$$\xi_{\tilde{\omega}} = \frac{v}{\tilde{\omega}} \qquad /3,17/$$

and $(v^{-1}\tilde{\omega})r \sim 1$ if $r \sim \xi_{\tilde{\omega}}$.

To understand the physics contained in the result (3,15) we are going to discuss the short-range as well as the long-range limits where the formula can be written into simpler forms. The change in e.d.s. consists of two parts, a nonoscillating and an oscillating one.

For making easier the detailed discussion of the result (3,15) we give it for the special case $\ell=0$

$$\rho(r;\omega) = \rho_o + \pi\rho_o^2 \mathrm{Im}\left\{ t_o(\tilde{\omega}-i\delta) \left[\mathrm{Re}\left(\left(\frac{\sin\left(k_o+i\frac{1}{\xi_\Delta}\right)r}{\left(k_o+i\frac{1}{\xi_\Delta}\right)r} - i\,\frac{\cos\left(k_o+i\frac{1}{\xi_\Delta}\right)r}{\left(k_o+i\frac{1}{\xi_\Delta}\right)r} \right) \frac{\Delta}{\tilde{\omega}-i\Delta} \right) \right.\right. \qquad /3,18/$$

$$\left.\left. + i\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2} \left(\frac{\sin\left(k_o+\frac{1}{\xi_{\tilde{\omega}}}\right)r}{\left(k_o+\frac{1}{\xi_{\tilde{\omega}}}\right)r} + i\,\frac{\cos\left(k_o+\frac{1}{\xi_{\tilde{\omega}}}\right)r}{\left(k_o+\frac{1}{\xi_{\tilde{\omega}}}\right)r} \right) + p_o\left(r,\tilde{\omega}\right) \right]^2 \right\}$$

where the coherence lengths given by (3,16) and (3,17) have been introduced.

a, short-range limit: $r \ll \xi_\Delta$ and $r \ll \xi_{\tilde{\omega}}$ for $\tilde{\omega} \ll \Delta$.

The special expression for $\ell=0$ shows that the terms containing the coherence lengths can be neglected in this limit. The validity of this approximation, however, is not restricted to the special case $\ell=0$. Neglecting the corresponding terms in (3,15) and replacing the Bessel functions of the third kind by the ones of the second kind, see (A,4), the following expression is obtained

$$\rho(r,\omega) = \rho_o + (2\ell+1)\pi\rho_o^2 \cdot$$

$$\mathrm{Im}\left\{ t_\ell(\omega-i\delta) \left[\mathrm{Re}\left(j_\ell(k_o r)\,\frac{\Delta}{\tilde{\omega}-i\Delta} \right) + \mathrm{Im}\left(n_\ell(k_o r)\,\frac{\Delta}{\tilde{\omega}-i\Delta} \right) \right.\right.$$

$$\left.\left. + i\left(j_\ell(k_o r) + i n_\ell(k_o r)\right)\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2} + p_\ell\left(r,\tilde{\omega}\right) \right]^2 \right\} \qquad /3,19/$$

For $\tilde{\omega}<<\Delta$ has been assumed, this formula can be further simplified by inserting $\tilde{\omega}=0$ into the contributions of the modified Green's functions with the result

$$\rho(r,\omega) = \rho_o - (2\ell+1)\pi\rho_o^2 \mathrm{Im}\left\{t_\ell(\omega-i\delta)\right\} j_\ell^2(k_o r) \quad . \qquad /3,20/$$

In (3,19) $p_\ell(r,\tilde{\omega})$ represents a negligible correction for $k_o r \gtrsim 1$.

a/1, density of states at the impurity site.

The e.d.s. at the impurity site can be derived using (3,20) and the expansion of the Bessel function $j_\ell(z)$ into power series

$$j_\ell(z) \sim \frac{z^\ell}{(2\ell+1)!!}\left[1 - \frac{z^2}{2(2\ell+3)} + \ldots.\right] \quad \text{for } z\to 0. \qquad /3,21/$$

Two cases have to be distinguished: $\ell=0$ and $\ell\neq 0$.
We get

$$\rho(o,\omega) = \rho_o - \pi\rho_o^2 \mathrm{Im}\left\{t_\ell(\tilde{\omega}-i\delta)\right\} \qquad \text{for } \ell=0 \qquad /3,22/$$

and

$$\rho(o,\omega) = \rho_o \qquad \text{for } \ell\neq 0 \qquad /3,23/$$

The density of states at the point r=0 changes due to the perturbation only in the case $\ell=0$, because in the other cases the incoming and outgoing scattering wave functions vanish at this point. In the derivation of the results given by (3,22) and (3,23) the assumption $\tilde{\omega}<<\Delta$ has not been used.

It is worth mentioning that $p_o(r,\tilde{\omega})$ and the n_ℓ Bessel functions appearing in (3,19) diverges as r tends to zero. These terms have been neglected in (3,20), because their coefficients are very small. Nevertheless, the result given by (3,22) and (3,23) remains valid, because these spurious divergent terms cancel each other.

a/2, density of states for $\ell(\ell+1)/k_o << r << \xi_\Delta$.

In the range $z >> \ell(\ell+1)$ the Bessel function $j_\ell(z)$ can be replaced in (3,20) by its asymptotic form given by (A,5). The result consists of two parts an oscillating and nonoscillating one as follows

$$\rho(r,\omega) = \rho_o + \Delta\rho_{o.}(r,\omega) + \Delta\rho_{n.o.}(r,\omega) \qquad /3,24/$$

where

$$\Delta\rho_{o.}(r,\omega) = \frac{2\ell+1}{2}\,\pi\rho_o^2\,\frac{1}{(k_o r)^2}\cos 2\left(k_o r-\tfrac{1}{2}\ell\pi\right)\mathrm{Im}\left\{t_\ell(\omega-i\delta)\right\} \qquad /3,25/$$

and

$$\Delta\rho_{n.o.}(r,\omega) = -\frac{2\ell+1}{2}\,\pi\rho_o^2\,\frac{1}{(k_o r)^2}\,\mathrm{Im}\left\{t_\ell(\omega-i\delta)\right\} \quad . \qquad /3,26/$$

b/ medium-range: $\ell(\ell+1)/k_o << r \sim \xi_\Delta$.

Making use of the asymptotic form (A,5) of the Bessel functions the formula of the e.d.s. (3,15) can be written in the form

$$\rho(r,\omega) = \rho_o + (2\ell+1)\pi\rho_o^2\,\frac{1}{(k_o r)^2}\left(\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2}\right)^2$$
$$\mathrm{Im}\left\{\left[e^{-\frac{r}{\xi_\Delta}}\left(1-i\frac{\tilde{\omega}}{\Delta}\right)\tfrac{1}{2}e^{i\left(k_o r-\frac{1}{2}\ell\pi\right)}+\left(1+i\frac{\tilde{\omega}}{\Delta}\right)\tfrac{1}{2}e^{-i\,k_o r-\frac{1}{2}\ell\pi}\right.\right.$$
$$\left.\left.-e^{-i\left(k_o r-\frac{1}{2}\ell\pi+\frac{r}{\xi_{\tilde{\omega}}}\right)}\right]^2 t_\ell(\omega-i\delta)\right\} \qquad /3,27/$$

where $p_\ell(r,\tilde{\omega})$ has been neglected.

The nonoscillating part arises from those terms of the square in (3,27) in which the two different oscillating exponential functions $\exp\{\pm ik_o r\}$ cancel each other. We obtain

$$\Delta\rho_{n.o.}(r,\omega) = -(2\ell+1)\pi\rho_o^2\,\frac{1}{(k_o r)^2}\left(\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2}\right)^2 \qquad /3,28/$$
$$\left\{e^{-\frac{r}{\xi_\Delta}}\mathrm{Im}\left[\left(1-i\frac{\tilde{\omega}}{\Delta}\right)e^{-i\frac{r}{\xi_{\tilde{\omega}}}}t_\ell(\omega-i\delta)\right]-\right.$$
$$\left.-\tfrac{1}{2}\,e^{-2\cdot\frac{r}{\xi_\Delta}}\left(\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2}\right)^{-1}\mathrm{Im}\left[t_\ell(\omega-i\delta)\right]\right\}.$$

c/ long-range limit:

It is important to notice that the nonoscillating part of the change in the e.d.s. falls off very rapidly beyond the coherence length ξ_Δ . The oscillating part consists of many terms. It contains a long-range term which is the only existing one outside of the coherence length ξ_Δ . For $r >> \xi_\Delta$ it is the following

$$\Delta\rho_{o.}(r,\omega) =$$
$$= (2\ell+1)\pi\rho_o^2\,\frac{1}{(k_o r)^2}\left(\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2}\right)^2\mathrm{Im}\left\{t_\ell(\omega-i\delta)e^{-2i\left(k_o r-\frac{1}{2}\ell\pi+\frac{r}{\xi_{\tilde{\omega}}}\right)}\right\}. \qquad /3,29/$$

This term corresponds to the Friedel oscillation as it will be seen in the next Sec.IV.

IV. Density of states given by the phase shift $\delta_\ell(\omega)$

In special physical problems the scattering amplitude can be expressed by phase shifts. If there is only one scattering channel, the scattering amplitude can be written in the following form

$$t_\ell(\omega \pm i\varepsilon) = \mp \frac{1}{2\pi i \rho_o}\left(e^{\pm 2i\delta_\ell(\omega)} - 1\right) = -\frac{1}{\pi\rho_o} e^{\pm i\delta_\ell(\omega)} \sin\delta_\ell(\omega) \quad /4,1/$$

where $\delta_\ell(\omega)$ denotes the phase shift of the predominating ℓ-type scattering.

Some of our previous results can be expressed by the phase shift in a very simple way.

The e.d.s. at the impurity site for $\ell=0$ given by (3,22) is

$$\rho(o,\omega) = \rho_o \cos^2\delta_o(\omega). \quad /4,2/$$

For the nonoscillating part of the e.d.s. given by (3,26) and (3,28) for $r \gg \ell(\ell+1)/k_o$ and $\tilde{\omega} \ll \Delta$ we get

$$\Delta\rho_{n.o.}(r,\omega) =$$

$$= -(2\ell+1)\rho_o \frac{1}{(k_o r)^2} e^{-\frac{r}{\xi_\Delta}} \left\{\sin\left(\delta_\ell(\omega) + \frac{r}{\xi_{\tilde{\omega}}}\right) - \frac{1}{2} e^{-\frac{r}{\xi_\Delta}} \sin\delta_\ell(\omega)\right\} \sin\delta_\ell(\omega) \quad /4,3/$$

The oscillating part is of interest in two limits. Making use of (3,21) the short-range limit $\ell(\ell+1)/k_o \ll r \ll \xi_\Delta$ and $\tilde{\omega} \ll \Delta$ is obtained.

$$\Delta\rho_o(r,\omega) = \frac{2\ell+1}{2}\rho_o \frac{1}{(k_o r)^2} \sin 2\left(k_o r - \frac{1}{2}\ell\pi + \frac{\pi}{4}\right) \sin^2\delta_\ell(\omega) \quad /4,4/$$

and in the long-range limit $(r \gg \xi_\Delta)$ considering (3,29) we get

$$\Delta\rho_o(r,\omega) \approx (2\ell+1)\rho_o \frac{1}{(k_o r)^2} \sin\delta_\ell(\omega) \cdot$$

$$\sin 2\left(k_o r - \frac{1}{2}\ell\pi + \frac{1}{2}\delta_\ell(\omega) + \frac{r}{\xi_{\tilde{\omega}}}\right) \quad /4,5/$$

It is worth mentioning that there appear different phases in the variable of the sines in expressions (4,4) and (4,5). The phase in (4,5) will be shown to be in good agreement with the phase of the Friedel oscillation. In the short-range limit the phase does not depend on the phase shift δ_ℓ, but it contains an additional $\pi/4$.

The charge oscillation around the impurity can be obtained by integrating (4,4) and (4,5) with respect to the energy up to the Fermi energy, ε_F . We obtain

$$\Delta\rho_{charge}(r) = -e\int d\omega \Delta\rho_o(r,\omega) \sim$$

$$\sim -e\Delta \frac{1}{(k_o r)^2}\rho_o \cos 2\left(k_o r - \frac{1}{2}\ell\pi\right)\sin^2\delta_\ell(\omega) \qquad /4,6/$$

for $\ell(\ell+1)/K_o << r << \xi_\Delta$ and

$$\Delta\rho_{charge}(r) \approx \frac{1}{2}e(2\ell+1)\rho_o v k_F \frac{1}{(k_F r)^3} \sin\delta_\ell \cos 2\left(k_o r - \frac{1}{2}\ell\pi + \frac{\delta_\ell}{2}\right)$$

/4,7/

for $r >> \xi_\Delta$, where $\varepsilon_o = \varepsilon_F$ and $k_o = k_F$ has been inserted, furthermore, the contribution to the integrals arising from the lower limit can not be given in general as it depends on the band structure or the cut-off . The phase is assumed to be independent of the energy, e denotes the electron charge. In the long-range limit the second expression, (4,7), yields the wellknown expression for the Friedel oscillation[1].

V. Conclusions

For an aribtrary conduction-electron-impurity scattering a formalism has been developed to determine the conduction electron density of states around a single impurity. It has been assumed that the scattering amplitude depends on the momenta of the incoming and outgoing electrons and the important contribution arises from the momentum region centered at k_o and with a width corresponding to an energy Δ . If such momentum dependence does not occur, Δ has to be replaced by the conduction electron band width D. The formalism can be applied to resonance scattering as well as to potential scattering of special form.

The change in the e.d.s. has different features in the short-range and long-range limits which are separated at a distance corresponding to the coherence length ξ_Δ . In the short-range region the change in the e.d.s. is always negative definite as it can be seen from (3,20) and in Fig. 1. The amplitude of this depression part takes its maximum value at the impurity site or at about one atomic distance depending on wether the scattering is of s-type or not. With increasing distance the change of the e.d.s. has a nonoscillating part eq. (3.28) illustrated in Fig. 2., which spreads over a distance determined by the coherence length ξ_Δ while in the long-

-range region only the oscillating terms survive,which correspond to the Friedel oscillation. The total change of the e.d.s. in the short range region is inversly proportional to the square of the distance r^{-2}, which dependence assures at small distances the convergence of the total e.d.s. inside a sphere. In the long-range limit it shows an r^{-3} dependence, in which case the total change of the e.d.s. corresponding to a sphere of radius R falls off like R^{-1}.

The different behaviour of the e.d.s. at the impurity site makes it possible to distinguish between scattering of s-type and of type of higher order by NMR experiments looking for the Knight shift and Korringa relaxation on the impurity nucleus. In the latter case these quantities are unchanged. However, in the case of s-type scattering we may expect drastic effects, namely, if the scattering can be described by a single phase shift, in the case of a resonance $\delta = \pi/2$ the e.d.s. given by (4,2) and represented in Fig. 1. becomes zero and therefore the Knight shift and Korringa relaxation caused by the direct conduction-electron-nuclear interaction must disappear. In the case of paramagnetic impurities interacting with the conduction electrons via s-d interaction the scattered waves are of d-type, therefore, no effect can be expected by NMR on the impurity nucleus.

If a coherence length is observed it might be posssible to distinguish whether it is due to some unusual form of the conduction electron band $D \ll \varepsilon_F$ or it is due to the momentum dependence of the conduction--electron-impurity scattering. In the first case it must depend only on the host metal, nevertheless, in the second case the coherence length must vary for different impurities.

Throughout the presented calculation a constant bulk e.d.s. and a special form of the cut-off function given by (2,4) is supposed. By dropping this assumption the results change only slightly[36] if the cut-off energy is smaller than the band width D as it is shown in Appendix II., where the results (3,22) and (4,2) for the impurity site are recalculated.

One may ask, how it is possible that the e.d.s. is always depressed at the impurity site while e.g., in the case of a simple attractive potential it does not happen. In this paper we have supposed a special momentum dependence which involves the vanishing of the potential at the impurity site. Therefore, our results do not hold for a simple attractive potential.

The most striking application of our results is to the Kondo effect. In this case the scattering amplitude shows a resonance at the Fermi energy and we may expect a momentum dependent scattering as well. The energy dependence of the scattering amplitude has been investigated extensively in the last few years, but the problem has not been solved yet. There are good solutions of the scattering problem worked out by Suhl and Wong[4], Hamann and Bloomfield[32], Brenig and Götze[33] etc. if only the one particle intermediate states are considered in the scattering process. However, recently it has been pointed out by Nozieres[34] from the low temperature side and by Fazekas and Zawadowski[35] from the high temperature side that the many particle intermediate states can play an important role, too.

The one particle scattering amplitude can be written as

$$\left(\alpha\sigma|T|\beta\sigma'\right) = t(\omega)\delta_{\alpha\beta}\delta_{\sigma\sigma'}+\tau(\omega)\vec{S}_{\alpha\beta}\vec{\sigma}_{\sigma\sigma'}, \qquad /5,1/$$

where $t(\omega)$ indicates the nonspinflip part of the scattering amplitude while $\tau(\omega)$ stands for its spin dependent part, furthermore, α, β and σ,σ' denote the spin indices of the initial and final impurity spin and conduction electron states respectively.

It is worth mentioning that it is common in the above mentioned solutions of the scattering problem that well below the Kondo temperature and at the Fermi energy $(\omega=0)$ $\tau(\omega)$ becomes zero and only the spin-conserving scattering channel is open. In this case the scattering can be described by a single phase shift $\delta = \pi/2$ and our result derived in Sec.IV. can be applied. The amplitude of the depression of the e.d.s. takes on its maximal value. If the energy variable ω moves off the Fermi energy or if the temperature is raised above the Kondo temperature, the amplitude of the investigated effect is gradually reduced in both cases as the scattering amplitude decreases.

As it is well known, below the Kondo temperature a magnetically polarized electron cloud is formed around the impurity spin. We have shown that the formation of the magnetic electron cloud is associated with depression of the e.d.s. inside the coherence length ξ_Δ. There is an essential difference between the change in the e.d.s. and the magnetic polarization considering their long-range parts. The first quantity does not contain any non-oscillating negative definite part while the magnetic polarization does, which is proportional to $\frac{1}{r}3.\log^{-2}\left(\frac{r}{\xi T_K}\right)$

The purpose of the following paper[37] is to extend our results to the case of an impurity layer where the effect becomes more pronounced and this makes possible the observation by tunneling experiments.

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Appendix I.

Introducing the notations given by (2,4), (2,5) and (3.14) in the definition (3,10) of the modified Green's function we get the quantity to be calculated

$$\mathcal{J}^{\ell}(r,\omega\pm i\delta) = \rho_o \int d\tilde{\varepsilon}\, j_\ell\left(\left(k_o+v^{-1}\tilde{\varepsilon}\right)r\right) \frac{1}{\omega-\tilde{\varepsilon}\pm i\delta} \cdot \frac{\Delta^2}{\Delta^2+\tilde{\varepsilon}^2} \qquad /A,1/$$

where the integral in the momentum space is replaced by another one with respect to the energy variable

$$\frac{1}{2\pi^2}\int dk.k^2 \rightarrow \rho_o \int d\tilde{\varepsilon} \qquad /A,2/$$

which identity is correct in the case of constant free e.d.s. The latter assumption is reasonable because in the integral the cut-off function $F(k)$, given by (2,4), makes the energy regions far from the Fermi energy i.e. $\frac{|\tilde{\varepsilon}|}{\Delta} > 1$ ineffective. Furthermore, in (A,1) the momentum in the neighbourhood of the Fermi energy is taken as a linear function of the energy, i.e.

$$k = k_o + v^{-1}\tilde{\varepsilon} \qquad /A,3/$$

where v is the velocity of the electrons at the energy ε_o and k_o is the value of the momentum at $\tilde{\varepsilon} = 0$.

The integration over the energy $\tilde{\varepsilon}$ can be performed by the contour integration method, however, particular attention must be paid to the asymptotic behaviour of the Bessel functions. Instead of the Bessel function of the second kind $j_\ell(z)$ and $n_\ell(z)$ it is convenient to deal with the Bessel functions of the third kind

$$h_\ell^{(1)}(z) = j_\ell(z)+in_\ell(z) \quad \text{and} \quad h_\ell^{(2)}(z) = j_\ell(z)-in_\ell(z) \qquad /A,4/$$

which show proper analytic behaviour in the asymptotic region, namely

$$h_\ell^{(1)}(z) \rightarrow i\,\frac{1}{z}e^{-i\left(z-\frac{1}{2}\ell\pi\right)} \quad \text{and} \quad h_\ell^{(2)}(z) \rightarrow -i\frac{1}{z}e^{+i\left(z-\frac{1}{2}\ell\pi\right)} \qquad /A,5/$$

for $z \gg \ell(\ell+1)$. The disadvantage of the use of these functions is that they have a pole at $z=0$, as

$$n_\ell(z) \sim \frac{(2\ell+1)!!}{2\ell+1}\left(\frac{1}{z}\right)^{\ell+1}\left[1+\frac{z^2}{2(2\ell-1)}+..\right] \text{ if } z \rightarrow 0 \qquad /A,6/$$

Disregarding the point $z=0$ the functions $h_\ell^{(1)}(z)$ and $h_\ell^{(2)}(z)$ are analytic on the upper and lower half plane, respectively, and

$$h_\ell^{(1)}(z^*) = \left(h_\ell^{(2)}(z)\right)^* \qquad /A,7/$$

holds.

Making use of (A,4) the modified Green's function can be written as a sum

$$\mathcal{G}^{\ell}(r,\omega\pm i\delta) = \mathcal{G}^{\ell(1)}(r,\omega\pm i\delta) + \mathcal{G}^{\ell(2)}(r,\omega\pm i\delta)$$

where

$$\mathcal{G}^{\ell(n)}(r,\omega\pm i\delta) = \frac{1}{2}\rho_o \int d\tilde{\varepsilon} h_\ell^{(n)}\left(\left(k_o+v^{-1}\tilde{\varepsilon}\right)r\right) \frac{1}{\tilde{\omega}-\tilde{\varepsilon}\pm i\delta} \frac{2}{\Delta^2+\tilde{\varepsilon}^2} \qquad /A,8/$$

$$/n=1,2/$$

and the integrals can be performed by the method of contour integration on the upper and lower half plane, respectively. The important contributions arise from the zeros of the denominators which are near the Fermi energy. The poles of the Bessel functions are very far from the Fermi energy and therefore they yield only a small correction which will be given by the function $p_\ell(r,\omega)$.

The staight forward calculation gives

$$\mathcal{G}^{\ell}(r,\omega-i\delta) = \rho_o\pi\left\{\mathrm{Re}\left[h_\ell^{(2)}\left(\left(k_o+iv^{-1}\Delta\right)r\right)\right] + \right.$$
$$\left. + ih_\ell^{(1)}\left(\left(k_o+v^{-1}\tilde{\omega}\right)r\right)\frac{\Delta^2}{\Delta^2+\tilde{\omega}^2} + p_\ell(r,\omega)\right\} \qquad /A,9/$$

where (A,7) has been taken into account. Furthermore, the contributions of the poles of the Bessel functions for $\ell=0$ and 2 are the following

$$p_0(r,\omega) = \frac{v}{r}\frac{\Delta^2}{\Delta^2+(k_o v)^2}\frac{1}{\omega+vk_o-i\delta} \qquad /A,10/$$

and

$$p_2(r,\omega) = -\frac{1}{4}\frac{v}{r}\frac{\Delta^2}{\Delta^2+(k_o v)^2}\frac{1}{\omega+vk_o-i\delta} -$$
$$-3\left(\frac{v}{r}\right)^2\left[\frac{1}{(\omega+vk_o-i\delta)^3}\frac{\Delta^2}{\Delta^2+(k_o v)^2} + \right.$$
$$+\frac{1}{(\omega+vk_o-i\delta)^2}\frac{2\Delta^2 vk_o}{\left(\Delta^2+(k_o v)^2\right)^2} +$$
$$\left. + \frac{1}{\omega vk_o-i\delta}\left(-\frac{\Delta^2}{\left(\Delta^2+(k_o v)^2\right)^2} + \frac{4v^2k_o^2\Delta^2}{\left(\Delta^2+(k_o v)^2\right)^3}\right)\right]$$

Appendix II.

It will be demonstrated how the results derived in this paper alter if the cut-off energy Δ is not much smaller than the band width D. The result given by (3,22) will be reinvestigated for s-type scattering at the impurity site.

The derivation of (3,22) is based on the expression (3,13) where the bulk e.d.s. occurs in the Green's function $\mathcal{G}$, too. Inserting the value $r=0$ and an energy dependent bulk e.d.s. $\rho_o(\omega)$ into (3,13); furthermore, assuming that $t(\omega)$ is pure imaginary we obtain

$$\rho(0,\omega) = \rho_o(\omega) + \frac{1}{\pi} \operatorname{Im} t(\omega-i\varepsilon)\left\{\left[\operatorname{Re}\mathcal{G}(0,\omega-i\varepsilon)\right]^2 - \left[\operatorname{Im}\mathcal{G}(0,\omega-i\varepsilon)\right]^2\right\} . \qquad /A,12/$$

Instead of making use of the cut-off procedure given by (2,4) we introduce sharp lower and upper cut-off energies E_ℓ and E_u, resp. In this way, the Green's function is

$$\mathcal{G}(0,\omega-i\varepsilon) = \int_{E_\ell}^{E_u} \frac{1}{\omega-\xi_p-i\varepsilon} \frac{d^3\vec{p}}{(2\pi)^3} \qquad /A,13/$$

where $\xi_p = \frac{p^2}{2m} - \mu$. It can be easily calculated and the result is

$$\operatorname{Re}\mathcal{G}(0,\omega-i\varepsilon) = 2\rho_o(\omega)\left\{-\frac{\sqrt{E_u}-\sqrt{E_\ell}}{\sqrt{\omega+u}} + \frac{1}{2}\left[\ln\left|\frac{\sqrt{\omega+\mu}+\sqrt{E_u}}{-\sqrt{\omega+\mu}+\sqrt{E_u}}\right| - \ln\left|\frac{\sqrt{\omega+\mu}+\sqrt{E_\ell}}{\sqrt{\omega+\mu}-\sqrt{E_\ell}}\right|\right]\right\}$$

and /A,14/

$$\operatorname{Im}\mathcal{G}(0,\omega-i\varepsilon) = \pi\rho_o(\omega) . \qquad /A,15/$$

In the previous result (3,22) the real part of $\mathcal{G}$ does not occur, because it vanishes in the special model investigated in the present paper. In this case the modification of the e.d.s. for $\omega = 0$ can be characterized by

$$\left(\frac{\operatorname{Re}\mathcal{G}}{\operatorname{Im}\mathcal{G}}\right)^2 = \frac{4}{\pi^2}\left\{\sqrt{\frac{E_\ell}{\mu}} - \sqrt{\frac{E_u}{\mu}} + \frac{1}{2}\left(\ln\frac{\sqrt{\frac{E_u}{\mu}}+1}{\sqrt{\frac{E_u}{\mu}}-1} - \ln\frac{\sqrt{\frac{E_\ell}{\mu}}+1}{-\sqrt{\frac{E_\ell}{\mu}}+1}\right)\right\}^2 \qquad /A,16/$$

where (A,14) and (A,15) have been considered. At present the e.d.s. does not vanish at the impurity site, for phase shift $\delta = \frac{\pi}{2}$; furthermore, the ratio of its remaining part to the bulk e.d.s. is given by (A,16) as it can be seen from (A,12). This ratio can be small, but not negligible for a wide region of cut-off energies. For the sake of simplicity one can use the values given by one parameter λ , $E_u = \lambda\mu$ and $E_\ell = \frac{1}{\lambda}\mu$,resp; then the ratio is

$$\frac{\rho(0,0)}{\rho_o(0)} = \frac{4}{\pi^2}\sqrt{\lambda}\left(1 - \frac{1}{\lambda}\right) . \qquad /A,17/$$

One can see that without a small cut-off (e.g. $\lambda=2$) the result changes by 30%, however, with smaller values as $\lambda = 1{,}25$ and $\lambda = 1{,}1$ only by 10% and 5%, respectively.

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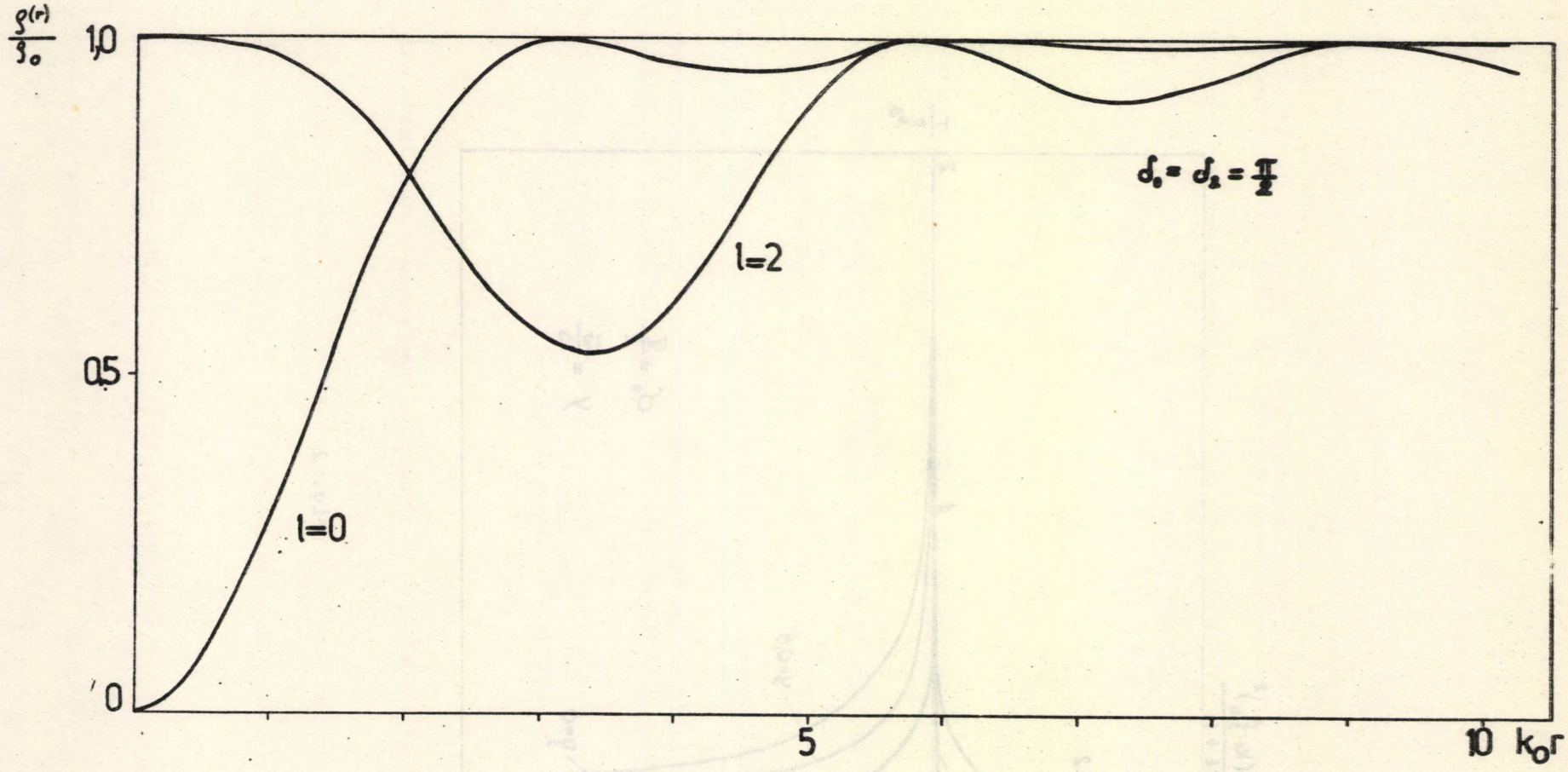

Fig. 1

61.820

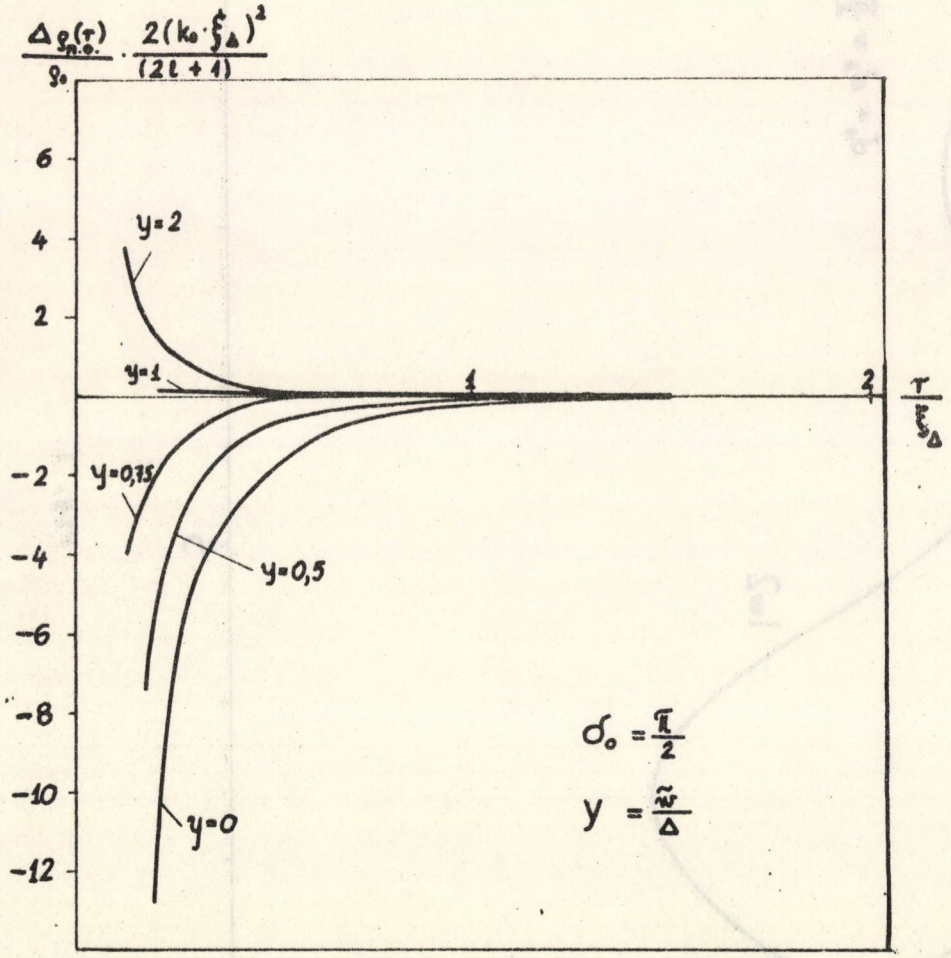
$\frac{\Delta\varrho(r)}{\varrho_0} \cdot \frac{2(k_0 \cdot \xi_\Delta)^2}{(2l+1)}$
6
4
2
-2
-4
-6
-8
-10
-12
y=2
y=1
y=0,75
y=0,5
y=0
1
2
$\frac{r}{\xi_\Delta}$
$\sigma_0 = \frac{\pi}{2}$
$y = \frac{\tilde{w}}{\Delta}$

Fig. 2