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# Electron Densities at Charged Impurities in Metals

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(29. I. 75)

*Abstract.* The enhancement of conduction electron density around charged impurities in metals is discussed in terms of scattering theory. A simple model for the effective potential is proposed which leads to an analytic form of the Jost function. The explicit expression for the enhancement factor allows the calculation of the electron density at positive muons and positrons by a simple integration. The results are in good agreement with recent elaborate numerical calculations as well as with the measured annihilation rates of positrons. The values obtained for the Knight shift of positive muons are of the correct order of magnitude.

## 1. Introduction

A thorough study of the electron distribution around point charges in metals has been presented by Sjölander and Stott [1]. They generalized the treatment of screening effects in an electron gas by Singwi et al. [2] to a two-component plasma and obtained an integral equation for the impurity-electron pair-correlation function. In an alternative approach, also elaborated in [1], the non-linear Hartree equations have been solved in a self-consistent manner. The equations have been evaluated numerically for positively and negatively charged fixed impurities as well as for impurity mass equal to the electron mass. In the latter case the results can be compared with the measured annihilation rate of positrons in metals. Good agreement with the experiments was obtained for metals with high conduction electron densities. For lower densities the calculations yielded an unreasonable increase of density enhancement. This breakdown of the method was ascribed to strong electron localization in a situation in which the system is close to a bound state. The same difficulties also showed up in the screening of a proton.

Our motivation to study the problem of density enhancement at impurities in metals is provided by the possible applications of positive muons in solid-state physics (we shall discuss further some aspects of this new field in Section 5). The positive muon with a mass of about 200 electron masses behaves in a metal like a light proton. We thus expect for muons the same screening properties as for protons.

Since the calculations of Sjölander and Stott indicate that bound states may occur we adopted the formalism of Kohn and Sham [3] to discuss the screening problem. In this scheme the theory of potential scattering can be applied directly. The key quantity is then the Jost function [4] from a knowledge of which we can deduce the enhancement factor as well as the bound states.

Self-consistent calculations of the effective potential,  $V_{\text{eff}}$ , in the Kohn-Sham formalism convinced us that the form of  $V_{\text{eff}}$  close to the impurity is very insensitive

to the details of the electron distribution so long as the condition of screening the total charge is fulfilled. Thus we approximated  $V_{\text{eff}}$  by a Hulthén potential where the screening parameter is determined by the Friedel sum rule [5]. This is of course quite similar to the usual approach to the screening problem by choosing a Yukawa potential, which gives phase shifts obeying the Friedel sum rule. In our case, however, we obtain an analytic expression for the Jost function. In addition, the electron density is not calculated from the Poisson equation but by summing the lowest lying states up to the Fermi energy.

Our model gives results which are in good agreement with the calculations of Sjölander and Stott [1] as well as with the recent result of Popovic and Stott [6] for the screening of a proton in an electron gas with a density corresponding to Al. Within our model the impurity will bind an electron for low densities of the electron gas. It is argued that this is due to the description of the conduction electrons by a homogeneous electron gas (jellium model). The presence of ions will prevent the occurrence of bound states in most cases since the low binding energy implies a Bohr radius larger than ionic spacing. An investigation of bound states of impurities, which is relevant for a real metal, cannot be made unless the band structure is taken into account. This is outside the scope of the present work but presents an interesting future problem, especially with regard to a direct experimental test using positive muons. The formation of muonium is easily verified by the typical quenching of polarization in longitudinal magnetic fields [7].

To introduce the necessary notation we give in the following section a brief account of the results of linear response theory. An interpolation formula for the dielectric function gives an analytic expression for the induced electron density which is valid close to the impurity. In Section 3 the density-functional approach of Kohn and Sham [3] to treat the inhomogeneous electron gas is discussed. The model potential mentioned above is then presented in the fourth section. In subsequent sections our results for positive muons, positrons and negatively charged impurities are compared with the calculations of other authors and with the available measurements.

## 2. Linear Response Theory

In the framework of linear response theory the Coulomb potential  $-Ze^2/r$  of a static point charge implanted into an electron gas of density  $n_0$  is screened according to

$$\tilde{V}(k) = -Ze^2 \frac{4\pi}{k^2 \epsilon(k)}. \quad (1)$$

The perturbed electron density  $n(r)$  is then calculated from the Poisson equation to be

$$n(r) = n_0 + Z \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\epsilon(k) - 1}{\epsilon(k)}. \quad (2)$$

The static dielectric function  $\epsilon(k)$  can easily be calculated for a free electron gas with the result

$$\epsilon(k) = 1 + \frac{k_s^2}{k^2} \left[ \frac{1}{2} - \frac{k_F}{2k} \left( 1 - \frac{k^2}{4k_F^2} \right) \ln \left| \frac{2k_F - k}{2k_F + k} \right| \right], \quad (3)$$

where  $k_F = (3\pi^2 n_0)^{1/3}$  denotes the Fermi wave-number and

$$k_s^2 = \frac{4k_F}{\pi a_B}, \quad (4)$$

with  $a_B$  being the Bohr radius. Various corrections to the Lindhard expression (3) accounting for exchange and correlation effects have been discussed in the literature (see e.g. [2], and Refs. cited therein). Langer and Vosko [8] have evaluated numerically equation (2) for  $\varepsilon(k)$  given by (3) as well as for the Hubbard dielectric function [9]. The most significant result is the oscillatory behavior of the induced electron density at large distances. The origin of these Friedel oscillations is the abrupt change of the electron density at the sharp Fermi surface which shows up mathematically in a logarithmic divergence of the first derivative of  $\varepsilon(k)$  at  $k = 2k_F$ . For distances  $r$  greater than about  $1/k_F$  the deviation from the mean density is small compared to 1 and the use of linear response theory seems adequate in this region.

Close to the impurity, however, the electron gas is strongly perturbed. To see the behavior for small  $r$  we may approximate expression (3) by a rational function which correctly describes the limiting behavior as  $k \rightarrow 0$  and  $k \rightarrow \infty$  (for better approximations, see [10]):

$$\frac{\varepsilon(k) - 1}{\varepsilon(k)} \approx \left( 1 + \frac{3k^4}{4k_s^2 k_F^2} \right)^{-1}. \quad (5)$$

The Fourier integral (2) can then be carried out with the result

$$\frac{n(r)}{n_0} = 1 + \frac{3\pi}{2} Z h^3 e^{-rk_F h} \frac{\sin(rk_F h)}{rk_F h} \quad (6)$$

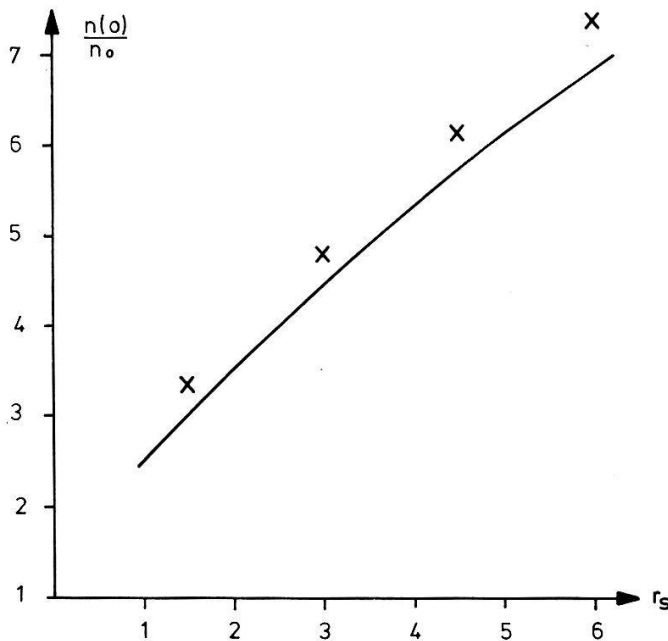


Figure 1

Enhancement at  $r = 0$  in linear response theory according to (6) for  $Z = 1$ . The crosses are the numerical results taken from Ref. [8].

where

$$h = (k_s^2/3k_F^2)^{1/4}. \quad (7)$$

The corresponding enhancement factors at  $r = 0$  are shown in Figure 1 for  $Z = 1$  as a function of  $r_s$  defined by

$$\frac{4\pi}{3} r_s^3 a_B^3 = 1/n_0. \quad (8)$$

For  $r < 1/k_F$ , the values obtained from (6) do not differ much from the numerical results of Langer and Vosko, but the large enhancements indicate anyway that linear response theory is no longer adequate in this region. This is clearly seen for negatively charged impurities, where even negative electron densities are obtained. The electron gas screens most of the impurity charge in a distance of order  $1/k_s$ , thus compensating the long-range part of the Coulomb potential. Near the impurity, however, the strong attractive Coulomb potential is still dominant and requires a treatment that goes beyond linear response.

### 3. Self-Consistent Theory for Inhomogeneous Electron Gas

The general density-functional formalism developed by Kohn and Sham [3] presents an adequate tool to handle the problem of the screening of an impurity charge. In this theory the ground-state properties of the inhomogeneous electron gas are expressed in terms of the local particle density. The general procedure is as follows.

A local, single-particle potential  $V_{\text{eff}}(\mathbf{r})$  generates a set of single-particle wave functions  $\psi_i(\mathbf{r})$  from the Schrödinger equation

$$\left( -\frac{\hbar^2}{2m} \Delta + V_{\text{eff}}(\mathbf{r}) \right) \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r}). \quad (9)$$

The ground-state density is calculated from

$$n(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2 \quad (10)$$

and the effective potential is given (in the special case of a point charge impurity) by

$$V_{\text{eff}}(\mathbf{r}) = -\frac{Ze^2}{r} + e^2 \int d^3r' \frac{n(r')}{|\mathbf{r} - \mathbf{r}'|} + V_{xc}[n(\mathbf{r})]. \quad (11)$$

The potential  $V_{xc}$  accounts for exchange and correlation effects and is a functional of the density  $n(\mathbf{r})$ . For slowly varying densities or in the high-density limit approximate expressions for  $V_{xc}$  may be taken from the theory of the homogeneous electron gas. For arbitrary  $n(\mathbf{r})$ , of course, no simple expression for this quantity is known. Once an approximate form of  $V_{xc}$  is assumed one has to solve the set of these equations in a self-consistent manner. This is a rather involved numerical task.

For the case of impurity screening Sjölander and Stott [1] have calculated  $n(r)$  by neglecting  $V_{xc}$ . The effective potential  $V_{\text{eff}}(r)$  is then connected with  $n(r)$  by the Poisson equation. Their results for both  $Z = 1$  and  $Z = -1$  differ drastically from the

linear-response values and are in agreement with the calculations from a self-consistent treatment of the dielectric function which was also given in Ref. [1]. Popovic and Stott [6] recently reported on a calculation of  $n(r)$  around a proton in an electron gas of density  $r_s = 2.06$  whereby they approximated  $V_{xc}[n(r)]$  by the functional form that this quantity assumes in a homogeneous electron gas.

The practical solution of (9) makes, of course, use of the theory of potential scattering for the spherically symmetric potential  $V_{\text{eff}}(r)$ . In particular, the requirement that the total introduced charge is screened leads to a condition on the asymptotic forms of the scattered waves. This is the Friedel sum rule [5] for the phase shifts of the partial waves at the Fermi wave-number  $k_F$ :

$$\frac{\pi}{2} \cdot Z = \sum_{l=0}^{\infty} (2l+1) \delta_l(k_F). \quad (12)$$

The quantity of interest for the Knight shift at the impurity or for the positron annihilation rate is the enhancement factor for  $s$ -waves, i.e. the ratio of the absolute square of the wave function at the scattering center to its value in the absence of a potential:

$$E(k) \equiv \frac{|\psi_{k,l=0}(r=0)|^2}{|\psi_{k,l=0}^{\text{free}}(r=0)|^2}. \quad (13)$$

This quantity is related to the Jost function [4, 11],  $f_{l=0}(k)$ , by

$$E(k) = |f_0(k)|^{-2}. \quad (14)$$

Furthermore, since the zeros of the Jost function on the negative imaginary  $k$ -axis correspond to bound states,  $f_l(k)$  is a key quantity in the discussion of the electron density enhancement at impurities.

#### 4. Model

In the course of calculating the screening of positive muons in metals according the scheme outlined above we noticed that the detailed form of  $V_{\text{eff}}(r)$  had very little influence on the value of  $E(k)$ . The global sum rule (12), which is of course implicitly contained in equations (9) to (11), puts rather stringent conditions on the behavior of  $V_{\text{eff}}$  near  $r = 0$ . Only the values of  $V_{\text{eff}}$  further away are not determined by (12) and have to be computed from (9) to (11). But it is precisely in this region where an iterative solution of the self-consistent equations converges poorly and depends crucially on the input values. Since we are mainly interested in the behavior near the impurity we therefore suppose a simple form of  $V_{\text{eff}}(r)$  with one parameter. The latter will be determined by the Friedel sum rule.

The model we use for  $V_{\text{eff}}(r)$  is the Hulthén potential

$$V_{\text{eff}}(r) = -Ze^2 \frac{\lambda}{e^{\lambda r} - 1} \quad (15)$$

which has been used for nucleon-nucleon scattering [12]. Near the origin,  $V_{\text{eff}}$  behaves like the Coulomb potential whereas for greater distances it is screened like  $\exp(-\lambda r)$ .



For this potential the Jost function for  $s$ -waves can be calculated analytically [4].

$$f_0(k) = \frac{\Gamma(1 + \alpha_+ + \alpha_-)}{\Gamma(1 + \alpha_+) \Gamma(1 + \alpha_-)} = \prod_{n=1}^{\infty} \frac{k + i \left( \frac{1}{an} - \frac{n\lambda}{2} \right)}{k - i \frac{n\lambda}{2}} \quad (16)$$

where

$$\alpha_{\pm} = \frac{ik}{\lambda} \left( 1 \pm \sqrt{1 - \frac{2\lambda}{ak^2}} \right) \quad (17)$$

and

$$a = \frac{\hbar^2}{Z\mu e^2}. \quad (18)$$

Here  $\mu$  is the reduced mass of the electron and the impurity. The product representation of  $f_0(k)$  immediately shows that the potential (15) has no bound state for  $\lambda > 2/a$ . From  $f_0(k)$  we can calculate the phase shifts  $\delta_0(k)$  from

$$S_0(k) = e^{2i\delta_0(k)} = f_0(k)/f_0(-k) \quad (19)$$

and the density enhancement  $E(k)$  (see (14)). The latter quantity can be obtained in closed form<sup>1)</sup>.

$$E(k) = \frac{2\pi}{ka} \cdot \frac{\text{Sh} \left( \frac{2\pi k}{\lambda} \right)}{\text{Ch} \left( \frac{2\pi k}{\lambda} \right) - \cos \left( \frac{2\pi k}{\lambda} \cdot \sqrt{\frac{2\lambda}{ak^2} - 1} \right)}. \quad (20)$$

At  $k = 0$  this reduces to

$$E(k=0) = \frac{2\pi^2}{\lambda a} \frac{1}{\sin^2 \sqrt{\frac{2\pi^2}{\lambda a}}}. \quad (21)$$

In order to determine the parameter  $\lambda$  from (12) we need to calculate the higher order phase shifts. This has been done numerically using the variable phase function approach [13]. For attractive potentials and for the range of  $k$ -values of interest, the phase shifts  $\delta_l(k)$  for  $l \geq 1$  are usually small and, except for  $p$ -waves, practically do not differ from the values obtained in Born approximation. The  $\lambda$ -values calculated are listed in Table I for  $a$ -values corresponding to a positive muon ( $a \approx a_B$ ) as well as for a positron ( $a = 2 \cdot a_B$ ).

<sup>1)</sup> If the argument of the square root in (20) is negative, the cosine term has to be replaced by

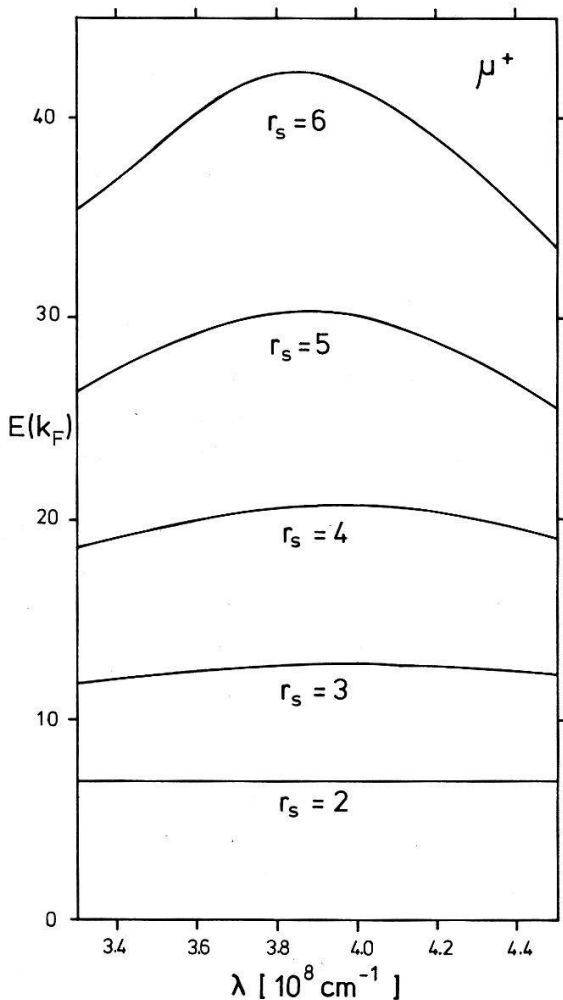
$$\text{Ch} \left( \frac{2\pi k}{\lambda} \sqrt{1 - \frac{2\lambda}{ak^2}} \right).$$

**Table I**  
 Values of  $\lambda$  (in  $10^8 \text{ cm}^{-1}$ ) obtained from (12) for electron densities ranging from  $r_s = 2$  to 6

$a$	$r_s$				
	2	3	4	5	6
0.532	3.79	3.43	3.42	3.44	3.52
1.058	2.42	2.07	1.90	1.80	1.75

For  $\lambda < \lambda_c = 2/a$  the Jost function has a zero on the negative imaginary axis and the potential has a bound state with binding energy  $E_1 = -(\hbar^2/8\mu)(\lambda_c - \lambda)^2$ . An inspection of Table I shows that this occurs for  $r_s > 2$  in the case of a proton impurity and for  $r_s > 4$  for a positron. This behavior is not peculiar to our model potential but has also been found in the calculations of Sjölander and Stott [1] (in both of their approaches). (For a discussion of bound states of positrons, see [14] and Refs. cited therein). If the impurity binds an electron, the potential has to be modified and the scattering of electrons at the bound system must be considered.

The occurrence of bound states is an artifact of our describing the conduction electrons by the jellium model. There is no experimental evidence that positronium is formed in metals. A meaningful theoretical discussion of bound states has to consider



**Figure 2**  
 Variation of the electron density enhancement at  $k_F$  with the parameter  $\lambda$  for various densities. The curves are calculated from (20) for a positive muon ( $Z = 1, a = 0.532 \times 10^{-8} \text{ cm}$ ).



the band structure. This is evident from the fact that the binding energies obtained in the jellium model are rather low. Thus the mean radius of the bound electron would extend over many lattice sites and the interaction is certainly modified by the neighboring ions. For a real bound state to exist in metals, the Bohr radius of the bound electron should be smaller than the smallest distance between impurity and ions. These aspects can be accounted for by taking Bloch waves instead of the plane waves for the unperturbed wave functions. Owing to the presence of metal ions we expect that the contribution of  $p$ - and  $d$ -wave functions will be enhanced at the expense of the  $s$ -waves.

From these arguments we can exclude positronium formation in metals. As concerns the formation of muonium or hydrogen, however, it is possible that a stable bound state can exist for Cs and Rb, at least if the muon is not at an interstitial place but at a vacancy. These interesting possibilities need further attention.

Despite these short-comings we may obtain reasonable results from the jellium model. The reason is due to the fact that the Jost function (16) for the  $k$ -values of interest does not depend very much on the parameter  $\lambda$ . This is demonstrated in Figure 2 where  $E(k_F)$  for a positive muon is plotted as a function of  $\lambda$  for various electron densities. The variation in the case of a positron impurity is even less pronounced (see Fig. 5). For the calculations in the following two sections we therefore replaced all values in Table I with  $\lambda < \lambda_c$  by  $\lambda = \lambda_c$ . We expect the error introduced by this approximation to be small for densities with  $r_s < 5$  whereas for lower densities we certainly have the correct order of magnitude provided, of course, that in fact no bound state exists.

## 5. Positive Muons in Metals

Currently extensive studies are made on the interaction of positive muons with matter [7] and it seems that muons can be a very valuable probe in solid state physics. The implanted  $\mu^+$  behaves very much like a hydrogen nucleus and the change of polarization of the initially fully polarized muons can be detected by means of the anisotropic angular distribution of the emitted positrons. In nonconducting solids the muon usually binds an electron (muonium formation) or is incorporated into a diamagnetic molecule<sup>2)</sup>. In metals, on the other side, the data obtained so far indicate that no muonium is formed. The thermalized muon goes preferably to interstitial sites or vacancies and its magnetic moment precesses freely in the local magnetic field. A systematic investigation on the location of stopped muons and on their diffusive or tunnelling behavior has not yet been made. An advantage of using  $\mu^+$  as a tool for studying the electron distributions and internal fields in para- and ferromagnetic metals is provided by the fact that the muon, like the proton, has no complicated core-electron structure. But whereas the solubility of hydrogen in many metals is rather low, the  $\mu^+$  can easily be implanted into every metal. On the other side, the positive unit charge will change the electron distribution in its neighborhood to a considerable degree. Measurements of  $\mu^+$ -precession in metals thus can only yield information on the conduction electrons if the enhancement of electron density at the muon is known. Our calculations are a first step towards the solution of this problem. A lot of systematic measurements and theoretical investigations have to be done in order to exploit the full information about the physics of solids, which can be obtained with positive muons.

<sup>2)</sup> These phenomena provide another interesting application of muons. In particular, the dipolar interaction of the  $\mu^+$  with nuclei within the compound allows an investigation of the crystal structure analogously to NMR measurements [15].

In the following we shall apply the model presented above to a discussion of the Knight shift and the electron density enhancement at positive muons. The numerical results apply equally well to the screening of protons since the reduced masses differ very little.

The Knight shift [16] arising from the contact interaction is directly proportional to the enhancement factor  $E$  evaluated at the Fermi wavenumber  $k_F$ :

$$\frac{\Delta H}{H} = \frac{8\pi}{3} E(k_F) \chi, \quad (22)$$

where  $\chi$  is the susceptibility of the electron gas. For a free electron gas the Pauli paramagnetic susceptibility has the value

$$\chi_P = \frac{3N\mu_B^2}{2\varepsilon_F} \quad (23)$$

whereas the diamagnetic (Landau) contribution is  $\chi_L = -1/3\chi_P$ . The Coulomb interactions generally enhance the spin susceptibility [17]. In real metals there are, of course, other contributions and the interpretation of NMR-Knight shift data is difficult [16] since (with the exception of Li and Na) there are no other independent measurements of  $\chi$  and a calculation of  $E$  must consider the core-electron structure, a problem not occurring for protons and muons.

In Figure 3 we present the Knight shifts calculated from (22) and (20) with  $\chi = \chi_P$  and  $\chi = 2/3\chi_P$ , respectively. The data are taken from measurements of Hutchinson et al. [18] which were not devoted to a systematic investigation of the Knight shift.

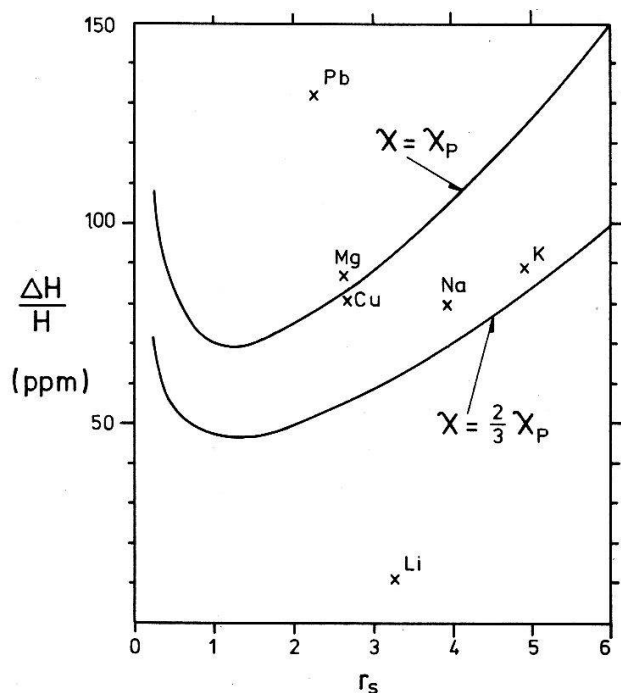


Figure 3  
Knight shift of the  $\mu^+$  calculated from (20) and (22) with  $\chi = \chi_P$  and  $\chi = \frac{2}{3}\chi_P$ . The crosses are measurements of Hutchinson et al. [18].

It is therefore not meaningful to compare the experimental values with the calculated and measured susceptibilities from NMR data until more precise  $\mu^+$  data are available<sup>3)</sup>. Our model gives the correct order of magnitude for the single metals with the exception of Li. The enhancement factors predicted by (20) are much bigger than expected from linear response theory. The steep rise in  $\Delta H/H$  at ultrahigh densities is due to the fact that in this region  $E(k_F) \rightarrow 1$  whereas  $\chi \propto r_s^{-1}$ .

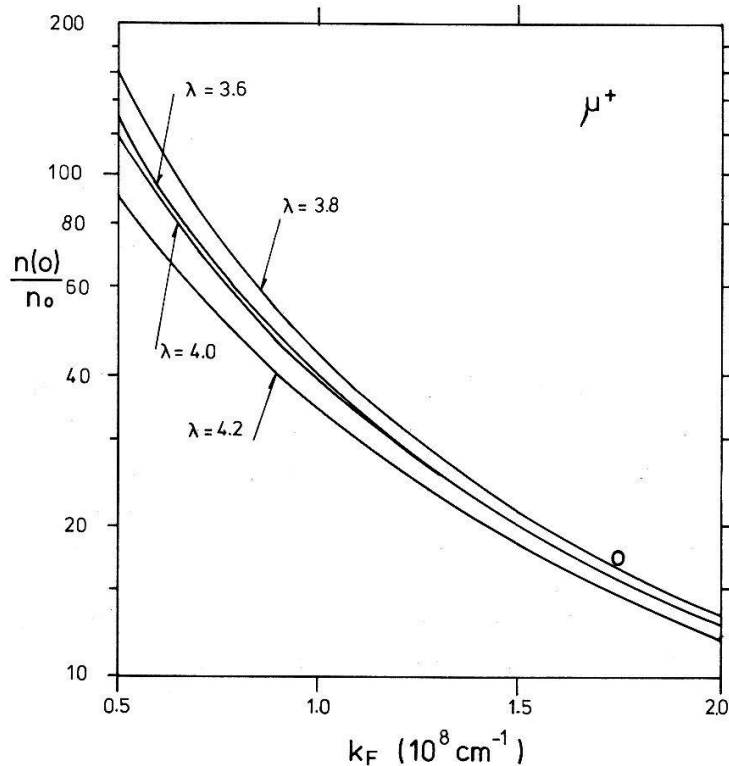


Figure 4  
Semilogarithmic plot of  $n(0)/n_0$  versus  $k_F$  calculated for various values of  $\lambda$  from a numerical integration of (24) using (20). The circle denotes the value reported by Popovic and Stott [6] for Al.

If we calculate the total electron density at the impurity according to

$$\frac{n(0)}{n_0} = \frac{3 \int_0^{k_F} dk k^2 E(k)}{k_F^3} \quad (24)$$

we obtain the values plotted in Figure 4. For high densities our results do not depend very much on  $\lambda$  and the model adopted thus seems reasonable. The recent calculations of Popovic and Stott [6] on the shielding of a proton in Al ( $r_s = 2.06$ ) give for  $n(0)/n_0$  a value of 17. For densities with  $r_s > 4$  the results depend strongly on  $\lambda$ . Huge enhancement factors of the order of 50 to 100 are, however, reasonable if we are close to a bound state. As already discussed in the previous section, we think that in this region reasonable quantitative predictions about the density enhancement cannot be made unless band structure effects are considered.

In contrast to the case of positrons considered in the following section there is no direct experimental test for  $n(0)/n_0$ . In the ferromagnetic state of the electron gas the

<sup>3)</sup> We are not aware of any Knight shift measurements of hydrogen dissolved in metals.

magnetization at the impurity is proportional to the difference of spin-up and -down electrons,  $n^\uparrow(0) - n^\downarrow(0)$ . The band splitting is always small, however, so that only the difference at the Fermi level which is proportional to  $E(k_F)$  is important. In addition, the exchange interaction plays a crucial role for the screening in the ferromagnetic state [19]. Therefore our results cannot be applied directly and further investigations about this point are necessary. This will be relevant for the interpretation of the recent measurements of the muon precession in ferromagnetic iron and nickel [20, 21]. The explanation of the observed hyperfine field in Ni, given in [22], is based on linear response screening which, in our opinion, is not adequate.

## 6. Positron Annihilation Rate

A full discussion of the screening of a light impurity is considerably more complicated than that of a heavy one where all properties can be regarded as static, since the correlated motion of the interacting particles must be taken into account. The electron density enhancement at a thermalized positron in a metal is of particular interest since the theoretical results can be compared to the measured positron annihilation rates. Starting with the work of Kahana [23] who approximately solved the Bethe-Salpeter equation for the electron-positron system, many theoretical efforts have been devoted to explain the measured positron lifetimes (for a review, see [24]).

In the framework of our simple model where we focus our attention on the scattering aspects we can discuss the screening of positrons simply by choosing the appropriate reduced mass. Putting  $a = 1.058 \times 10^{-8}$  cm in (20) we find that the dependence of  $E(k)$  on the screening parameter  $\lambda$  in the appropriate range is even weaker than for a proton. This is shown in Figure 5. Calculating the density enhancement from the

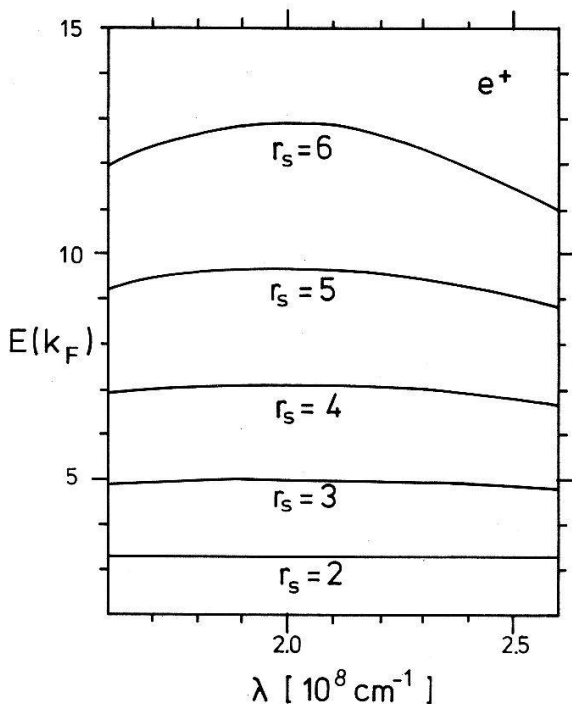


Figure 5  
Variation of the electron density enhancement at  $k_F$  with the parameter  $\lambda$  (in  $10^8 \text{ cm}^{-1}$ ) for a positron ( $a = 1.058 \times 10^{-8}$  cm).

integral (24) we directly obtain the positron annihilation rate

$$\Gamma = \frac{n(0)}{n_0} \Gamma_0 \quad (25)$$

where  $\Gamma_0$  is given by

$$\Gamma_0 = \frac{3}{2} r_s^{-3} \Gamma_{\text{para}} = \frac{3\alpha^4 c}{16a_B r_s^3} \approx \frac{12}{r_s^3} \times 10^9 \text{ sec}^{-1}. \quad (26)$$

Our results are plotted in Figure 6, together with some experimental values and two recent theoretical curves. Most theories lead to an annihilation rate which increases strongly for low electron densities, similar to the curve of Ref. [1]. The work of

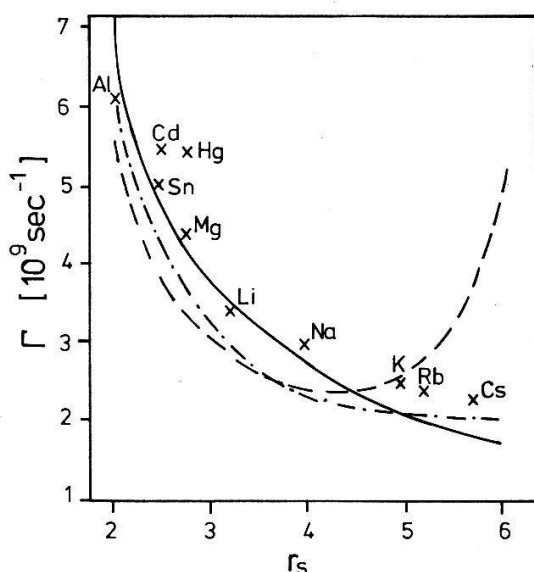


Figure 6

Positron annihilation rate versus  $r_s$ . Full curve: result from our model; dashed line: Sjölander and Stott [1]; dashed-dotted line: Bhattacharyya and Singwi [25]. The crosses indicate experimental value taken from the compilation of West [24].

Bhattacharyya and Singwi [25], however, seems to describe the data correctly<sup>4</sup>). These authors solve a nonlinear integral equation accounting for three-particle correlations and fit an unknown parameter to the data at  $r_s = 6$ . Our simple approach again gives reasonable values for the density enhancement and leads to a monotonic decrease of the annihilation rate.

## 7. Repulsive Potential

Sjölander and Stott [1] have calculated the electron distribution around negatively charged impurities by solving their integral equation for the pair-correlation function and, for fixed point impurities, also by a self-consistent treatment of the non-linear Hartree equations. We now compare those results with the predictions we obtain from our model if the quantity  $a$  (see (18)) has values  $-0.529$  and  $-1.058$  Å, respectively.

<sup>4</sup>) An estimated core contribution of 15% is usually subtracted from the data to yield the contribution from conduction electrons alone.

For repulsive potentials the quantity  $E(k) = |f_0(k)|^{-2}$ , given by (20), starts from

$$E(k=0) = \frac{2\pi^2}{\lambda|a|} \frac{1}{\text{Sh}^2 \sqrt{\frac{2\pi^2}{\lambda|a|}}} \tag{27}$$

and increases monotonically with  $k$  to the limiting value  $E(k \rightarrow \infty) = 1$ . Compared to the case of an attractive potential the relative contributions from  $p$ - and  $d$ -wave scattering are stronger. The screening parameters obtained from the sum rule (12) are listed in Table II.

Table II  
Values of  $\lambda$  (in  $10^8 \text{ cm}^{-1}$ ) obtained from (12) for electron densities ranging from  $r_s = 2$  to 6

$a$	$r_s$				
	2	3	4	5	6
-0.529	2.88	2.22	1.86	1.62	1.38
-1.058	2.18	1.83	1.44	1.27	1.12

Calculating the electron density at the impurity according to (24) we find for the fixed point impurity strong depletions which are plotted in Figure 7 as a function of the unperturbed electron density. The results compare rather well with the nonlinear Hartree-Fock values of Ref. [1], whereas the solution of the integral equation leads to negative densities for higher values of  $r_s$ . The density depletions at an impurity having the mass of an electron are shown in Figure 8 together with the results from the pair-correlation function obtained by Sjölander and Stott.

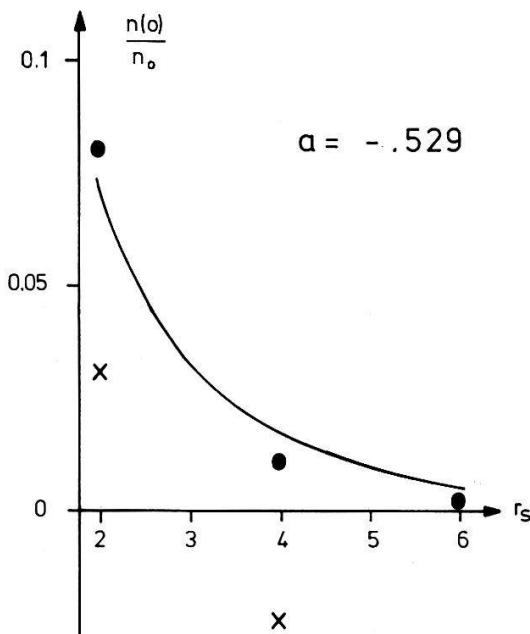


Figure 7  
Density depletion obtained from (24) for  $a = -0.529 \times 10^{-8} \text{ cm}$ . The results from the nonlinear Hartree equations (●) and from the pair-correlation function treatment (x) are taken from Ref. [1].



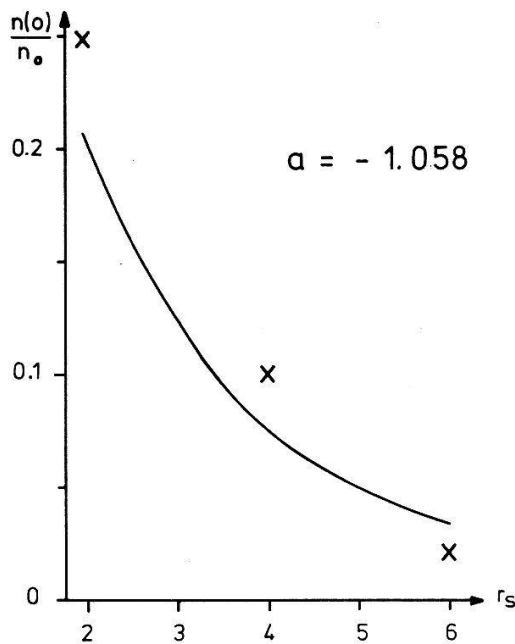


Figure 8

Density depletion for  $a = -1.058 \times 10^{-8}$  cm. The pair-correlation function values (x) are taken from Sjölander and Stott [1].

At this point we should like to mention that the behavior of  $n(r)/n_0$  as a function of  $r$  leads to a variation similar to that obtained in Refs. [1] and [6], at least for  $r < 1/k_F$ . Although we have restricted ourselves to a discussion of the Jost function, the enhancement at arbitrary  $r$  can easily be found. For the potential (15) the solution of the radial ( $s$ -wave) part of the Schrödinger equation, which behaves like  $\exp(-ikr)$  for large  $r$ , is given in terms of the hypergeometric function  $F$  as (note that  $u_k^{l=0}(r=0) = f_0(k)$  is the Jost function)

$$u_k^{l=0}(r) = e^{-ikr} F(\alpha_-, \alpha_+, 1 + \alpha_- + \alpha_+; e^{-\lambda r}) \quad (28)$$

with  $\alpha_{\pm}$  given by (17). This can then easily be compared to the free solution.

## 8. Conclusion

The problem of calculating the electron distribution around an impurity is an interesting question in the many-body theory of the electron gas where the interplay of the various contributions arising from Coulomb interaction, exchange and correlation effects can be studied. These aspects have been treated in the work of Sjölander and Stott. Our model completely neglects the microscopic origin of the screening. The advantage, however, is the simple form we obtain for the quantities of interest in explaining experimental data. This is in contrast to the extensive numerical work which cannot be avoided in a microscopic treatment but which at the same time may mask some physical insight. We suggest that further calculations using the Kohn-Sham density functional formalism should discuss the Jost function. This concept is particularly effective in discussing the enhancement factor and bound states.

The obtained results indicate that the scheme of Kohn and Sham, who reduce the complicated many-body problem of the inhomogeneous electron gas to a single-particle problem, is very useful even if the functional form of the exchange and correlation potential is unknown. Close to the impurity the Coulomb potential is dominant and the

particular form of the screening has little influence on the density enhancement of conduction electrons once the Friedel sum rule is satisfied. This seems to be true also in the case of light impurities. Our simple results for the positron annihilation rate agree remarkably well with the experiments and with microscopic calculations.

From a pragmatic point of view we may say that our model suffices to explain the behavior of muons and positrons in the jellium model. Improvements should concentrate on the influence of band structure effects. This would be a rewarding investigation with regard to the bound state effects.

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