

gradient is in general sufficient to yield a nonzero voltage across the shock front. This is the same mechanism which has been invoked to explain⁵ the acoustoelectric effect. The shock results in a region of local charge density accompanying the shock front as it propagates down to the medium, in agreement with the ideas of Mineev *et al.*³

We wish to point out that aside from the details of band structure, the same phenomena are expected to occur upon shocking a semiconductor. The effect has been observed³ in semiconductors, and we have given a tentative explanation of the details elsewhere.⁷

There is also the possibility that a Hall-effect measurement, without the presence of an external

Hall current, will give nonzero results. Such measurement would give useful information concerning the interaction of a shock wave with the electronic structure of a material (perhaps a large amplitude-phonon drag effect). Such signals would undoubtedly be easier to observe in semiconductors, where shock effects have already been observed⁸ in the presence of an external Hall current.

ACKNOWLEDGMENT

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Electron Distribution around Mobile and Fixed Point Charges in Metals

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A new approach is presented to the calculation of the charge density induced around a charged point particle in the electron gas; this approach includes contributions beyond those considered in linear-response theory. The method can be used to treat impurities with infinite as well as finite mass. Results from calculations with various charges, positive and negative, are presented. In particular, results for the electron density distribution around a positron are presented. The positron-annihilation rates obtained are compared with results of other authors and with experiments.

I. INTRODUCTION

A new treatment of the screening effects in an electron gas has recently been presented by Singwi *et al.*¹ Particular attention was given to the strong Coulomb repulsion between two electrons that are close to each other. This was achieved by constructing an effective electron-electron interaction which took into account the depletion of particle density around a particular electron by means of the static pair-correlation function. The latter was finally determined from the calculated dielectric function in a self-consistent manner. This theory led to a considerable improvement upon

earlier treatments of the static pair-correlation function as well as some other properties of the electron gas.

Here we present a generalization of the above treatment which provides a new method going beyond linear-response theory, for calculating the electron distribution around a point charged particle in the electron gas. The particle may have a positive or negative charge and may be at a fixed location (infinite mass) or have a finite mass, in which case it will be affected by recoil effects. An interesting example would be a positron in thermal equilibrium in an electron gas.

A brief outline of our method and the results of

some preliminary calculations appeared in an earlier paper.² The philosophy of our approach is as follows. We consider a two-component system consisting of electrons with an equilibrium density n^- and of impurity particles with density n^+ . The charge neutrality of the whole system is maintained by a uniform charged background. To this system we apply infinitesimally weak external potentials $V^-(\vec{x}, t)$ and $V^+(\vec{x}, t)$ which act separately on the electrons and impurity particles, respectively, and which vary in both space and time. By calculating the linear response of the electron density to the external potential $V^+(\vec{x}, t)$, for instance, we obtain an expression for the electron distribution around an impurity particle. Then letting the impurity particle density n^+ tend to zero we obtain a result valid for the case of a single impurity in the electron gas. We shall assume an effective interaction between the electrons, as well as between the impurities and the electrons which has a form similar to that employed in the papers of Singwi *et al.* In this way we take into account, in an approximate way, the strong Coulomb interaction between particles that are close to each other. If we should assume that the impurity-electron interaction is weak and use this to approximate our final expressions, we obtain a result for the electron distribution around the impurity which is the same as that obtained from ordinary linear-response theory.

The material is presented in the following order. In Sec. II the mathematical formulation is given leading to an integral equation which has been solved numerically. Some of the results so obtained have been compared with results based on the nonlinear Hartree approximation, and a brief summary of the latter is given in Sec. III. A comparison of the numerical results of these two theories for the case of an infinitely heavy impurity is presented in Sec. IV. Section V contains result for the case of an impurity having the mass of the electron. In particular, the electron distribution around a positron is calculated; the result is compared with that of other calculations; and then estimates of the positron lifetime are made and compared with the observed results for some simple metals. Finally, in Sec. VI we make some concluding remarks.

II. MATHEMATICAL FORMULATION

We consider a two-component system consisting of electrons with charge $-e$ and mass m and of point impurity particles with charge Ze and mass M , where Z may be positive or negative. In the absence of any external disturbance the dynamics of the system is governed by a Hamiltonian H_0 . We now apply weak external potentials $V^-(\vec{x}, t)$ and $V^+(\vec{x}, t)$ which act only on the electrons and

impurity particles, respectively. The dynamics is then governed by the new Hamiltonian

$$H = H_0 + \int d\vec{x} [\rho^+(\vec{x}, t) V^+(\vec{x}, t) + \rho^-(\vec{x}, t) V^-(\vec{x}, t)], \quad (1)$$

where ρ^+ and ρ^- denote the operators for the charge densities contributed by the two components. We shall use the notations n^+ and n^- for the corresponding particle number densities.

From the linear-response theory we obtain the following expressions for the corresponding induced mean charge densities:

$$\begin{aligned} \langle \rho^+(\vec{x}, t) \rangle_{\text{ind}} &= \frac{-i}{\hbar} \int_{-\infty}^t dt' \int d\vec{x}' \langle [\rho^+(\vec{x}, t), \rho^+(\vec{x}', t')] \rangle V^+(\vec{x}', t') \\ &\quad - \frac{-i}{\hbar} \int_{-\infty}^t dt' \int d\vec{x}' \langle [\rho^+(\vec{x}, t), \rho^-(\vec{x}', t')] \rangle V^-(\vec{x}', t'), \end{aligned} \quad (2a)$$

$$\begin{aligned} \langle \rho^-(\vec{x}, t) \rangle_{\text{ind}} &= \frac{-i}{\hbar} \int_{-\infty}^t dt' \int d\vec{x}' \langle [\rho^-(\vec{x}, t), \rho^+(\vec{x}', t')] \rangle V^+(\vec{x}', t') \\ &\quad - \frac{-i}{\hbar} \int_{-\infty}^t dt' \int d\vec{x}' \langle [\rho^-(\vec{x}, t), \rho^-(\vec{x}', t')] \rangle V^-(\vec{x}', t'), \end{aligned} \quad (2b)$$

where $\langle [,] \rangle$ are the equilibrium values of the commutators entering in conventional response theory³ and should be calculated with no external disturbance present. We notice that an external potential acting only on the impurities will, through the impurity-electron interaction, induce a change in the electron density.

By analogy to the conventional procedure used in treatments of the one-component system we introduce frequency- and wave-number-dependent dielectric functions $\epsilon^{\alpha\beta}(\vec{q}, \omega)$, where α, β represent + or -, and write the Fourier transforms of Eqs. (2a) and (2b) in the form

$$\langle \rho^\alpha(\vec{q}, \omega) \rangle_{\text{ind}} = \sum_\beta \left(\frac{1}{\epsilon^{\alpha\beta}(\vec{q}, \omega)} - \delta_{\alpha\beta} \right) \frac{V^\beta(\vec{q}, \omega)}{4\pi/q^2}. \quad (3)$$

By comparing Eqs. (2a) and (2b), and (3) we find that

$$\begin{aligned} \frac{1}{\epsilon^{\alpha\beta}(\vec{q}, \omega)} - \delta_{\alpha\beta} &= -\zeta_\alpha \zeta_\beta \frac{4\pi e^2}{q^2} \left(\frac{i}{\hbar V} \int_0^\infty dt e^{i\omega t} \langle [n_{-\vec{q}}^\alpha(t), n_{\vec{q}}^\beta(0)] \rangle \right), \end{aligned} \quad (4)$$

where $\zeta_+ = Z$, $\zeta_- = -1$, and V is the volume of the system; we have also made use of the translational invariance of the unperturbed system. The quantities $n_{\vec{q}}^\alpha(t)$ are the operators for the spatial Fourier transforms of the particle number den-

sities of the two components.

The Fourier transforms of the static density-density correlation functions, denoted by $\langle n_{\vec{q}}^{\alpha} n_{\vec{q}}^{\beta} \rangle$, are given in terms of the corresponding dielectric functions by the relations

$$\langle n_{\vec{q}}^{\alpha} n_{\vec{q}}^{\beta} \rangle = -(\xi_{\alpha} \xi_{\beta})^{-1} \frac{\hbar q^2 V}{4\pi^2 e^2} \int_0^{\infty} d\omega \operatorname{Im} \left(\frac{1}{\epsilon^{\alpha\beta}(\vec{q}, \omega)} \right). \quad (5)$$

These quantities are closely related to the desired density distributions around a particular particle. We introduce for convenience four structure factors $\gamma^{\alpha\beta}(\vec{q})$ through the relations

$$\langle n_{\vec{q}}^{\alpha} n_{\vec{q}}^{\beta} \rangle = V n^{\alpha} [\delta_{\alpha\beta} + n^{\beta} \gamma^{\alpha\beta}(\vec{q})], \quad (6)$$

where we have used n^+ and n^- to denote the equilibrium particle number densities. The partial pair-correlation functions are then given by

$$g^{\alpha\beta}(\vec{r}) - 1 = (2\pi)^{-3} \int d\vec{q} e^{-i\vec{q}\cdot\vec{r}} \gamma^{\alpha\beta}(\vec{q}). \quad (7)$$

The quantity $g^{\alpha\beta}(\vec{r})$ gives the probability of finding a particle of type α a distance r from another of type β . The first term in the brackets in Eq. (6) arises from the self-part of the density-density correlation and the corresponding term is therefore absent in our expressions for $g^{\alpha\beta}(\vec{r})$. It follows from Eq. (6) that $\gamma^{+-}(\vec{q}) = \gamma^{-+}(\vec{q})$.

In calculating the dielectric response functions we shall follow the procedure developed in Ref. 1. The induced densities are calculated as if our system were composed of free particles responding to effective potentials. This leads to [cf. Eqs. (2a) and (2b)]

$$\langle \rho^{\alpha}(\vec{q}, \omega) \rangle_{\text{ind}} = (\xi^{\alpha} e)^2 \chi_0^{\alpha}(\vec{q}, \omega) V_{\text{eff}}^{\alpha}(\vec{q}, \omega), \quad (8)$$

where $\chi_0^{\alpha}(\vec{q}, \omega)$ are the free-particle response functions given by the expression

$$\chi_0^{\alpha}(\vec{q}, \omega) = \frac{-i}{\hbar V} \int_0^{\infty} dt e^{i\omega t} \langle [n_{\vec{q}}^{\alpha}(t), n_{\vec{q}}^{\alpha}(0)] \rangle. \quad (9)$$

The mean value of the commutator in Eq. (9) is calculated for a noninteracting system. For the effective potentials we choose

$$V_{\text{eff}}^{\alpha}(\vec{x}, t) = V^{\alpha}(\vec{x}, t) + \sum_{\beta} \int d\vec{x}' \Psi^{\alpha\beta}(\vec{x} - \vec{x}') \times \langle \rho^{\beta}(\vec{x}', t) \rangle_{\text{ind}}, \quad (10)$$

where

$$\nabla \Psi^{\alpha\beta}(\vec{x}) = g^{\alpha\beta}(\vec{x}) \nabla \phi(\vec{x}), \quad (11)$$

and we have written $\phi(\vec{x}) = 1/|\vec{x}|$, the bare Coulomb potential. By this choice of the effective potential we take into account the fact that a single particle experiences, besides the external potential, an induced one, arising from the disturbance of the

surrounding particle densities. If we choose $g^{\alpha\beta}(\vec{x}) = 1$, this gives us the ordinary Hartree field. We are then, however, neglecting the fact that the unperturbed mean densities around a particle, which are actually disturbed by the external potential, may be depleted or enhanced from the uniform mean densities depending on whether the particle interaction is repulsive or attractive. This is taken into account here in an approximate way by inserting the static pair-correlation functions $g^{\alpha\beta}(\vec{x})$ which are determined through a self-consistent procedure. The nonlinearity in the response of the *electron density to the impurity charge* enters in our treatment only through the functions $g^{\alpha\beta}(\vec{x})$. Putting $g^{\alpha\beta}(\vec{x}) = 1$ we recover the ordinary linear-response result.

Inserting the above effective potentials in Eq. (8) we obtain two coupled equations for the induced densities. We may write

$$[1 - e^2 \Psi^{--}(\vec{q}) \chi_0^{-}(\vec{q}, \omega)] \langle \rho^{-}(\vec{q}, \omega) \rangle_{\text{ind}} - e^2 \Psi^{+-}(\vec{q}) \chi_0^{-}(\vec{q}, \omega) \langle \rho^{+}(\vec{q}, \omega) \rangle_{\text{ind}} = e^2 \chi_0^{-}(\vec{q}, \omega) V^{-}(\vec{q}, \omega), \quad (12a)$$

$$- (Ze)^2 \Psi^{+-}(\vec{q}) \chi_0^{+}(\vec{q}, \omega) \langle \rho^{-}(\vec{q}, \omega) \rangle_{\text{ind}} + [1 - (Ze)^2 \Psi^{++}(\vec{q}) \chi_0^{+}(\vec{q}, \omega)] \langle \rho^{+}(\vec{q}, \omega) \rangle_{\text{ind}} = (Ze)^2 \chi_0^{+}(\vec{q}, \omega) V^{+}(\vec{q}, \omega), \quad (12b)$$

where

$$\Psi^{\alpha\beta}(\vec{q}) \left(1 + \int \frac{d\vec{q}'}{(2\pi)^3} \frac{\vec{q} \cdot \vec{q}'}{q'^2} \gamma^{\alpha\beta}(\vec{q} - \vec{q}') \right) \frac{4\pi e^2}{q^2}. \quad (13)$$

Solving the above equations we get explicit expressions for the quantities $(1/\epsilon^{\alpha\beta} - 1)$, appearing in Eqs. (3)–(5). Finally, we may, through Eq. (5), determine $\gamma^{\alpha\beta}(\vec{q})$ in a self-consistent way.

It is sufficient for our purpose to let $V^+ = 0$, thus, assuming that the external potential acts only on the electrons. A considerable simplification enters if the impurity density n^+ is small. Because $\chi_0^{+}(\vec{q}, \omega)$ is proportional to n^+ , we may then in Eq. (12b) replace $[1 - (Ze)^2 \Psi^{++}(\vec{q}) \chi_0^{+}(\vec{q}, \omega)]$ by unity and also neglect the second term in Eq. (12a). This gives us

$$\langle \rho^{+}(\vec{q}, \omega) \rangle_{\text{ind}} = (Ze)^2 \Psi^{+-}(\vec{q}) \chi_0^{+}(\vec{q}, \omega) \langle \rho^{-}(\vec{q}, \omega) \rangle_{\text{ind}} \quad (14a)$$

and

$$\langle \rho^{-}(\vec{q}, \omega) \rangle_{\text{ind}} = e^2 [1 - e^2 \Psi^{--}(\vec{q}) \chi_0^{-}(\vec{q}, \omega)]^{-1} \times \chi_0^{-}(\vec{q}, \omega) V^{-}(\vec{q}, \omega). \quad (14b)$$

The induced electron density is the same as for the pure electron gas and we may, through Eq. (3), express it in terms of the dielectric function $\epsilon^{--}(\vec{q}, \omega)$ of the pure electron gas. The disturbance of the impurity density is proportional to n^+ . We may

again through Eq. (3) introduce $\epsilon^{+-}(\vec{q}, \omega)$ and write Eq. (14a) in the following form:

$$\frac{1}{\epsilon^{+-}(\vec{q}, \omega)} = (Ze)^2 \left(1 + \int \frac{d\vec{q}'}{(2\pi)^3} \frac{\vec{q} \cdot \vec{q}'}{q'^2} \gamma^{+-}(\vec{q} - \vec{q}') \right) \times \phi(\vec{q}) \left(\frac{1}{\epsilon^{--}(\vec{q}, \omega)} - 1 \right) \chi_0^+(\vec{q}, \omega), \quad (15)$$

where we repeat that $\epsilon^{--}(\vec{q}, \omega)$ is here the dielectric function for the pure electron gas.

Now taking the imaginary part of $1/\epsilon^{+-}(\vec{q}, \omega)$ from Eq. (15) and inserting it in Eq. (5), we obtain an integral equation for $\gamma^{+-}(\vec{q})$:

$$\gamma^{+-}(\vec{q}) - f(\vec{q}) \int \frac{d\vec{q}'}{(2\pi)^3} \frac{\vec{q} \cdot \vec{q}'}{q'^2} \gamma^{+-}(\vec{q} - \vec{q}') = f(\vec{q}), \quad (16)$$

where we have written

$$f(\vec{q}) = \frac{Z\hbar}{\pi n^+ n^-} \int_0^\infty d\omega \text{Im} \left[\left(\frac{1}{\epsilon^{--}(\vec{q}, \omega)} \right) \chi_0^+(\vec{q}, \omega) \right]. \quad (17)$$

The angular integration in Eq. (16) may easily be performed to yield a simple equation for $\gamma^{+-}(\vec{q})$:

$$\gamma^{+-}(\vec{q}) - \frac{q^3}{4\pi^2} f(\vec{q}) \times \int_0^\infty dx x^2 \left[1 + \left(\frac{1-x^2}{2x} \right) \ln \left| \frac{1+x}{1-x} \right| \right] \gamma^{+-}(qx) = f(q). \quad (18)$$

The free-particle response function entering the expression for $f(q)$ is easily obtained from Eq. (9) and is explicitly given by

$$\chi_0^+(q, \omega) = \frac{n^+}{\hbar} \left(\frac{1}{\omega - (\hbar q^2/2M) + i\eta} - \frac{1}{\omega + (\hbar q^2/2M) + i\eta} \right), \quad (19)$$

where η is a positive infinitesimal and M is the mass of the impurity particle. Finally, we obtain an explicit expression for $f(q)$:

$$f(q) = -\frac{Z}{n^-} \text{Re} \left(\frac{1}{\epsilon^{--}(q, \hbar q^2/2M)} - 1 \right) + \frac{Z}{\pi n^-} \int_0^\infty d\omega \text{Im} \left(\frac{1}{\epsilon^{--}(q, \omega)} \right) \times \wp \left(\frac{\hbar q^2/2M}{\omega^2 - (\hbar q^2/2M)^2} \right), \quad (20)$$

where \wp represents the principal value. For a fixed impurity ($M = \infty$) we have

$$f(q) = -\frac{Z}{n^-} \left(\frac{1}{\epsilon^{--}(q, 0)} - 1 \right). \quad (21)$$

We see that from a knowledge of the dielectric function for the pure electron gas we can calculate $f(q)$ for any chosen value of the impurity particle mass and then by solving Eq. (18) we obtain the equilibrium density of electrons around the impurity particle.

If we ignore the integral term in Eq. (18), we recover for $\gamma^{+-}(q)$ the result obtained by considering merely the linear response of the electrons to the disturbance caused by the impurity. Clearly, this would only be valid approximation for $\gamma^{+-}(q)$ for a weak electron-impurity interaction. The numerical results that we shall present will show that the correction to linear response is actually very large even for $Z = \pm 1$.

III. NONLINEAR HARTREE APPROXIMATION

An alternative procedure for calculating the electron density around a fixed charged impurity in the electron gas has been followed by Stott *et al.*⁴ using the nonlinear Hartree approximation. There, one solves the single-particle Schrödinger equation for the electrons:

$$[-(\hbar^2/2M)\nabla^2 + V(\vec{r})] \Psi_{\vec{k}}(\vec{r}) = E_{\vec{k}} \Psi_{\vec{k}}(\vec{r}), \quad (22)$$

where the potential $V(\vec{r})$ is determined from the Poisson equation

$$\nabla^2 V(\vec{r}) = -4\pi [eZ\delta(\vec{r}) + \langle \rho^-(\vec{r}) \rangle + en^-]. \quad (23)$$

The first term in the bracket of Eq. (23) represents the charge distribution of the impurity, the second term is the electron charge distribution, and the third term accounts for the positively charged background. The mean electron density is given in terms of the eigenfunctions of Eq. (22) through the relation

$$\langle \rho^-(\vec{r}) \rangle = -e \sum_{E_{\vec{k}} \leq E_f} |\Psi_{\vec{k}}(\vec{r})|^2, \quad (24)$$

where the label \vec{k} includes spin. We take account of the Pauli principle in an *ad hoc* way by placing one of the N^- electrons in each of the lowest N single-particle states. Apart from regarding this as merely a self-consistent Hartree calculation, we could alternatively think of this as an application of the theory developed by Hohenberg, Kohn, and Sham^{5,6} in which the ground-state properties of a many-particle system are expressed in terms of the local particle density where the latter is written in terms of single-particle eigenfunctions. This method is, in principle, exact; our approximation here corresponds to neglecting the exchange and correlation contributions to the effective single-particle potential.

It is well known⁷ that by linearizing Eqs. (22)–(24) we obtain the random-phase-approximation (RPA)

result for the electron distribution. Our main point here is to obtain the solution beyond this approximation.

At this point we are already able to make some comparisons between the treatments presented in this section and Sec. II. In the nonlinear Hartree approximation one automatically guarantees the particle density to be positive or zero [see Eq. (24)] whereas this is not the case in the other treatment. In fact, the pair-correlation function we calculate from the integral equation is slightly negative for large r_s and for small distances from a repulsive impurity particle. The nonlinear Hartree approximation takes correlation and exchange effects into account only to the extent that the RPA does. However, in the procedure outlined in Sec. II such effects are more properly included. At present, one does not know precisely the degree to which these effects are included in the treatment. Both procedures are not restricted to weak potentials and are therefore of considerable interest. The theory of Sec. II is easily applied to impurities of finite mass, which does not seem possible in the case of the nonlinear Hartree approximation. Because of the difference in the two methods, it is of interest to compare the numerical results one obtains. This may clarify some of the physical assumptions and possibly help to improve both theories.

IV. RESULTS FOR FIXED POINT IMPURITY

Before presenting the results, we shall give some details of the calculational procedure. In the nonlinear Hartree calculation the radial Schrödinger equation was solved using a trial potential $V(\vec{r})$. The radial wave functions and a number of scattering phase shifts were calculated for a set of occupied \vec{k} values which characterize the radial eigenstates. Using these results, the corresponding Hartree potential was calculated from Eqs. (23) and (24) and it was employed in choosing an improved trial potential for a new calculation. This routine was repeated until sufficient self-consistency was achieved. The Friedel sum rule, relating the phase shifts to the charge on the impurity, was satisfied to high numerical accuracy ($\sim 0.01\%$) and this guarantees the charge neutrality of the system.

In solving Eq. (18) we used a finite-interval Fredholm method. In order to handle the integrand for large values of q we utilized the relation

$$\gamma^{+-}(q) \rightarrow g^{+-}(0)f(q) \quad (25)$$

for $q \rightarrow \infty$, a result which follows directly from Eq. (16). The number of intervals used in the integration procedure was increased until sufficient convergence was attained. In determining $f(q)$ we used the dielectric function for the pure electron gas as calculated by Singwi *et al.*⁸

A. $Z < 0$

We first present results for a negatively charged fixed point impurity. In Fig. 1 we show $g^{+-}(\vec{r})$ for various r_s values within the range of metallic conduction electron densities and with $Z = -1$; the curves are obtained from linear-response theory (curves 1), from our integral equation (18) (curves 2) and from the nonlinear Hartree theory (curves 3). The pair-correlation function by definition should never take negative values and we notice that linear response gives quite unsatisfactory results over a sizable region in \vec{r} space and it becomes worse in this respect as r_s increases. The fact that the total depletion of particle density, given by

$$\int d\vec{r} [g^{+-}(\vec{r}) - 1] = Z, \quad (26)$$

is correctly reproduced implies that too much charge is moved away from the impurity to larger distances. This leads to an overestimate in the amplitude of the oscillations in the charge density for large distance. Curves 2 and 3 are rather close together and even though Eq. (18) does not guarantee a positive $g^{+-}(\vec{r})$ the violation of this condition is very slight. This is consistent, with the observations of Singwi *et al.*^{1,8} on the pair-correlation function for the pure electron gas.

Figure 2 shows results for a point impurity with $Z = -3$ and $r_s = 2.07$ a. u. appropriate for aluminum. Linear response is much worse than for $Z = -1$ [the $(g^{+-}(\vec{r}) - 1)$ from linear response being linear in Z]. Nonlinear Hartree theory and Eq. (18) give qualitatively very similar results. The density obtained from Eq. (18) is still only very slightly negative for small distances bearing in mind that the total density depletion is now three.

B. $Z > 0$

The results for a positively charged fixed point impurity (for $Z = +1$ the case of a proton in the electron gas) are somewhat controversial and we see no point in presenting our numerical results in the form of figures. Our calculations for $Z = +1$ based on Eq. (18) gave for $r_s = 2$ a. u. a very large density enhancement around the impurity [$g^{+-}(0) = 39$]. For $r_s > 2$ a. u., $g^{+-}(\vec{r})$ became negative and large in the region near the impurity. The nonlinear Hartree calculations for all reasonable choices of trial potential gave a bound s state for $r_s \geq 2$ a. u. This leads us to suspect that the failure of our new method in this range of electron density is due to the appearance of a bound state, which this method was not designed to treat. One of the trial potentials used in the Hartree calculations was the Coulomb potential screened by the dielectric function of Singwi *et al.* and this also led to a bound state. This potential must therefore

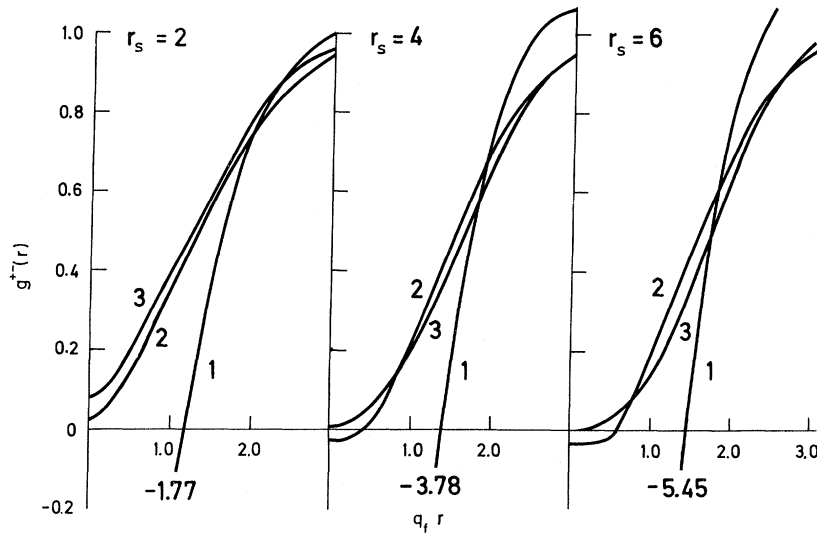


FIG. 1. Electron distribution around a fixed impurity $g^{+}(r)$ vs $q_f r$ for $Z = -1$, and $r_s = 2, 4$, and 6 a.u. calculated using linear-response theory (curves 1), from the integral equation (18) (curves 2) and using nonlinear Hartree theory (curve 3). The number associated with curves 1 is the degree of density depletion at $r = 0$.

be regarded as strong, invalidating the use of linear-response theory. The screening has removed the long-range part of the bare Coulomb potential, which is the feature of the bare potential responsible for the infinity of bound states for the hydrogen atom. However, it has not significantly weakened the strong attractive part of the potential near the impurity. It is this part that leads to a bound state in the case we are considering. We noticed that the binding energy is considerably reduced from that for the state of hydrogen atom. Consequently, the bound-state wave function extends over a larger region and the amplitude is correspondingly smaller.⁹ Unfortunately, the calculational method we employed was not suitable for making a fully self-consistent Hartree calculation when bound states appeared. We intend to rectify this in the future. At present, we do not consider our results conclusive concerning the existence or nonexistence of a bound state.

V. RESULTS FOR FINITE-MASS POINT IMPURITY

Calculations have been performed for the impurity mass equal to the electron mass and for both positive and negative unit charge. Because of its finite mass the impurity will now be influenced by recoil effects. We would expect the depletion of density around the negatively charged impurity to be less pronounced than before. In the case of the positively charged impurity the enhancement of electron density should, similarly, be less than for the fixed impurity.

A. $Z < 0$

Figure 3 presents the results for various r_s values and $Z = -1$ obtained from linear response (curves 1) and from the integral equation (18)

(curves 2). For comparison we also show the pair-correlation function for electrons of opposite spin, $g_1^+(\vec{r})$, for the pure electron gas as given by Singwi *et al.*⁸ (curves 3). We notice that the recoil effects have considerably reduced the degree of density depletion near the impurity, making linear response somewhat better. However, it still gives a $g^{+}(\vec{r})$

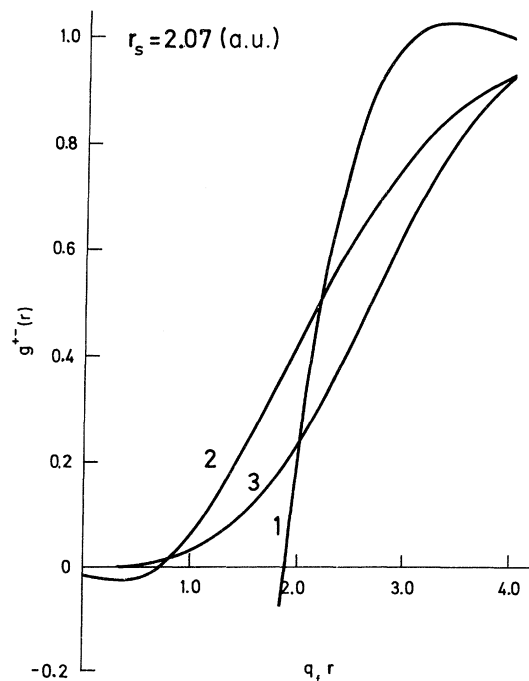


FIG. 2. Electron distribution around a fixed impurity $g^{+}(r)$ vs $q_f r$ for $Z = -3$, and $r_s = 2.07$ a.u. calculated using linear-response theory (curve 1), from the integral equation (18) (curve 2) and using nonlinear Hartree theory (curve 3).

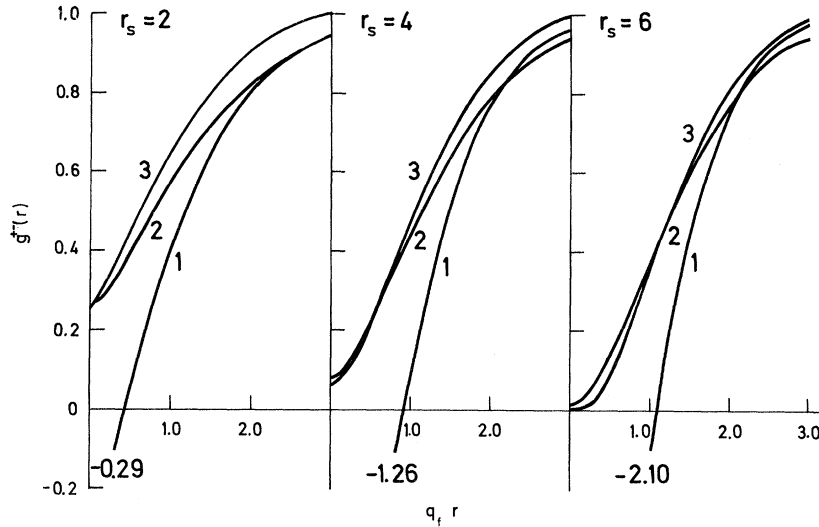


FIG. 3. Electron distribution around an impurity having the mass of the electron $g^{+-}(r)$ vs $q_f r$ for $Z = -1$, and $r_s = 2, 4$, and 6 a.u. calculated using linear-response theory (curves 1) and from the integral equation (18) (curves 2). The $g_{+1}(r)$ for the pure electron gas taken from Ref. 8 is also shown for each r_s value (curves 3). The number associated with curves 1 is the degree of density depletion at $r=0$.

which is negative at small distances. In fact, for $r_s > 1.5$ a.u., $g^{+-}(0)$ is negative. The density obtained from Eq. (18) is now positive over the whole range $r_s = 2-6$ a.u. and we find $g^{+-}(\vec{r})$ to be nearly the same as $g_{+1}(\vec{r})$ for the pure electron gas, particularly so for the larger values of r_s . The differences between the two quantities is due to the fact that the electrons are not distinguishable from each other whereas the point impurity, even though it has the mass and charge of an electron, is still distinguishable from the electrons. As we can see from the figure, these exchange effects become small as r_s increases.

We have noticed that the full pair-correlation function for the pure electron gas, as calculated by Singwi *et al.*, lies rather close to the $g^{+-}(\vec{r})$ obtained for the fixed point impurity with $Z = -1$. In order to illustrate this we have, in Fig. 4, plotted $g^{+-}(\vec{r})$ from nonlinear Hartree theory and the pure electron gas $g(\vec{r})$ from Ref. 8 for $r_s = 3$ a.u. Effects due to recoil and the Pauli principle, appearing in $g(\vec{r})$, seem to cancel each other to a large extent.

B. $Z > 0$

Figure 5 illustrates results for an impurity carrying unit positive charge and having a mass equal to the electron mass (this could be the case of a positron in the electron gas). We present results from linear-response theory (curves 1) and those obtained from Eq. (18) (curves 2). We notice a large nonlinear effect in the density buildup close to the impurity as r_s increases. This density enhancement is much less pronounced in the case of the linear-response results. We conclude that linear-response theory greatly underestimates the enhancement in the metallic range of r_s values. It should be noted that in all cases the total induced

density around the impurity is Z . This implies that linear response distributes this density over too large a region.

We have calculated the total induced density within a sphere of radius r_s around the impurity both from linear response and from our nonlinear theory (see Table I).

First of all we notice that the induced density extends further from the impurities with $Z = -1$ than for those with $Z = +1$. This is apparent also

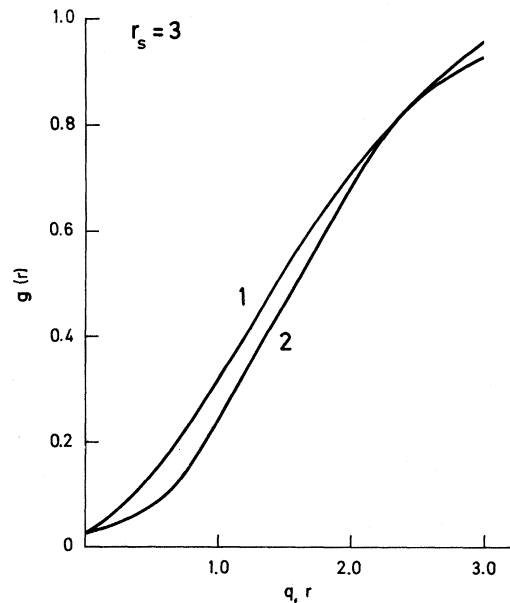


FIG. 4. Pair-correlation function $g(r)$ for the pure electron gas taken from Ref. 8 (curve 1) and the electron distribution around a fixed impurity $g^{+-}(r)$ for $Z = -1$ calculated using nonlinear Hartree theory (curve 2); $r_s = 3$ a.u. and the curves are plotted against $q_f r$.

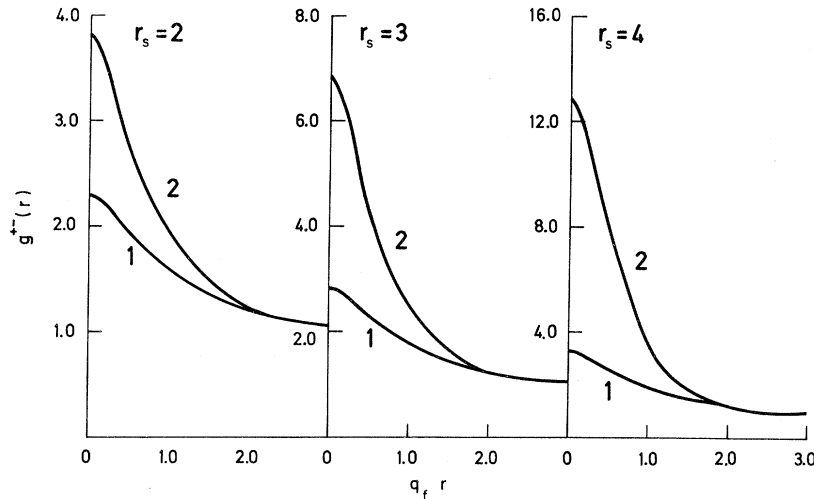


FIG. 5. Electron distribution around an impurity having the mass of the electron $g^{+-}(r)$ vs $q_f r$ for $Z=+1$, and $r_s=2, 3$, and 4 a.u. calculated using linear-response theory (curves 1) and from the integral equation (18) (curves 2).

from Figs. 3 and 5. This effect is due to there being no restriction on the degree to which the density near an attractive impurity may be enhanced apart from the cost in kinetic energy and provided the total induced density fulfills the charge neutrality condition. As a consequence, in these cases we see $g^{+-}(0) \gg 1$ for large values of r_s . In contrast, the electron density around a repulsive impurity may only be reduced at any point by an amount n^- from the average density r_s and the range of the induced density is at least r_s . We also notice from Table I that the nonlinear results for $r_s=4$ and $Z=+1$ indicate that the impurity is overscreened within the radius r_s . This is compensated for in $g^{+-}(\vec{r})$ at larger r by substantial oscillations about unity. Further investigation is needed in order to say whether this is a reasonable result.

The present calculations enable us to calculate the positron-annihilation rate λ in an electron gas using the relation¹⁰

$$\lambda = \frac{1.2}{r_s^3} g^{+-}(0) \times 10^9 \text{ sec}^{-1}. \quad (27)$$

Our results are presented in Fig. 6 and are compared both with earlier calculations of Carbotte,¹¹ using the Bethe-Salpeter equation, and of Bergersen and Terrell.¹² The theoretical calculations are compared with the experimental results of Weisberg and Berko.¹³ The results of our new method compare favorably with those of other authors in the metallic range up to $r_s \sim 5$ a.u. However, the theoretical results lie consistently below the experimental results for the simple metals.

The electron-gas model used to describe positrons in metals is inadequate on two counts. Of lesser importance for the simple metals is the effect of the periodic crystal potential on the valence electrons. We believe, in addition, that the penetration of the positron into the ion cores and the

subsequent annihilation with a core electron contributes substantially to the total annihilation rate. Both of these effects will lead to a broad component in the two-photon angular correlation curves. The area of this broad component in the case of lithium metal amounts to a fraction ($\sim 15\%$)¹⁴ of the total and this fraction represents the contribution to the total annihilation rate which accounts approximately for the discrepancy between our results and the experiments.

Our results are unreliable for $r_s \geq 5$ a.u. The method breaks down in the same manner as for the heavy impurity with $Z=+1$ and the range of r_s in which the nonlinear Hartree method indicated a bound state. We suspect that the breakdown of the method is connected to the appearance of strong electron localization, but further investigation of this point is required.

VI. CONCLUSION

We have found that an impurity particle carrying

TABLE I. The number of displaced electrons within a sphere of radius r_s about the impurity particle for a variety of cases.

$Z < 0$	$r_s = 2$ a.u.	$r_s = 4$ a.u.	$r_s = 6$ a.u.
$Z = -1, M = \infty$			
Results from Eq. (18)	-0.460	-0.544	-0.579
$Z = -1, M = \infty$			
Nonlinear Hartree	-0.404	-0.594	-0.642
$Z = -1, M = m$			
Results from Eq. (18)	-0.307	-0.394	-0.441
$Z > 0$	$r_s = 2$ a.u.	$r_s = 3$ a.u.	$r_s = 4$ a.u.
$Z = +1, M = m$			
Results from Eq. (18)	+0.588	+0.893	+1.312

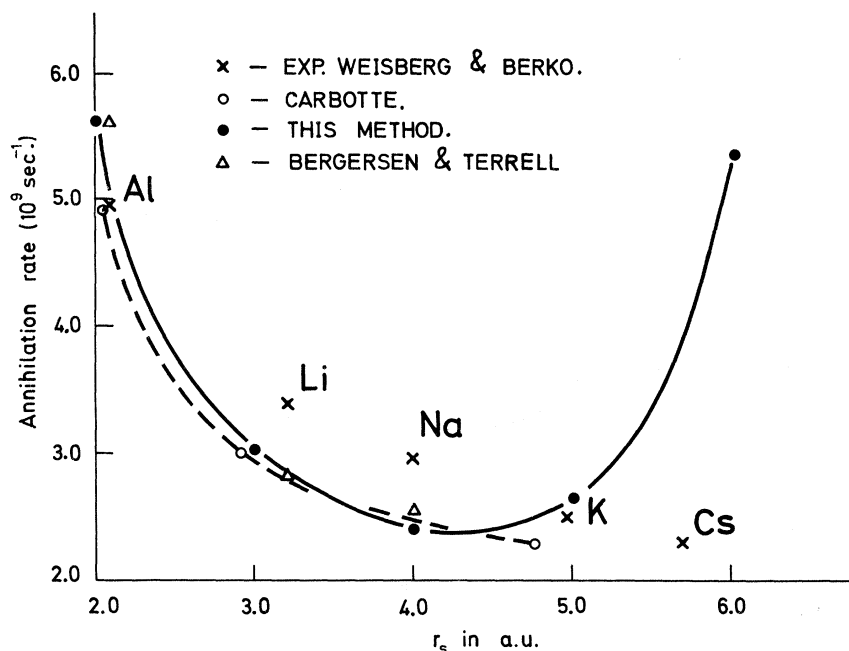


FIG. 6. Positron-annihilation rate λ vs r_s , calculated from the integral equation (18) (●), other theoretical results of Carbotte (Ref. 11) (○), and Bergersen and Terrell (Ref. 12) (Δ). The experimental results of Weisberg and Berko (Ref. 13) are also indicated (x).

unit electric charge is a strong perturbation on an electron gas within the metallic range of densities. Linear-response theory leads to an unreasonable distribution around the impurity. In particular, for a unit negatively charged impurity linear-response theory gives a negative electron density near the impurity both for a fixed impurity particle and for one having the electron mass.

Calculations that go beyond linear response have been performed. The cases of impurities with large mass and the electron mass have been treated by a new method which takes some account of exchange and correlation effects. The case of a heavy impurity was also treated using nonlinear Hartree theory. These two approaches in the case of a negatively charged fixed impurity gave similar results for the electron density around the impurity. The results are reasonable physically, being essentially positive, and the corrections to linear-response theory are substantial in the metallic range of electron density.

In the case of the heavy impurity carrying positive unit charge the new method breaks down in

most of the metallic density range; the nonlinear Hartree calculations indicate a strong localization of electrons near the impurity and the possibility of a bound state cannot be ruled out, although this point is under further investigation. We believe that this strong localization may be related to the breakdown of our new method. The new method breaks down in a similar fashion for an impurity having the mass and charge of a positron for $r_s \geq 5$ a.u. At higher densities the new method leads to good results for the positron-annihilation rate.

One should notice that for large enhancements the two terms on the left-hand side of Eq. (18) cancel each other nearly completely. Approximations have been made in choosing our effective potential and even a small error of the integral term in Eq. (18) could have a large effect on $\gamma^+(q)$. It could then easily introduce an unphysical overcompensation leading to a negative density distribution. Judged from this point of view it may seem surprising that the method works so well in the positron case in spite of the rather large enhancement effects.

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Optical Properties of Rb between 3.3 and 10.5 eV*

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The optical and dielectric constants of Rb have been determined from reflectance measurements for photons of energy between 3.3 and 10.7 eV. Reflectance measurements were made as a function of incident angle at a Rb-substrate interface in an ultrahigh-vacuum system. The refractive index (n) was determined from the critical angle for total internal reflection, and the absorption coefficient (k) from the slope of the reflectance curve at the critical angle. The real part of the dielectric function (ϵ_1) and the optical conductivity ($\sigma = \omega\epsilon_2/4\pi$) were derived from n and k . In σ , we find a broad strong peak centered at 7 eV. It is attributed to absorption processes involving plasmon-assisted interband transitions and to direct interband transitions to "f" bands. ϵ_1 is analyzed in terms of a nearly-free-electron model to obtain a value for the contribution of core polarization to ϵ_1 of $4\pi\alpha = 0.25 \pm 0.02$, and an effective mass of $m_{\text{eff}} = (1.03 \pm 0.02)m_0$.

INTRODUCTION

The alkalis are the simplest of the metals, in that their properties most nearly match those predicted using a simple nearly-free-electron (NFE) model of metals. Optical measurements on Na, K, Rb, and Cs in the visible and infrared region give results in generally good agreement with the NFE model.^{1,2} These results and optical measurements on Na at higher energies suggest that there may be additional absorption above the plasma frequency that cannot be accounted for by the absorption mechanisms usually included in the NFE model.³ We have recently reported measurements of the optical and dielectric constants of Cs for photon energies between 4 and 10 eV that conclusively demonstrate the existence of such an additional absorption process in this material.^{4,5} A broad absorption peak with a maximum at 5 eV was found in the optical conductivity which we interpreted as absorption resulting from the simultaneous excitation of a collective mode and an interband transition.

In this paper we report experimental determinations of the index of refraction (n), the absorption coefficient (k), the real part of the dielectric response function (ϵ_1), and the optical conductivity

(σ) for Rb for photon energies of 3.3–10.7 eV. A broad peak centered at 7 eV is observed in the conductivity. The peak is somewhat weaker and broader and lies at a higher energy than the corresponding peak found for Cs. A Kramers-Kronig analysis applied to the imaginary part of the dielectric response function ($\epsilon_2 = 4\pi\sigma/\omega$) is used to calculate the effect of the interband transitions and of the broad high-energy absorption peak on ϵ_1 . These contributions are subtracted from ϵ_1 so that the remaining portion represents the ϵ_1 expected for a NFE model containing only free-carrier absorption. This corrected value of ϵ_1 is used to obtain values of the core polarization and the effective mass, which are the adjustable parameters of such a free-electron model. The values obtained are compared with those obtained by other authors.

EXPERIMENTAL PROCEDURES

The basic experimental procedures used in this work have been described in detail elsewhere.^{3,5} The sample chamber is shown schematically in Fig. 1. In brief, Rb was deposited on the flat surface of a transparent semicylinder substrate. The reflectance of light incident on the Rb film through the substrate was measured as a function of angle. A semicylinder is used so that incident and re-