Single-Particle Excitations in a Dense Electron Gas Containing a Positive Point Charge*

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We have investigated the perturbative solution of the equation for the one-particle Green's function for the ideal problem of a dense infinite electron gas with neutralizing uniform positive background and a static "source" consisting of a fixed positive point charge of atomic number Z. The densities appropriate to the perturbation expansion are so high as to limit the quantitative applicability of the model to very dense metals or dense degenerate astronomical systems such as white dwarfs. Lowest order expressions for the non-Hermitian effective Hamiltonian of the single-particle excitation spectrum are derived. According to an interpretation discussed in a previous paper, the eigenvalues and eigenfunctions of the effective Hamiltonian correspond also to single-electron energy levels and wave functions associated with ground-state properties of the system. Some general properties of the induced charge density and of the corresponding polarization potential are discussed. The theory predicts the existence of a discrete spectrum of bound holes and its disappearance beyond a certain limiting value of the density, n: $n^{1/3}\simeq Z^2a_0^{-1}$, where a_0 is the Bohr radius. This is a consequence of the fact that the lowest order polarization potential is a shielded Coulomb potential (Yukawa potential) with a range inversely proportional to the classical plasma frequency. This potential, derived here by a formal limiting process, is well known from the electron theory of metals where its derivation has been based on a linearized Thomas-Fermi treatment. In order for the discrete spectrum of bound holes to have physical reality it is necessary that the level width of these holes be less than the spacing of bound levels or less than the distance to the continuum limit. This condition is verified, at high densities, by a lowest order calculation of the level width in the same formal high-density limit that yielded the Yukawa potential. Approximate numerical estimates for the level width are then given for a considerably wider range of densities and values of Z. It is shown that, to a fair approximation, the level width depends on only two parameters: the ratio of the interparticle spacing to the Bohr radius and the ratio of the binding energy to the Fermi energy, provided that these parameters are less than or comparable to unity. It turns out that away from the limit of very small binding energies, the plasmon-emission mode gives an important contribution to the level width. An interesting consequence of the present work is that for low binding energies the "orbits" of bound holes may be considerably larger than the interparticle spacing. Some physical applications of the results, particularly to the problems of electron capture by a nucleus in a dense medium, and the x-ray spectrum of atoms in metals are briefly discussed.

I. INTRODUCTION

We shall be concerned here with the application of a nonrelativistic field-theory method to an ideal many-fermion system consisting of a dense infinite electron gas at zero temperature, with neutralizing positive background and a fixed positive point charge of atomic number Z.[1]

The field-theory method is the widely used Green's function approach.[2–7] In a previous paper[8] some aspects of this method were considered for the more general problem of a static external potential, $V(x)$, and a two-body interaction $v(x-x')$. In the present example, V and v have the forms

$$V(x)=-Ze^2/r, \tag{1}$$

$$v(x-x')=e^2/|x-x'|. \tag{2}$$

The model of the dense electron gas has been intensively studied for a number of years and is now qualitatively well understood.[9] The field-theory treatment of this problem is more recent.[5,10–12] A comprehensive field-theory analysis of the uniform dense electron gas has been given by Dubois.[5] This work forms an important part of the background of the present investigation.

As is well known, the high-density limit of the electron gas corresponds to a lowest order expansion in terms of Feynman graphs. This is, of course, the reason why so many authors, including the present author, have been attracted to this domain of densities.

High densities here means that the interparticle spacing is less than or approximately equal to the Bohr radius. Such densities are found only in extremely dense metals, which even so apparently lie on the border line of validity of the perturbation expansion.[5,9] But they are also found in some dense degenerate astronomical systems, in white dwarfs for example, where the electron density gets as high as one desires.[13–15]

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[1] A brief account of part of this work was published in Bull. Am. Phys. Soc. **6**, 447 (1961).

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[3] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).

[4] A. Klein and R. Prange, Phys. Rev. **112**, 994 (1958).

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[7] T. Kato, T. Kobayashi, and M. Namiki, Suppl. Progr. Theoret. Phys. (Kyoto) No. 15, 3–60 (1960).

[8] A. J. Layzer, preceding paper [Phys. Rev. **129**, 897 (1963)]. We shall refer to this article, hereafter, as I. The terminology and results of this paper will be freely employed here.

[9] We refer to the review article of D. Pines for a discussion of this earlier work and for references to the extensive original literature. D. Pines, *The Many-Body Problem* (W. A. Benjamin, New York, 1961) (Collection).

[10] J. Quinn and R. Ferrell, Phys. Rev. **112**, 812 (1958).

[11] J. Langer and S. Vosko, J. Phys. Chem. Solids **12**, 196, (1960). I wish to thank Professor J. Lebowitz for bringing this paper to my attention.

[12] J. S. Langer, Phys. Rev. **124**, 1003 (1961); **120**, 714 (1960).

[13] E. Schatzman, *White Dwarfs* (Interscience Publishers, Inc., New York, 1958). I wish to thank Dr. E. Spiegel for bringing this work to my attention.

One hopes then that in addition to illustrating some general features of nonuniform many-fermion systems, this model will be of "practical" use in applications to the description of properties of metals or white dwarfs as influenced by point inhomogeneities of charge and, from another point of view, to the description of nuclear processes in such dense media as influenced by electronic shielding.

To see clearly how the density of the system and the strength of the source potential are related to the perturbation expansion, it is convenient to adopt the standard units

$$\hbar = m = p_F = 1, \tag{3}$$

where p_F is the unperturbed Fermi momentum. This is related to the background density, n, through the usual formula

$$\lambda\!\!\!^{-}_F{}^{-3} = 3\pi^2 n, \tag{4}$$

where $\lambda\!\!\!^{-}_F$ is the Fermi wavelength

$$\lambda\!\!\!^{-}_F \equiv \hbar/p_F. \tag{5}$$

The unit of length is now the Fermi wavelength and the unit of energy is twice the Fermi energy. We introduce also the ratio, β, of the Fermi wavelength to the Bohr radius of the electron a_0:

$$\beta \equiv \lambda\!\!\!^{-}_F / a_0. \tag{6}$$

Then β and Z are the only dimensionless parameters in the problem.

In these units the unperturbed Green's function G_0 and the potentials v and V have the following forms in momentum space[16]:

$$G_0(p,w) = \frac{\theta(1-p)}{w - p^2/2 - i\eta} + \frac{\theta(p-1)}{w - p^2/2 + i\eta}, \tag{7}$$

$$v(q,w) = 4\pi\beta/q^2, \tag{8}$$

$$V(q) = -Zv(q). \tag{9}$$

We see that G_0 is free of the parameters β and Z, while v is proportional to β and V to βZ. Thus, we verify that the formal conditions for the validity of the perturbation expansion are

$$\beta \lesssim 1, \tag{10a}$$

$$Z\beta \lesssim 1. \tag{10b}$$

The last condition states that if an expansion in powers of the source potential is also to be valid the interparticle spacing must be comparable or smaller than the "Bohr radius" of a hydrogenic atom of atomic number Z.[17]

We shall be mostly concerned here with the single-particle excitation spectrum of our model. For the uniform system this question has been considered by several authors[5,18] and we shall mainly consider here effects related to the presence of the additional point "source."

In order to investigate this problem we shall obtain, via a Feynman diagram expansion, lowest order expressions for the effective Hamiltonian describing single-particle excitations and entering into the so-called Schwinger equation for the one-particle Green's function $G(x,t;x',t')$.[19,3,7,8]

For a static external field the energy transform of the Schwinger equation takes the operator form

$$[w - p^2/2 - V(x) - \Sigma(w)]G(w) = 1, \tag{11}$$

where $G(w)$ is the frequency transform of the Green's function operator and $\Sigma(w)$ is the transform of the so-called self-energy operator.

$\Sigma(w)$ is the sum of a local, Hermitian, and w-independent polarization potential $P(x)$ and a mass operator or exchange potential $M(w)$. (The exchange potential is nonlocal, non-Hermitian and energy dependent.)

The polarization potential $P(x)$ is the classical field due to the average distribution of electrons and may be written in the closed form

$$P(x) = -e\int v(x-x')\rho(x')d^3x', \tag{12}$$

where $\rho(x)$ is the number density of electrons at the point x, the sum of the average or background density and the induced density.

In terms of Feynman diagrams, $P(x)$ is given by the totality of polarization insertions at a single point in an electron line.

The exchange potential is determined by the remaining class of insertions. The lowest order expression for $M(w)$ [see Eq. (40)] is the familiar exchange potential first derived by Bloch.[20]

As is well known, lowest order expressions for the induced charge density, in an approximation linear in the external potential, can be written down on the basis of various approximations to the static dielectric

[14] J. Greenstein, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1958), Vol. 50. I wish to thank Professor Greenstein for an informative discussion of problems connected with dense astronomical systems.

[15] S. Chandrasekhar, *An Introduction to the Study of Stellar Structure* (University of Chicago Press, Chicago, 1939), especially Chap. 11.

[16] We ignore here the complication caused by the shift of the chemical potential which may be remedied by shifting the unperturbed energies and performing the appropriate "mass renormalization" subtractions. See J. Luttinger and J. Ward, Phys. Rev. 118, 1570 (1960); reference 12; and footnote 52 of I.

[17] For some of the results obtained here, however, the restriction (10b) may be dropped (see Sec. 4).

[18] A. Glick and R. Ferrell, Ann. Phys. (New York) 11, 359 (1960).

[19] J. Schwinger, Proc. Natl. Acad. Sci. U. S. 37, 452, 455 (1951).

[20] F. Bloch, Z. Physik 57, 545 (1929). See also H. Bethe, in *Handbuch der Physik*, edited by S. Flügge (Verlag Julius Springer, Berlin, 1933), Vol. 24, Part 2, p. 484, and reference 10.

constant of the electron gas.[21–23,5] More recently, Langer and Vosko[11] have derived these expressions within the context of the exact nonlinear field theory.

In the simplest of these approximations, commonly known as the pair approximation, the momentum space transform of the induced number density, $\rho_i(q^2)$, takes the form

$$\rho_i(q^2)=Z\beta b_1(q^2)/[q^2+\beta b_1(q^2)], \tag{13}$$

where

$$b_1(q^2)=\frac{2}{\pi}\left[1+\frac{1}{q}\left(1-\frac{q^2}{4}\right)\ln\left|\frac{1+q/2}{1-q/2}\right|\right], \tag{14}$$

and the Fourier transform has been normalized according to the relation

$$f(q)=\int f(x)e^{iqx}d^3x. \tag{15}$$

Roughly speaking, the corresponding charge density in position space is of the form associated with a screened Coulomb potential. Langer and Vosko,[11] however, made the important observation that the logarithmic singularity of $\rho_i(q^2)$ at the momentum transfer $q=2$ (twice the Fermi momentum) gives rise to a small (of order β) oscillatory long-range behavior of the induced density in position space of the form ($R\equiv|x|$) (see Lighthill[24]):

$$\rho(x)\sim\beta\left\{a(\beta)\frac{\cos 2R}{R^3}+b(\beta)\frac{\sin 2R}{R^4}(\ln R+c)\right\}. \tag{16}$$

On the same grounds,[24] the polarization potential, $P(x)$, must also have this asymptotic behavior.

In the presence of an attractive external potential, a new type of single-particle excitation is expected to enter. This is a "bound hole" localized around the source and associated with a bound single-electron energy level occupied in the ground state. The real and imaginary parts of discrete complex eigenvalues of the *homogeneous* Schwinger equation correspond to the energies and lifetimes of such bound holes.[2–8]

As a physical example of such a bound hole excitation we cite the case of orbital electron capture by a nucleus in a dense medium.

Since the effective potential, $V+\Sigma(w)$, is of shielded rather than pure Coulombic form, the number of bound levels should be finite rather than infinite. Since the range of the shielded potential decreases with increasing particle density, the number of bound states should decrease in this process and one anticipates that there will occur a limiting density, for given atomic number Z, beyond which no bound states are possible. This type of behavior would be consistent with the qualitative phenomena of "pressure ionization" in dense matter.[25–27]

The present analysis confirms the above conjectures though, because of the mathematical complexity of the problem, they cannot be regarded as rigorously established.

These questions are considered quantitatively in Sec. 3 where lowest order expressions for the self-energy operator are given. We derive also lowest order expressions for the lifetimes of bound holes.

In Sec. 4, rough numerical estimates are given for the level width of bound holes over a considerably wider range of densities and values of Z than in the previous limiting case. It turns out that away from the limit of very small binding energies (relative to the Fermi energy) the plasmon-emission process gives an important contribution to the level width of bound holes.

A summary and discussion of the results is given in Sec. 5. In that section we also consider briefly some physical applications of the results obtained here for the single-particle excitation spectrum.

2. PROPERTIES OF INDUCED CHARGE DENSITY

We consider first some general properties of the induced charge density and the corresponding polarization potential of the Schwinger equation. We include a brief discussion of the derivation, by our methods, of the pair-approximation result (13).

Let us first dispose of the complication of the uniform positive background. Actually, we should have included in our Feynman diagrams external-potential vertices due to the uniform background. Now, since the density of the unperturbed system is the same as that of the background, the vertex due to the latter [Fig. 1(a)] is cancelled by the lowest order polarization diagram [Fig. 1(b)]. Furthermore, since the density of the interacting and unperturbed systems is the same, in the absence of the source, the lowest order polarization diagram has, in fact, the same value as the totality of source-free polarization diagrams at the same point [Fig. 1(c)]. Thus, we may eliminate the uniform background from consideration provided that we adopt

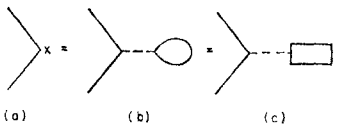

FIG. 1. Diagrams illustrating the cancellation of the effect of the uniform background. The cross represents the potential due to the uniform background.

[21] J. Lindhard, Kgl. Danske Videnskab. Selskab. Mat.-fys. Medd. **28**, 8 (1954).
[22] P. Nozières and D. Pines, Nuovo Cimento **9**, 470 (1958).
[23] J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957); **A243**, 336 (1957); **A244**, 199 (1958).
[24] M. J. Lighthill, *Fourier Analysis and Generalized Functions* (Cambridge University Press, New York, 1960), Chap. 4.
[25] J. C. Slater and H. M. Krutter, Phys. Rev. **47**, 559 (1935).
[26] P. M. Morse, Astrophys. J. **92**, 27 (1940).
[27] E. Schatzman, reference 13, Chap. 4.

the following simple convention.[28] *All vertices due to the uniform background and simultaneously all source-free polarization insertions in an electron line are to be ignored.*

This convention, of course, is equivalent to subtracting out the unperturbed charge density, ρ_0, from the total density ρ in all expressions involving ρ, a type of renormalization procedure which is appropriate to this problem.

We turn now to a consideration of the induced charge density. The direct potential, defined here as the sum of the external and polarization potentials, can be written in the operator form

$$V_d = K^{-1}V, \tag{17}$$

where V, as usual, is the external potential.

More explicitly, we have

$$V_d(x) = \int d^3x'\, K^{-1}(x,x')V(x'). \tag{18}$$

Or, in momentum space,

$$V_d(q) = \int d^3q'\, K^{-1}(q,q')V(q'). \tag{19}$$

K^{-1} is itself a functional of the external potential V. The inverse operator K will be called the generalized dielectric constant. If the external potential is spherically symmetric, it is easy to see that K is rotationally invariant. In the limit $Z \to 0$, K is diagonal in momentum space and $K(x,x')$ is a function of $(x-x')^2$.

The quantity $K^{-1}(q,q')$ corresponds to the totality of polarization diagrams with initial dotted line labeled by q and a final "source" vertex $V(q')$ as illustrated in Fig. 2, in addition to a simple vertex corresponding to the external potential alone. These polarization diagrams can be broken down into diagrams involving repeated insertions in dotted lines of strongly connected diagrams, as in the example of Fig. 2(b). The totality of such strongly connected insertions will be called Q.

It is easy to verify that Q is a Hermitian operator.

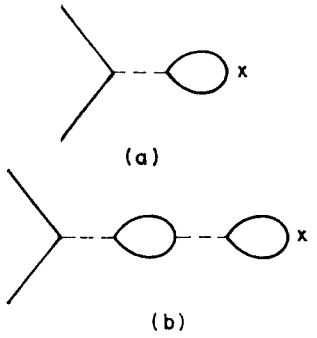

FIG. 2. Polarization diagrams with (a) a single strongly connected insertion, (b) two strongly connected insertions.

[28] I wish to thank Professor M. Ruderman for the idea of looking at the cancellation in this simple way.

For spherically symmetric external potential, Q, like K, is rotationally invariant. Furthermore, Q is a real symmetric matrix in position space. This last property guarantees the reality of the induced charge density when using the dielectric constant approach.[29]

For suitably normalized Q one has then for K^{-1} the operator expansion

$$K^{-1} = 1 - vQ + vQvQ - vQvQvQ + \cdots, \tag{20}$$

whose sum is

$$K^{-1} = (1+vQ)^{-1}. \tag{21}$$

Thus, the generalized dielectric constant has the form

$$K = 1 + vQ. \tag{22}$$

From (17) and (22) one can write also

$$(1+vQ)V_d = V, \tag{23}$$

or

$$(v^{-1}+Q)V_d = v^{-1}V = -Z. \tag{24}$$

The induced number density ρ_i is obtained by taking the negative Laplacian of the induced potential. Thus, we obtain from (17) and (21)

$$\langle q|\rho_i\rangle = q^2\langle q|\,(K^{-1}-1)V\rangle, \tag{25}$$

$$\langle q|\rho_i\rangle = -q^2\left\langle q\left|\frac{vQ}{1+vQ}V\right.\right\rangle. \tag{26}$$

Let us consider first the subclass $\bar{Q}$ of Q consisting of source-free diagrams. Since $\bar{Q}$ is diagonal in momentum space, (26) becomes simply

$$\langle q|\rho_i\rangle = -\frac{q^2v(q)\bar{Q}(q)}{1+v(q)\bar{Q}(q)}\langle q|V\rangle. \tag{27}$$

Since $v(q) = 4\pi\beta/q^2$ and $V(q) = -Zv(q)$, we see from (27) that

$$\rho_i(q) = 4\pi\beta Z\bar{Q}(q)/[q^2 + 4\pi\beta\bar{Q}(q)], \tag{28}$$

where the Fourier transforms $\rho(q)$, $V(q)$ are normalized as usual according to the relation

$$f(q) = \int f(x)e^{iq\cdot x}d^3x. \tag{29}$$

Assuming that $\bar{Q}(q)$ approaches a limit different from zero as $q \to 0$, as we shall see is, indeed, the case, we

[29] These properties of Q follow from similar properties of the zero-frequency transform, D, of the "density propagator" $D(t-t')$. The latter is defined by $\langle x|\,D(t-t')\,|x'\rangle = \langle T\rho(x,t)\rho(x',t')\rangle$ where $\rho(x) \equiv \psi^\dagger(x)\psi(x)$.

Except for a real constant of proportionality, we have, namely, $Q = D(1+vD)^{-1} = D - DvD + \cdots$. Note also that $K^{-1} = 1 + vD$.

The stated properties for D follow from the representation

$$\langle x|\,D\,|x'\rangle = c\lim_{\sigma\to 0}\int_{-\infty}^{\infty} d\tau\, e^{-\sigma|\tau|}\{\theta(\tau)\langle\rho(x)e^{i(H-E)\tau}\rho(x')\rangle + \theta(-\tau)\langle\rho(x')e^{-i(H-E)\tau}\rho(x)\rangle\},$$

where c is a real constant.

FIG. 3. Feynman diagram for $Q_0(q,w)$.

note, in particular, from (28) and (29) that

$$\rho_i(0)=\int \rho_i(x)d^3x=Z. \tag{30}$$

This expresses the fact that the total induced charge exactly cancels the source charge, leaving the system, in this approximation at least, electrically neutral. We must expect that (30) holds true in the exact theory also since charge neutrality is a necessary condition for the electrostatic stability of the ground state.[30] We shall return to this point later.

The derivation of the neutrality condition (30) points up the fact, characteristic of the long-range Coulomb interaction, that the conventional perturbation expansion of ρ in powers of β, which would regenerate a series of the type (20), is invalid for $q^2\lesssim\beta$. As is well known, the terms of this series exhibit successively stronger "infrared" divergences at $q^2=0$ which cancel when the sum is taken. A correct perturbative procedure is, instead, to make the same lowest order approximation to Q in both numerator and denominator of (26) leaving the denominator unexpanded.

The lowest order expression for ρ_i, in the above sense is obtained by making the replacement $\tilde{Q}\to Q_0(q)$ in (27) where $Q_0(q)$ corresponds to the limit $w\to 0$ of the simple "bubble" diagram of Fig. 3, denoted by $Q_0(q,w)$.

The correctly normalized expression for $Q_0(q,w)$ is

$$Q_0(q,w)=\frac{2i}{(2\pi)^4}\int d^3k dw'\, G_0(k,w')G_0(q+k,w+w'). \tag{31}$$

For w different from zero Q_0 has an imaginary part which contributes to the lowest order lifetime of a single-particle excitation, as discussed in the next section. According to Dubois[5] and Lindhardt,[21] $Q_0(q,w)$ has the following value:

$$\begin{aligned}\mathrm{Re}Q_0(q,qu)&=\frac{1}{2\pi^2}\left\{1+\frac{1}{2q}\left[1-\left(u+\frac{q}{2}\right)^2\right]\ln\left[\frac{(u+q/2)+1}{(u+q/2)-1}\right]\right.\\&\left.-\frac{1}{2q}\left[1-\left(u-\frac{q}{2}\right)^2\right]\ln\left[\frac{(u-q/2)+1}{(u-q/2)-1}\right]\right\},\end{aligned} \tag{32}$$

$$\mathrm{Im}Q_0(q,qu)=\frac{1}{2\pi}|u|,\quad |u|+\frac{q}{2}<1, \tag{33a}$$

$$=\frac{1}{4\pi}\frac{1}{q}\left\{1-\left(|u|-\frac{q}{2}\right)^2\right\},\quad \left|\frac{q}{2}-|u|\right|<1<\frac{q}{2}+|u|, \tag{33b}$$

$$=0,\quad \left|\frac{q}{2}-|u|\right|>1. \tag{33c}$$

In the limit $w\to 0$, the imaginary part of Q_0 disappears and one obtains from (32)

$$4\pi Q_0(q)=b_1(q^2)=\frac{2}{\pi}\left[1+\frac{1}{q}\left(1-\frac{q^2}{4}\right)\ln\left|\frac{1+q/2}{1-q/2}\right|\right]. \tag{34}$$

Substituting this into (28) we obtain the familiar "pair-approximation" result (13) for the induced charge density.

Before proceeding to the discussion of single-particle excitations we return briefly to the question of the neutrality of the system in the exact theory as pledged earlier. We have already seen, formula (30), that neutrality is achieved in the linear approximation in which Q is replaced by the totality of source-free diagrams.

Let us separate out the source-free approximation by writing Q and V_d in the form

$$Q=\tilde{Q}+Q',\quad V_d=\tilde{V}+V', \tag{35}$$

where $\tilde{V}$, proportional to Z, is the solution of (23) with $Q=\tilde{Q}$. V' involves higher powers of Z. The lowest order diagram for Q' is shown in Fig. 4.

From (23) one easily derives the following equation for V' in terms of $\tilde{Q}$, $\tilde{V}$, and Q':

$$V'=-(v^{-1}+Q)^{-1}Q'\tilde{V}. \tag{36}$$

In lowest order, corresponding to the approximation Q_0 for Q, $\tilde{V}$ has the general form

$$\tilde{V}_0(q)=\mathrm{const}/[q^2+\beta b_1(q)]=b'(q^2), \tag{37}$$

where b_1 and b' are bounded functions of q^2 [the exact form of b_1 is given in (34)]. We note also from (34) that $Q_0(q^2)$ is a bounded function of q^2.

It is now easy to show from (36) that the induced charge density corresponding to V' will not affect the neutrality relation (30) provided that suitable boundedness requirements in momentum space are imposed on

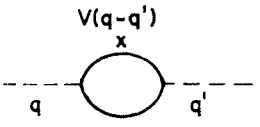

FIG. 4. Lowest order Feynman diagram for Q'.

[30] At first sight the requirement of charge neutrality may be puzzling since one imagines that an extra charge Ze has been inserted (adiabatically) into an enclosed system which was originally neutral. However, it must be kept in mind that in calculating local properties, such as the density, we are really dealing with a limiting process in which the volume of the container becomes arbitrarily large while attention is focussed on a fixed point of space. In this case, boundary effects do not appear in the final result and, in particular, charge neutrality will be preserved.

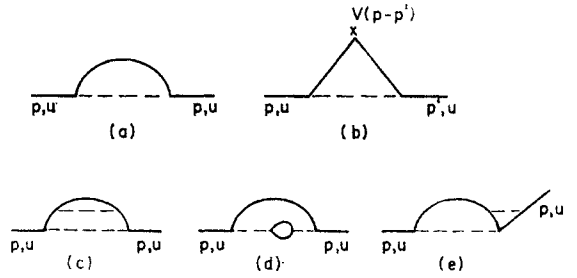

FIG. 5. Lowest order mass operator diagrams.

$\bar{Q}$, $\bar{V}$, and Q' which are suggested by the lowest order results (34) and (37).

Let us assume, for example, that the *exact* $\bar{Q}(q)$ is a bounded function with $\bar{Q}(0)\neq 0$. It then follows that the exact $\bar{V}(q)$ can be expressed as a bounded function of q^2 times the factor $(q^2+c)^{-1}$ for some positive $c\neq 0$:

$$\bar{V}(q^2)=b(q^2)(q^2+c)^{-1}. \tag{38}$$

The same is true, of course, of a factor $(v^{-1}+\bar{Q})^{-1}$. Let us assume now that a series expansion of $(v^{-1}+Q)^{-1}$ about $(v^{-1}+\bar{Q})^{-1}$ has the usual desirable convergence properties. Then (as one easily sees by induction on the nth term of the expansion) in order for the total charge induced by V' to be zero, it is sufficient to assume in addition that Q' has the property

$$\int \frac{d^3q'}{q'^2+c}|Q'(q,q')|=b(q^2), \tag{39}$$

for all positive $c\neq 0$, where $b(q^2)$, as usual, denotes a bounded function of its argument.

This is true, for example, if $Q'(q,q')$ can be expressed as a bounded function times $[(q-q')^2+c]^{-1}$, where c is a positive or zero constant. This Coulomb type of dominating behavior is suggested by the lowest order diagram for Q'. (See Fig. 4.)

While the verification of these properties is a difficult matter, even within the framework of perturbation theory, it is nevertheless satisfying that plausible conditions of this kind, guaranteeing charge neutrality for the exact theory, can be formulated.

3. LOWEST ORDER EQUATION FOR SINGLE-PARTICLE EXCITATIONS

We shall now consider in some detail the lowest order equation describing single-particle excitations. This is obtained by using the pair approximation (13) for the electron density in the Schwinger equation (11) together with the lowest order "mass operator" term corresponding to diagram (a) of Fig. 5.

Diagrams (b) through (e) of Fig. 5 are formally of one higher order in β or $Z\beta$ than diagram (a), due to the presence of an additional interaction line or an external potential. It is not difficult to show that diagrams (a), (b), and (c) do not have imaginary parts. Thus, in particular, the imaginary part of the mass operator enters only in order β^2.[31] This circumstance permits one to neglect the non-Hermitian part of the effective Hamiltonian in lowest order. That is, single-particle excitations are stable in lowest order.

Diagram (a) is easily evaluated [see formula (77) of I]. The resulting expression is, in fact, identical with the familiar lowest order exchange contribution to the single-particle energies in the source-free case.[20]

$$\langle p|M_a|p'\rangle=M_a(p)\delta^3(p-p'), \tag{40}$$

$$M_a(p)=-\beta b_2(p^2), \tag{41}$$

$$b_2(p^2)=\frac{1}{2\pi^2}\int\frac{d^3k}{k^2}\theta[1-|p-k|]$$

$$=\frac{2}{\pi}\left[\frac{1-p^2}{4p}\ln\left|\frac{1+p}{1-p}\right|+\tfrac{1}{2}\right]. \tag{42}$$

As before, $b(x)$ denotes a *bounded* function of x.[32] Note that M_a is independent of w. $M_a(0)$, like the mass renormalization term in quantum electrodynamics, which it *formally* resembles, represents a constant (state-independent) shift in the single-particle energies which is the same for free and bound electrons in the medium. Unlike the Q.E.D. case, however, this shift has observable physical consequences.[33]

According to the foregoing discussion, the complete lowest order equation for single-particle excitations reads as follows:

$$\{w'-p^2/2+\beta[b_2(p^2)-b_2(0)]\}\psi_w(p)$$

$$=\frac{Z\beta}{2\pi^2}\int\frac{d^3p'}{q^2+\beta b_1(q^2)}\psi_w(p'), \tag{43}$$

where

$$w'=w+\beta b_2(0), \tag{44}$$

and $b_1(q^2)$, $b_2(p^2)$ are given by (13) and (42). This equation describes an independent particle model in which single electrons move in an effective potential consisting of a direct potential, determined by the pair approximation for the total density of electrons, plus a momentum term which in a quadratic approximation simply changes the effective mass of the electron (and shifts all energies by a constant amount).

Of particular interest are the bound-state excitations, if any, associated with discrete negative values of w'. It is physically clear that these excitations must correspond to bound *holes* rather than particles. To confirm the hole character of the excitations and estimate the lifetime of the holes, one must determine

[31] This formal estimate is confirmed by the detailed calculations given later, which show that the leading order is in fact $\beta^2\ln\beta$.

[32] It is interesting to note that the functional forms of b_2, and b_1, are related: $b_2(x^2)=\frac{1}{2}b_1((2x)^2)$.

[33] The shift should enter, for example, into the energetics of electron capture by a nucleus in a dense medium.

the sign and magnitude of the imaginary part of the effective Hamiltonian. We shall return to this point later.

To see whether bound states occur, it is convenient to introduce a further approximation in which the bounded functions $b_1(q^2)$ and $b_2(p^2)$ are replaced by their values at zero argument. (The nature of this approximation will be investigated more closely later on.) The direct potential now becomes a Yukawa potential and the mass operator term simply reduces to a constant. Thus, in this approximation, Eq. (43) becomes, after taking the position space transform,

$$\{w'-p^2/2-(\beta Z/r)\exp[-(4\beta/\pi)^{1/2}r]\}\psi_0(r)=0, \quad (45)$$

where ψ_0 denotes the approximate wave function.

The radial equation corresponding to (45) is of the general form ($\phi=r\psi$), for S states:

$$(d^2\phi/dr^2)+[a+b(e^{-r}/r)]\phi=0. \quad (46)$$

This equation has been investigated by a number of authors in connection with the two nucleon problem[34,35] and the problem of Debye shielding in plasmas.[36,37] It has been noted that unless the parameter b exceeds a certain critical value there is no bound state. According to the numerical work of Hulthén and Laurikainen,[34] the condition for binding is

$$b\geq 1.68. \quad (47)$$

This condition, translated for Eq. (45) reads

$$Z^2\beta\geq(1/\pi)(1.68)^2\cong 0.898. \quad (48)$$

Thus, if the density is too high, binding is destroyed. The condition (48) is in competition with the condition (10) for the validity of our perturbation expansion. We see that for both conditions to be met, the density (or Z) must lie in the range determined by

$$0.898Z^{-2}\leq\beta\lesssim Z^{-1}. \quad (49)$$

It should be emphasized that the Yukawa approximation is not adequate for the wave function either very close to or very far from the source. This is because the approximation disregards the high momentum components of the effective Hamiltonian and also the logarithmic singularities, in momentum space, of the direct potential and the mass operator due to the Fermi momentum cutoff.

In this connection, it is interesting to note that the logarithmic singularity at the Fermi momentum of the *exchange* potential may be expected to give rise to an oscillating long-range behavior, of order β, similar to (16), for the wave functions of the discrete spectrum. Thus, the bound-state wave functions are considerably more diffuse than in the Yukawa approximation.

Nevertheless, the Yukawa approximation is, in a certain sense, a well-defined lowest order limit of (43). We have in mind a particular limit procedure in which β tends to zero while $Z^2\beta$ is held fixed. (Under these circumstances $Z\beta$ will also approach zero.)

To show this formally, let us perform the scale transformation

$$p\rightarrow\beta Z p, \quad r\rightarrow(\beta Z)^{-1}r. \quad (50)$$

The "Schrödinger" equation (43) then becomes

$$[w_s'-p^2/2+\gamma^{-1}[b_2(\beta\gamma p^2)-b_2(0)]]\psi_s(p)$$
$$=\frac{1}{2\pi^2}\int\frac{d^3p'}{q^2+\gamma^{-1}[b_1(\beta\gamma q^2)]}\psi_s(p'), \quad (51)$$

where

$$\gamma\equiv\beta Z^2, \quad (52)$$

and

$$w_s'=[w+\beta b_2(0)]/(\beta Z)^2=w_s+\gamma^{-1}b_2(0). \quad (53)$$

Here, ψ_s is the scaled wave function and $w_s=w/(\beta Z)^2$.

If, now, β and $Z\beta$ approach zero while γ is held fixed, we obtain in the limit the equation

$$[w_s'-p^2/2]\psi_s(p)=\frac{1}{2\pi^2}\int\frac{d^3p'}{q^2+4(\pi\gamma)^{-1}}\psi_s(p'). \quad (54)$$

In position space this is

$$\{w_s'-p^2/2-(1/r)\exp[-(4/\pi\gamma)^{1/2}r]\}\psi_s(r)=0. \quad (55)$$

Equation (55) is, indeed, the scaled form of (45).

It is useful to note the conversion formula giving w in rydbergs in terms of the dimensionless quantity w_s in (54):

$$w=2Z^2w_s \text{ Ry}. \quad (56)$$

We observe also that the continuum starts at $w_s'=0$, which corresponds, from (53), to a value of w_s given by

$$w_{s,0}=-\gamma^{-1}b_2(0)=-(2/\pi)\gamma^{-1}. \quad (57)$$

We see that the limit of the continuum of single-particle energies is "pushed down" by the interaction (see references 25–27).

We have shown above that the Yukawa approximation (55) is a formal limit of Eq. (51) as β and $Z\beta$ approach zero with $\gamma=Z^2\beta$ fixed. It is legitimate to inquire now as to the validity of this formal limiting process.

Unfortunately, a rigorous mathematical investigation of this important point is a difficult matter, beyond the scope of the present paper, and we must content ourselves with comments of a heuristic nature.[38]

We restrict attention to the discrete spectrum since this is the simpler case to discuss. It is, in fact, mis-

[34] L. Hulthén and K. V. Laurikiainen, Revs. Modern Phys. 23, 1 (1951). I wish to thank Dr. H. Nickle for bringing this reference to my attention.

[35] J. Blatt and V. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), Chap. 2. I would like to thank Dr. L. Rosenberg for informing me of this reference.

[36] G. Ecker and W. Weizel, Ann. Physik 17, 126 (1956).

[37] G. Harris, Phys. Rev. 125, 1131 (1962).

[38] This point could be settled by numerically solving Eq. (51) for a range of values of β and γ.

leading to talk about limit processes for continuum wave functions outside the context of particular matrix elements of interest.

For the eigenvalues and eigenfunctions of the discrete spectrum, it is reasonable to assume that the above formal limit process is valid. We refer here to the "scaled" form (51) of the original Eq. (43).

First, we note that there is no difficulty in formally applying ordinary lowest order perturbation theory for the discrete eigenvalues and eigenfunctions of (51) and that this gives results in agreement with the above assumption. This, however, is not a very reliable test.[39]

In order to rigorously establish the validity of the passage from (51) to (54) for a region of values of w_s' about a single point of the unperturbed discrete spectrum it is sufficient to show, according to a theorem of Riesz and Sz-Nagy, that the perturbed "Hamiltonian" operator approaches the unperturbed one "relatively uniformly" as the perturbation parameter (in our case the parameter β) approaches zero.[40]

This property of relative uniform convergence is apparently assured in our problem by the bounded nature of the functions b_1 and b_2 and the good boundedness properties in momentum space of the Yukawa potential.[41]

It should be noted that the source-induced Yukawa potential which we have justified here by a formal limiting process has long been known and used—for the impurity problem—in the electron theory of metals, where its introduction has been based on a linearized Thomas-Fermi treatment. (For a recent discussion, see Pines.[42] The original derivation is apparently due to Mott.[43])

This contact with the semiclassical Fermi-Thomas method permits one to ascribe a more extended region of validity to the Yukawa potential than emerges from the present formal analysis.

An important condition for the validity of the semiclassical analysis is that the average potential due to the source be much less than the Fermi energy. We might guess then that our special formal limiting process in which $\beta \to 0$ with γ fixed is actually valid in the case of *weak binding*—and high densities—that is, when the binding energy of the bound state in question is sufficiently small compared to the Fermi energy. This speculation is strengthened by the following level-width estimates, particularly of Sec. 4, where at the same time a more precise definition of the "weak binding" limit is provided.

Calculation of Level Width

Let us now consider in more detail the imaginary part Γ of the eigenvalues of the exact Eq. (11) in the bound-state case. We must show, in particular, that the sign of Γ is that appropriate to holes rather than particles. Furthermore, if these bound excitations are to be discrete, Γ must be smaller, though not necessarily much smaller, than the *separation* between bound levels.[44]

Actually, the question of the sign of Γ in perturbation theory can be answered on general grounds since it is known (see I, Sec. 2) that the non-Hermitian part of $\Sigma(w)$ is a negative *operator* if $w<\mu$ and, in particular, if w is negative. (Here, μ is the chemical potential.) As is easily seen this property must be true also in lowest order perturbation theory. Of course, explicit calculation must give the same result.

As we have already remarked, the lowest order imaginary part is due to diagrams (d) and (e) of Fig. 5. Thus, Γ is given in the lowest order by the imaginary parts, Γ_d and Γ_e, of the expectation values of M_d and M_e using wave functions that are solutions of Eq. (43).

Actually, the familiar problem of the "infrared divergence" at low momentum transfer forces us to consider along with diagram (d) diagrams with an arbitrary number of bubble insertions. Since the lowest order mass-operator diagram has no imaginary part, we can add this to M_d without affecting Γ_d. If we do this, then the net effect of all these bubble insertions is to replace the interaction, v, of the lowest order diagram by the "effective interaction" vK_0^{-1} where $K_0=1+vQ_0$ is the time-dependent dielectric constant in the pair approximation.

Physically, diagrams M_d and M_e correspond to the creation of electron-hole pairs or plasmons in the decay of a single-particle (hole) excitation to a lower state of excitation. This has been shown explicitly by Dubois, who has introduced effective momentum dependent coupling constants for these modes of decay.[45] (See also Quinn and Ferrell,[46] and Quinn.[47])

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[39] It gives the wrong answer, for example, in the case of the Stark effect.

[40] F. Riesz and R. Sz-Nagy, *Functional Analysis* (Frederick Ungar, New York, 1955), translation of 2nd French ed., Chap. 9, p. 372. The operator sequence A_n is said to converge relatively uniformly to the (Hermitian) operator A if

$$\text{l.u.b.}_f \frac{\|(A-A_n)f\|}{\|f\|+\|Af\|} \to 0$$

where l.u.b. means least upper bound and where f ranges over the Hilbert space.

[41] We argue roughly that the numerator of the relevant ratio (see footnote 40) approaches zero with β except for functions f concentrated in a high momentum region of order $1/\beta$. However, for these f, the denominator becomes very large, like β^{-2}, and, therefore, the ratio still approaches zero (like β^2).

[42] D. Pines, in Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1955), Vol. 1.

[43] N. F. Mott and H. Jones, *The Theory of Metals and Alloys* (Oxford University Press, New York, 1936), p. 87.

[44] This is a physical criterion corresponding to the requirement that the linewidth of the emission spectrum for a transition between bound holes be less than the transition energy. We recall that $e^{-2|\Gamma|t}$ is the probability for decay of the excitation in time t. See I, Sec. 2.

[45] D. Dubois, reference 5. See especially formulas (3.10), (3.12), (3.13), (1.14) and (1.15) of the second article. A number of misprints in these formulas have been corrected here.

[46] J. Quinn and R. Ferrell, reference 10.

[47] J. Quinn, Phys. Rev. **126**, 1453 (1962).

Dubois has pointed out also that M_e is the exchange interference correction to the pair portion of M_d. The plasmon is stable in the pair approximation and the plasmon decay mode arises mathematically as a delta function contribution to Γ_d from a pole of the inverse dielectric constant at the plasma frequency.

In writing the decay probabilities in this form, one adopts an S matrix and Feynman diagram point of view conventional in relativistic field theory. The initial state is a hole, in our case a bound hole, and the final state is a free hole plus either an electron-hole pair or a plasmon. Of course, in this many-particle case all initial and final states are actually unstable. The pair "coupling constant" $g(p,q)$ given below in (64) is essentially the momentum-energy transform of the time-dependent effective interaction, analogous to the photon propagator of electrodynamics. The plasmon, treated as a boson, is coupled directly to the electron field by the coupling constant $g_p(q)$ given in (66), which arises from the residue of the pole of the effective interaction at the plasma frequency.

Since M_d and M_e are diagonal in momentum one can write Γ_d and Γ_e as weighted averages, with weight function $|\psi_w(p)|^2$ of the transition rate for the decay of source-free hole excitations of definite momentum, p. One can then simply take over Dubois' expressions for the latter. The only unusual point in this regard is that the energy, $-w$, of the "free" hole excitation of momentum p is positive, since we are actually dealing with a hole in a bound state. However, momentum and energy conservation apply just as in the true free-excitation case.

Thus, we have

$$\Gamma_i=\int d^3p\ |\psi_w(p)|^2\Gamma_i(p), \quad i=d,\ e. \tag{58}$$

The transition rate $\Gamma_i(p)$ can be written as an integral of a differential transition rate $\Gamma_i(p,q)$ corresponding to a definite momentum transfer, q, upon de-excitation of the hole to a (true) free-hole excitation with momentum $p-q$:

$$\Gamma_i(p)=\int d^3q\,\theta[1-|p-q|]\Gamma_i(p,q). \tag{59}$$

For $\Gamma_i(p,q)$ we take over bodily, with only minor alterations, the expressions and terminology of Dubois[45]:

$$\Gamma_{d,\mathrm{pr}}(p,q)=\frac{1}{8\pi^2}g^2(p,q)\int_{|p_1|<1<|p_1+q|}d^3p_1 \times\delta(\tfrac{1}{2}q^2+q\cdot p_1-\Delta), \tag{60}$$

$$\Gamma_e(p,q)=\frac{1}{8\pi^2}(-\tfrac{1}{2})g(p,q)\int_{|p_1|<1<|p_1+q|}d^3p_1 \times g(p,\bar{q})\delta(\tfrac{1}{2}q^2+q\cdot p_1-\Delta). \tag{61}$$

Here $\bar{q}$ is the "exchange momentum transfer" (for *holes*).

$$\bar{q}\equiv p_1-p, \tag{62}$$

$$\Gamma_{d,\mathrm{pl}}(p,q)=\frac{1}{8\pi^2}g_p^2(q)\frac{\delta(\Delta-\Lambda(q))}{2\Lambda(q)}\theta(q_c-q). \tag{63}$$

The coupling constants for pair creation $g(p,q)$ and $g(p,\bar{q})$ are given by

$$(2\pi)^{-3}g^2(p,q)=\tfrac{1}{2}(\beta/\pi^2q^2)^2|K_0(q,\Delta)|^{-2}, \tag{64}$$

where K_0 as before is the dielectric constant in the pair approximation.

In the formulas above, Δ is the energy transfer in the de-excitation of the hole:

$$\Delta=|w'|+(p-q)^2/2. \tag{65}$$

Here, we have noted that since the "mass renormalization" constant w_0 of formula (57) affects both initial and final hole excitation states only the "renormalized" energy w' enters in the expression for energy transfer.

In the approximation we are considering, K_0 may be replaced by unity in the expression for Γ_e since there is no infrared divergence at low q values for the exchange correction.

In formula (63), $g_p(q)$ is the plasmon coupling constant and $\Lambda(q)$ is the momentum-dependent plasmon frequency. According to Dubois[45]

$$\frac{g_p^2(q)}{(2\pi)^3}=\frac{3\Lambda_p^4}{8\pi q^2}\left[1+\frac{5}{9}\frac{q^2}{\Lambda_p^2}+\cdots\right], \tag{66}$$

$$\Lambda^2(q)=\Lambda_p^2\left[1+\frac{12}{5}\frac{q^2}{\Lambda_p^2}+\cdots\right], \tag{67}$$

where Λ_p, the classical plasma frequency, is given, as usual, by

$$\Lambda_p=(4\beta/3\pi)^{1/2}. \tag{68}$$

q_c is the plasmon cutoff momentum determined by the equation

$$\Lambda(q_c)=\tfrac{1}{2}q_c^2+q_c. \tag{69}$$

An alternative closed expression for $\Gamma_{d,\mathrm{pr}}(p,q)$ may also be given and is often more convenient[48]:

$$\Gamma_{d,\mathrm{pr}}(p,q)=\frac{2}{\pi}\frac{\beta^2\mathrm{Im}Q_0(q,\Delta)}{|q^2+4\pi\beta Q_0(q,\Delta)|^2}. \tag{70}$$

The real and imaginary parts of Q_0 are given in formulas (32) and (33).

An exact analytic evaluation of Γ_d and Γ_e is not possible. Let us consider first the special lowest order approximation defined previously in which β and Z

[48] Compare formulas (3.6) and (3.20) of Dubois, reference 5. Dubois' derivation of (3.20) is valid also in the present bound-state case. Let us note that these closed expressions can be used to derive expressions (60), (61), and (63) without using the S-matrix approach.

approach zero while $\gamma \equiv Z^2\beta$ is held fixed at a value greater than that needed for binding. We shall call this the fixed-γ approximation.

In the fixed-γ approximation the (relative) binding energy, w, is of order β as one sees from Eqs. (53) and (54). Similarly, the wave function "selects" (relative) momenta of order $\beta^{1/2}$. Thus, as $\beta \to 0$, the level width tends to a value appropriate to a source-free hole excitation of zero energy and momentum.

We shall consider only terms of order β^2 (or bigger) which is the nominal order of diagrams M_d and M_e (two vertices). Actually, Γ_d is of order $\beta^2 \ln\beta$ in the fixed approximation due to an infrared divergence at low q values.

On the other hand, it is not difficult to show that the plasmon decay mode is of higher order than β^2 in the fixed-γ approximation. Indeed, the energy-momentum relation of a plasmon forbids the decay of a strictly zero momentum and energy hole excitation to a lower state of excitation via the creation of a single plasmon. Even when one takes into account the distribution of momenta permitted by the wave function, this "phase-space suppression" turns out to be sufficient to make the plasmon decay mode of technically higher order in β than the pair contribution.[49]

After a short calculation, details of which are given in Appendix 1, we obtain the following lowest order results for the imaginary part of diagrams of the type M_d and M_e, in rydbergs[50]:

$$\tfrac{1}{2}\Gamma_d = [a \ln(1/\beta) + b] \text{ Ry}, \tag{71}$$

$$\tfrac{1}{2}\Gamma_e = c \text{ Ry}, \tag{72}$$

where

$$a = 1/\pi,$$
$$b = 1/\pi[-1 - \ln(4/\pi) + (\pi/2)\gamma(|w_s'| + \tfrac{1}{2}\langle p^2\rangle_\gamma)],$$
$$c = -\pi/24.$$

Here the symbol $\langle\ \rangle_\gamma$ denotes the expectation value with respect to scaled Yukawa-potential wave functions, solutions of (55), for fixed γ. Note that the constants a and c are independent of the bound state and are, in fact, the same as for a source-free excitation with $p = w = 0$.

For the total width of the excitation level in the fixed approximation one then obtains the result

$$\tfrac{1}{2}\Gamma = (1/\pi)[\ln(\pi/4\beta) - 1 - (\pi^2/24) + (\pi/2)\gamma(|w_s'| + \tfrac{1}{2}\langle p^2\rangle_\gamma)] \text{ Ry}. \tag{73}$$

We see that as the density increases indefinitely with γ held fixed, the absolute level width will approach infinity, like $\ln\beta$. Since from (56), with fixed γ, the binding energy is of order $1/\beta$ in absolute units (rydbergs), the bound-state level spacing Δw_n also approaches ∞ and in a manner such that the ratio $(\Gamma/\Delta w_n)$ approaches zero like $\beta \ln\beta$. This assures the existence of a discrete spectrum in the limit $\beta \to 0$ with γ fixed.

One must demand also that the first bound level be separated from the continuum by an amount greater than the linewidth. This is clearly also guaranteed in the limit $\beta \to 0$.

4. SOME NUMERICAL ESTIMATES

Although the result just given for the level width in the limit $\beta \to 0$ with γ fixed is interesting from the point of view of establishing with some degree of mathematical rigor the actual existence of the discrete spectrum of bound holes, the region of quantitative accuracy of this formula is limited to extremely high densities. It is, therefore, desirable to get a rough, necessarily nonrigorous, estimate of the level width for a wider range of densities. At the same time, this would permit one to assess more precisely the region of validity of the fixed γ result. To this rather lengthy task we devote the present section. We shall, of course, maintain the restriction that β be not (appreciably) larger than unity. However, we shall not take the limit $\beta \to 0$ and we shall not at first place a restriction on the magnitude of Z.

The approximation we shall use is the following. We shall assume that the major contribution to Γ for $\beta \lesssim 1$ comes from the expectation value of diagrams of type M_d with respect to an appropriately chosen wave function. Thus, in particular, we shall neglect the exchange interference diagram, M_e, the contribution of which has been shown to be small in the fixed-γ approximation.

We neglect also, as before, all higher order mass operator diagrams. Since $\beta \lesssim 1$, this is a reasonable first approximation for the class of diagrams not involving external source vertices. (Multiple emission processes are included in this set of discarded diagrams.) Diagrams with external source vertices, however, have factors of $Z\beta$ associated with them, which we do not assume to be necessarily small.

We justify dropping external source diagrams on the grounds that the influence of the source on the decay of the bound hole is primarily to determine, through the wave functions, a distribution of momenta for the decay of "free" holes.

Thus, we neglect, in particular, the possibility of the decay of the hole to *another bound state* and, more generally, we neglect the influence of the source on the final decay states and on the "coupling constants."[51]

Clearly, these approximations will be poor when the bound state in question approaches the corresponding state of the isolated atom that is when the binding

[49] A further justification of the neglect of the plasmon contribution to the linewidth to lowest order in β is given in the next section.

[50] The leading $\ln\beta$ term was announced at the Chicago meeting of the American Physical Society, November, 1961.

[51] An approximate expression for the decay rate to a lower bound state is given at the end of this section.

energy becomes significantly larger than the Fermi energy. Therefore, we do not expect our results to be particularly meaningful beyond the range $w \lesssim 1$.[52]

We come now to the question of the choice of wave function. We shall attempt to make as general a choice as possible since the exact form of the effective Schrödinger equation is unknown except in the limiting case previously considered.

Now, if one neglects the small nonlocal potential due to the mass operator, as we shall, the (radial) wave function falls off exponentially in position space for large distances with a range that depends only on the binding energy[53]

$$\psi_w(r) \underset{r\to\infty}{\sim} \exp[-(2w)^{1/2}r]. \tag{74}$$

The corresponding normalized momentum-space wave function is

$$(4\pi)^{1/2}\psi_w(p) = (32/\pi)^{1/2}[(2w)^{5/4}/(p^2+2w)^2]. \tag{75}$$

This is the wave function we shall adopt as a starting point in the present approximate calculation.[54] It has the interesting property that it depends only on the single parameter of the (relative) binding energy, w, rather than on the full set of parameters characterizing the exact solution, namely, β, Z and the quantum numbers of the bound state. Of course, it gives a rigorous solution for the ground state of the isolated hydrogen atom.[55]

Let us consider now in more detail the pair portion of Γ_d. After some elementary manipulations, Eqs. (70) and (59) for $\Gamma_{d,\mathrm{pr}}(p)$ can be put into the following form in which phase-space limitations are explicitly exhibited in the limits of integration:

$$\frac{\pi}{2}\Gamma_{d,\mathrm{pr}}(p) = \frac{2}{p}\int_{z_-}^{z_+} dz z^2 \times \int_{y_-}^{y_+} dy \frac{f_2(z,y)}{[z^2+\beta f_1(z,y)]^2+\beta^2 f_2^2(z,y)} \text{ Ry}. \tag{76}$$

Here we have introduced the standard variable $z=q/2$. The variable y is the energy transfer in the decay of the hole divided by the momentum transfer q. f_1 and f_2 are, respectively, the real and imaginary parts of Q_0 multiplied by π as given by formulas (32) and (33) with u replaced by y. The limits of integration $z_\pm$ and $y_\pm$ are defined by

$$z_+ = \min\left[\frac{p+1}{2}, \frac{1+(2+2w)^{1/2}}{2}\right], \tag{77a}$$

$$z_- = \max\left[\frac{p-1}{2}, \frac{w+\frac{1}{2}p^2}{2(1+p)}\right], \tag{77b}$$

$$y_+ = \min\left[\frac{w+\frac{1}{2}}{2z}; \frac{w+\frac{1}{2}(p+2z)^2}{2z}; z+1\right], \tag{77c}$$

$$y_- = \max\left[\frac{w+\frac{1}{2}(p+2z)^2}{2z}; z-1\right]. \tag{77d}$$

f_2 has the form (33a) for y less than $1-z$ and the form (33b) elsewhere.

In spite of the factor of $1/p$ in (76), this expression is finite in the limit $p \to 0$ due to the limits of the y integration.

It is easy to verify from the limits of integration that $\Gamma_{d,\mathrm{pr}}(p)$ vanishes unless p lies in the region

$$\max[0, (2w+2)^{1/2}-2] < p < (2w+2)^{1/2}+2. \tag{78}$$

This interval always contains the point $p^2=2w$. To get Γ_d we must integrate $\Gamma_d(p)$ with the weight function $\psi_w^2(p)d^3p$. Now, we see from (75) that $p^2\psi_w^2(p)$ has a maximum near $p^2=2w$ with a half-width for p of order $(2w)^{1/2}$. On the other hand, $\Gamma_{d,\mathrm{pr}}(p)$ has a wider distribution in p for small w.

For the above reasons, we make the further approximation that the pair portion of Γ_d is adequately represented in the region $w \lesssim 1$ by evaluating the integrand at $p^2=2w$:

$$\Gamma_{d,\mathrm{pr}} = \int \Gamma_{d,\mathrm{pr}}(p)\psi_w^2(p)d^3p \simeq \Gamma_{d,\mathrm{pr}}(p=(2w)^{1/2}). \tag{79}$$

To evaluate the right-hand side of (79) it is still necessary, in general, to carry out a double integration numerically. In a few special cases, however, this integration can be performed exactly or asymptotically or reduced to a single integral. Thus, one finds that in the limit $p^2, w \to 0$ (for $\beta \neq 0$),

$$\frac{\pi}{2}\Gamma_{d,\mathrm{pr}}(p^2=w=0) = 2\int_0^{1/2} \frac{z^3 dz}{[z^2+\beta f_1(z,z)]^2+\beta^2 f_2^2(z,z)} \text{ Ry}. \tag{80}$$

[52] Here and in the remainder of this section we adopt for notational simplicity the convention that the symbol "w" stands for the renormalized *binding energy*, a positive quantity.

[53] We have already observed that the logarithmic singularity of the *exchange* potential at $p=1$ is responsible for a small long-range falloff of the wave function similar to that of the polarization potential. This effect actually dominates the asymptotic behavior of the bound-state wave function at very large distances from the nucleus. However, according to perturbation theory, this long-range tail should not be important, in the high-density region, for expectation values such as that involved in computing the linewidth.

[54] The wave function (75) can be improved by taking into account the change in effective mass, m^*, of the electron. To do this one should replace w by $(m^*/m)w$. According to the lowest order Hamiltonian of Eq. (43), $(m^*/m)=(1+2\beta/3\pi)^{-1}$.

[55] The wave function (75) satisfies, of course, the relation $\langle p^2\rangle = 2w$, the virial theorem for bound states in a Coulomb potential. The virial theorem goes somewhat differently for, say, a Yukawa potential, but one does not expect a radical change in this relation between the rms value of momentum and the binding energy. After all, for a given bound state, one can always approximate the effect of a Yukawa potential by using a Coulomb potential with the appropriate "effective charge" (by averaging the screening factor).

This yields the leading logarithmic term of (61) in the limit $\beta \to 0$.

For $\beta=0$ and $w<1/18$ one obtains the asymptotic formula

$$(\pi/2)\Gamma_{d,\mathrm{pr}}(p=(2w)^{1/2}) \underset{w\to 0}{\sim} 1/w+2\ln(1/w) -2\ln 2-4-13/24.\ \mathrm{Ry}. \quad (81)$$

For $\beta=0$, $w=\frac{1}{2}$ and $p^2=1$:

$$(\pi/2)\Gamma_{d,\mathrm{pr}}(p^2=1=2w)=\tfrac{3}{4}[(99/80)-\tfrac{2}{5}\sqrt{3}]\ \mathrm{Ry} \simeq 0.41\ \mathrm{Ry}. \quad (82)$$

Let us turn now to the plasmon portion of Γ_d. We neglect the dispersion of plasmon frequency and, therefore, consider only the first term in the expansions (66), (67). A simple calculation then yields the result

$$\frac{\pi}{2}\Gamma_{d,\mathrm{pl}}(p)\simeq\frac{\pi}{2}\beta^{-1}\Lambda_p\theta[1-2(\Lambda_p-w)] \times\theta(\Lambda_p-w)\frac{\ln(q_+/q_-)}{p}\ \mathrm{Ry}, \quad (83)$$

where

$$q_+=\min[q_c,\ p+(2\Lambda_p-2w)^{1/2}], \qquad q_-=\min[q_c,\ |p-(2\Lambda_p-2w)^{1/2}|], \quad (84)$$

and

$$q_c\simeq(1+2\Lambda_p)^{1/2}-1. \quad (85)$$

Note that from momentum and energy considerations the plasmon portion vanishes if w is less than $\Lambda_p-\frac{1}{2}$ or larger than Λ_p. [Λ_p is given by Eq. (68).]

We are interested, of course, in the integrated expression

$$\Gamma_{d,\mathrm{pl}}=\int d^3p\,\Gamma_{d,\mathrm{pl}}(p)\psi_w^2(p). \quad (86)$$

Since $\Gamma_{\mathrm{pl}}(p)$ goes to infinity logarithmically in p at the point $p^2=2(\Lambda_p-w)$, it is no longer a good approximation to replace the weighted average (86) by the value of the integrand at $p^2=2w$. Instead, one might try to approximate the integral by evaluating the square of the wavefunction at $p^2=2(\Lambda_p-w)$. This gives the result

$$\Gamma_{d,\mathrm{pl}}\simeq\psi_w^2[p^2=2(\Lambda_p-w)]\int d^3p\,\Gamma_{d,\mathrm{pl}}(p). \quad (87)$$

The integral on the right-hand side can be evaluated exactly, yielding

$$(\pi/2)\Gamma_{d,\mathrm{pl}}\simeq 16w^{5/2}(\Lambda_p-w)^{1/2}\beta^{-1}q_c\Lambda_p^{-3} \times\theta(\Lambda_p-w)\theta[1-2(\Lambda_p-w)]\ \mathrm{Ry}. \quad (88)$$

Comparison of (88) with the results of a numerical integration of (86) shows that (88) is always somewhat too large but becomes better with increasing β and is quite good for β in the neighborhood of unity.

From (88) one sees that in the fixed γ approximation, when w is of the order of β, $\Gamma_{d,\mathrm{pl}}$ approaches zero like $\beta^{3/4}$ Ry and is, therefore, indeed of higher order than the pair portion of Γ_d, as we have previously claimed.

The final numerical results we shall present here were obtained by the numerical evaluation of the double integral of the approximation (79) for the pair portion of Γ_d and a numerical integration of (86) with the wave function (75) for the plasmon portion of Γ_d. A range of values of w and β lying in the interval 0 to 1 was taken. The results for the partial and total contributions to $(\pi/2)\Gamma_d$ are given in Table I. (See also Fig. 6.)

The coefficient $\pi/2$ multiplying Γ was chosen for convenience in comparing the numerical results with the analytical asymptotic expressions (73) and (81) and has no physical significance. Inasmuch as the probability of decay of the bound hole goes like $\exp(-2\Gamma t)$ a more conventional linewidth parameter would be 2Γ, slightly larger than the normalization adopted here.

TABLE I. Partial and total level widths vs w and β for bound holes.

β / w	0	0.1		0.2		0.3		0.4		0.6		0.8		1.0	
	b	a	b	a	b	a	b	a	b	a	b	a	b	a	b
0.00	inf.		1.37		0.87		0.63		0.48		0.31		0.22		0.16
0.05	21.10	0.96	3.59	0.32	1.74	0.17	1.11	0.11	0.79	0.06	0.47		0.28		0.20
0.10	8.33	4.09	8.10	1.46	3.48	0.79	2.01	0.51	1.35	0.28	0.75	0.18	0.48		0.22
0.15	4.24	7.53	10.78	3.16	5.15	1.78	3.12	1.17	2.05	0.64	1.10	0.43	0.72		0.21
0.20	2.56	4.34	6.95	4.84	6.57	2.94	4.17	1.99	2.87	1.12	1.57	0.75	1.03	0.54	0.75
0.25	1.70		1.98	5.28	6.78	3.93	5.07	2.81	3.67	1.65	2.11	1.12	1.41	0.82	1.02
0.30	1.20		1.37		1.30	4.22	5.25	3.45	4.26	2.18	2.66	1.51	1.80	1.12	1.33
0.35	0.88		0.98		1.07	1.85	2.78	3.56	4.31	2.61	3.10	1.88	2.18	1.42	1.63
0.40	0.67		0.74		0.80		0.80	1.88	2.59	2.84	3.32	2.19	2.50	1.70	1.91
0.45	0.52		0.56		0.60		0.65		0.61	2.38	2.85	2.36	2.70	1.92	2.14
0.50	0.41		0.44		0.47		0.51		0.53	0.85	1.29	2.10	2.43	2.05	2.28
0.60	0.27		0.29		0.30		0.32		0.34		0.37		0.31	1.56	1.81
0.70	0.19		0.20		0.20		0.22		0.23		0.25		0.26		0.23
0.80	0.14		0.15		0.15		0.16		0.16		0.17		0.19		0.20
0.90	0.11		0.11		0.11		0.12		0.12		0.13		0.13		0.14
1.00	0.08		0.08		0.08		0.09		0.09		0.09		0.10		0.11

[a] a is the plasmon emission width in rydbergs from formula (86); b is the total width, equal to a plus pair width from formula (79); w is the ("renormalized") binding energy divided by twice the Fermi energy; β is the ratio of the Fermi wavelength to the Bohr radius of the electron.

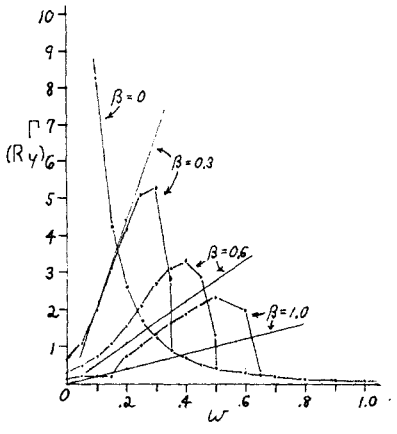

FIG. 6. The broken curves show the level width Γ as a function of the relative binding energy, w, for several values of β, from data of Table I with straight-line interpolation between computed points. Physical bound holes must lie on the portion of the curves below the solid straight lines, which show the locus of equal level width and binding energy for each value of β.

The following main features of the dependence of Γ on w and β may be noted. In general, for $\beta \gtrsim 0.1$, Γ begins at $w=0$ with values determined by pair emission alone, then increases with w and has a single pronounced peak, at a value of several rydbergs, to which *plasmon* emission contributes dominantly. (The pair portion is comparatively flat as a function of w.) The plasmon portion then cuts out sharply at the classical plasma frequency.[56] Γ continues to fall as w increases and at $w=1$ the values of Γ for all β have fallen to a roughly common value of about 0.1 Ry.[57]

The peak value of the linewidth is lowered as β is increased and it is displaced slightly toward higher values of w. Thus, the peak value is about 10 Ry for $\beta=0.1$ at $w=0.15$ and goes down to about 2 Ry for $\beta=1$ at $w=0.50$.

For $\beta=0$, only the pair portion contributes. Γ decreases monotonically with w starting at infinity at $w=0$ like $1/w$ in a manner given in detail by the asymptotic formula (81).

For $\beta \gtrsim 0.6$, the plasmon contribution comes in sharply, and in fact discontinuously in our approximation, at $w=(\Lambda_p-\frac{1}{2})$, the minimum binding energy for plasmon emission. (In our units the Fermi energy is $\frac{1}{2}$).

The region $0<\beta<0.1$ is not covered by Table I. In this region, presumably, pair emission tends to be the dominant process throughout. Values of Γ in the immediate neighborhood of $w=0$ should be adequately approximated by the fixed-γ approximation result (73) with p^2 replaced by $2w$.

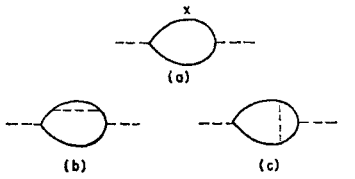

FIG. 7. Polarization diagrams entering into the next order of perturbation theory.

The results of Table I are interesting in that they show a characteristic dependence of the linewidth of the bound hole on the density of the system and on the relative binding energy of the corresponding bound state.

Table I can also be used to obtain a correction to the Hulthén-Laurikainen criterion (48) for the existence of bound holes and at the same time a correction to the location of the edge of the physical continuum. We recall that the first bound-hole state must have a linewidth less than its binding energy to prevent the level from merging into the continuum.

To investigate this point, we shall adopt values of the binding energy arising in the Yukawa potential approximation, as tabulated by Harris.[58]

Keeping in mind the relation $W=(2w)/\beta^2$ between the relative binding energy and the absolute binding energy, W, in rydbergs and using the Yukawa potential eigenvalues of Harris,[58] one finds that for the higher values of β there is a significant change in the critical binding condition due to linewidth. For example, for $\beta=0.6$ one finds that the minimum value of Z for bound holes to exist is changed from $Z=2$ (He) to $Z=3$ (Li).[59]

Some interesting points show up in this connection and it is worth going into the matter in somewhat greater detail. For $\beta \lesssim 0.3$ one finds from Table I that W is always greater than Γ for $w \gtrsim 0.05$, though plasmon emission broadens the level width considerably. For $\beta=0.4$ to 0.6 the minimum value of w for binding, w_m, occurs near the end of the plasmon peak at $w=0.4$ and 0.5, respectively. For $\beta=0.8$ and 1.0, w_m occurs immediately following the plasmon cutoff, $w_m=0.6$ and 0.7, respectively.

For $\beta=1.0$ one finds an interesting situation: A bound hole can also exist if w is in the neighborhood of 0.15 ($W=0.3$ Ry). For still lower densities, that is, entering the region of ordinary metallic densities, one would presumably find that the domain of values of w for the possible existence of bound holes consists of two isolated intervals with the plasmon emission region excluded. One should, therefore, observe at these densities a gap in the emission spectrum of bound holes

[56] Of course, the sharp cutoff on plasmon emission is partly due to our approximation, in which the dispersion of plasma frequency has been neglected. Moreover, plasmon emission could still take place in *multiple* processes, neglected here, for example the emission of two plasmons or the emission of a plasmon plus an electron-hole pair.

[57] As one sees from the form of the denominator in the pair emission formula (76), the reason for the lack of dependence on β of the linewidth, at these comparatively large values of w, beyond the plasmon-emission cutoff, can be found in the rather large minimum momentum transfer in the decay. The latter is determined by w according to formula (77b). This is also part of the cause for the rapid decrease in pair emission at these energies. Another reason for this decrease is that the solid angle (of q) for pair emission is continually narrowed about the "backward" direction (with respect to p) as w increases in order to maintain conservation of energy and momentum.

[58] G. Harris, Table II of reference 37.

[59] This rough calculation neglects the effect of the change in effective mass. See also footnote 54. This would also change the Hulthèn-Laurikainen criterion (48).

marked by the absence of transitions to or from bound states with binding energies in the single, unaccompanied plasmon emission region $(\Lambda_p-\frac{1}{2})<w<\Lambda_p$.

From general considerations, the linewidth of a bound level should show up also in the absorption spectrum and, therefore, the single-particle bound states in question should be effectively missing.

Because of the simplifying approximations made in the present treatment of the plasmon portion and since the region in question occurs for values of β and w greater than or comparable to unity, the above interesting prediction must be taken with a grain of salt. Certainly, a more accurate analysis of the plasmon portion, employing better wave functions and taking into account the dispersion of plasmon frequency, is justified.

Before closing this subsection, we comment briefly on the region of validity of the fixed-γ approximation result (73). One sees from the above work that this is a *weak-binding* and high-density result whose domain of applicability is characterized by the fact that the relative binding energy, w, is appreciably less than β which in turn should be appreciably less than unity.

Region of Stronger Binding

The previous estimates of level widths can be improved by dropping the approximation (79) and by making use of more accurate wave functions as provided, for example, by the numerical solution of an effective Schrödinger equation with a Thomas-Fermi potential or the numerical solution of (the nonlocal) Eq. (43) which is somewhat better than Thomas-Fermi at very small and very large distances. In this way, one can even hope to obtain a rough approximation for the pair-emission and plasmon-emission rates in the *strong binding* region $w>1$.

This is the appropriate place to discuss also the contribution to the level width of bound holes arising from the transition of the hole to another bound state. In order to estimate this effect, it is convenient to adopt an S-matrix point of view and regard the transition as taking place by means of the previous lowest order Feynman diagrams and "coupling constants." Thus, we have now initial and final bound-hole states in addition to a final free electron-hole pair or plasmon.

After a brief and straightforward calculation one obtains in this way the approximation[60]

$$\Gamma_{ww'}\simeq\int d^3q\,\Gamma_d(q,\Delta)\left|\int\psi_w(p)\psi_{w'}(p-q)d^3p\right|^2, \quad (89)$$

where

$$\Delta\equiv w-w'. \quad (90)$$

Here $\Gamma_{ww'}$ is the (electronic) decay rate for transition of a hole of binding energy w to another of binding energy w'. ψ_w and $\psi_{w'}$ are the wave functions of the two bound states. $\Gamma_d(q,\Delta)$ is the sum of the pair and plasmon portions of $\Gamma_d(p,q)$ with Δ in those formulas replaced everywhere by $w-w'$. [See formulas (63) and (70).]

Since in our approximation the plasmon energy is q independent, there will be no plasmon-emission contribution to $\Gamma_{ww'}$ unless $w'-w$ happens to coincide with the plasma frequency.

[60] The integral involving the wave functions is essentially the q-momentum transform of the product of the wave functions in position space. It is, therefore, small unless the overlap of the wave functions is appreciable.

5. SUMMARY AND CONCLUDING REMARKS

In the preceding sections we have considered some properties of the effective Hamiltonian entering into the so-called Schwinger equation or effective Schrödinger equation describing single-particle excitations, for the particular case of a dense electron gas containing a fixed positive point charge of atomic number Z. Formula (43) gives the lowest order Schwinger equation for this problem with respect to a perturbation expansion in powers of the dimensionless parameters β and βZ. (β is the ratio of the Fermi wavelength to the Bohr radius.) The lowest order energies and wave functions may be obtained by a numerical solution of Eq. (43).

The lowest order equation (43) has an Hermitian and energy-independent effective Hamiltonian and, therefore, is within the framework of the "h approximation" discussed in I. In this approximation the ground-state wave function is an antisymmetrized product of the wave functions satisfying (43) with eigenvalues less than the chemical potential μ. The single-particle excitation states are found by adding particles or holes in these single-electron states with excitation energies equal to the corresponding eigenvalues.

We have been particularly concerned with the discrete spectrum of "bound-hole" excitations. One of the more interesting results of the present investigation, though not rigorously established, is the actual presence of a discrete spectrum and its disappearance beyond a certain value of the density corresponding to a value of the parameter $\gamma=Z^2\beta$ roughly equal to unity.

We have introduced a particular type of limiting process, especially appropriate to the investigation of the discrete spectrum, in which the parameter γ is kept fixed while the parameter β approaches zero. We may call this the fixed-γ approximation or limiting process.

For the fixed-γ approximation, Eq. (43) reduces formally in the limit $\beta\to 0$ to an ordinary Schrödinger equation with a Yukawa potential, formula (54), an equation of a type which has been intensively investigated in connection with the deuteron and plasma problems. According to the numerical work of Hulthén and Laurikainen,[34] this equation has bound states only for $\gamma\gtrsim 0.898$.

In the important case of hydrogen ($Z=1$) this critical binding condition is unfortunately not very accurate since it corresponds to a value of β near unity. On the other hand, for $Z>1$, the critical value of γ occurs at

values of β, as well as $Z\beta$, that are appreciably less than unity.

The Yukawa potential obtained by our formal limiting process is actually a familiar expression, due originally to Mott, following from a linearized Thomas-Fermi treatment.[43]

In formula (73), values were given for the lifetimes of bound holes for the two lowest orders of the fixed-γ approximation in terms of the unperturbed solutions of the Yukawa approximation. This calculation confirms the important point that at least in the limit $\beta \to 0$ the level width is small compared to the separation of bound levels. If this were not the case, the discrete spectrum of bound holes would have no real physical existence. Formula (73) shows also that the level width at high densities is of the order of rydbergs.

In Sec. 4 we obtained approximate numerical estimates for the level width of bound holes over a considerably wider range of densities and source charges. These results are summarized by Table I. It turns out that in the range $w \lesssim 1$, the linewidth, to a fair approximation, can be expressed in terms of only two parameters, β and w. Here w is the relative binding energy of the bound state—the ratio of the binding energy to (twice) the Fermi energy.

Table I lists separately the important plasmon-emission contribution to the linewidth. This comes into play, in general, as soon as one leaves the limit of very small binding energies and disappears for binding energies greater than the maximum plasmon energy, which is approximately the classical plasma frequency.

The magnitude of the linewidth is responsible for a correction to the Hulthén-Laurikainen criterion (48) for the existence of bound holes. In order to prevent the first bound level from merging into the continuum, one must demand namely that it be separated from the continuum limit by an amount greater than the level width. We find, for example, that for $\beta=1$ this linewidth effect is responsible for shifting the minimum value of Z for the binding of holes from $Z=1$ (hydrogen) to $Z=2$ (helium).

It is interesting to note that the dimensions of the "orbits" of bound holes can be considerably larger than the interparticle spacing since very weakly bound holes may be very remote from the nucleus. Specifically, we see from the form of the approximate wave function (74) that a measure of the range of the orbit is the inverse square root of the relative binding energy, w, while in the same units the interparticle spacing is of order unity. This conclusion is affected somewhat by the level-width correction, which requires a minimum value of w before the level is actually separated from the continuum.[61]

Our calculations permit us to assess more accurately the region of validity of the fixed-γ approximation, which yielded the Yukawa potential in the limit $\beta \to 0$. It appears that this approximation is valid in the *weak-binding* and high-density limit in which, more precisely, the relative binding energy w is small compared to β which, in turn, is small compared to unity. This conclusion is consistent with the considerations needed for the Thomas-Fermi derivation of the Yukawa potential.

This weak-binding limit, as we have defined it, may actually go beyond the region where $Z\beta$ is less than unity, a restriction imposed by our original perturbation approach. This extension of the domain of validity of the perturbation theory may be ascribed to the fact that in avoiding the problem of the infrared divergence at low momentum transfers we have summed over an infinite set of polarization diagrams.

A number of interesting and important questions remain open and deserve detailed study. These questions are, for example, (a) a mathematically more rigorous delineation of the domains of validity of the perturbation expansion, (b) the extension of the perturbation calculation to higher orders, (c) alternative nonperturbative treatments, (d) the elaboration of the theoretical model to physically more "realistic" situations and, finally, (e) the question of the experimental verification of the results concerning the single-particle excitation spectrum.

In concluding the present section, we would like to comment briefly and qualitatively on a few rather isolated aspects of problems coming under the headings (b), (d), and (e).

It is easy to see what diagrams are expected to enter into the next higher order of perturbation theory. Formally, at least, these are diagrams with an extra dotted line or external potential vertex since such diagrams have extra factors of β or βZ. These diagrams are the three polarization diagrams of Fig. 6 and the four mass-operator or exchange diagrams of Figs. 5(b)–5(e). This approximation already goes beyond the "h approximation" discussed in I, since the operators corresponding to diagrams M_d and M_e of Fig. 5 are non-Hermitian and energy dependent.

From the point of view of physical applications, the present ideal model has the usual advantages and disadvantages of ideal models: It is simple enough to give a rough description of a variety of physical situations. On the other hand, if we wish an accurate account of any particular physical example, the model must be refined and extended.

Speaking in general terms, the model can be applied to situations in which a fixed or slowly moving point inhomogeneity of charge, or "source," is present in a dense neutral system composed of positive ions (the "background") and electrons at temperatures low enough that the electrons (but not the ions) form a degenerate Fermi gas.

The point "source" can be either an "impurity"

[61] According to Table I the minimum value of w is about 0.5 for $\beta=0.6$ and goes down to less than 0.05 for $\beta=0.1$.

nucleus of atomic number Z, which is the most straightforward interpretation, or it may represent a particular nucleus of the background.[62]

If the electron density is sufficiently high, the background atoms will be completely ionized. At the lower densities of incomplete ionization the theoretical separation of the background is more arbitrary. In this case, it is natural to regard only the unbound electrons as belonging to the electron gas and the partially ionized "cores" as belonging to the background. The degree of ionization can be estimated, self-consistently, on the basis of results obtained here and the remark of the previous paragraph.

The chief deficiency of the model is in the simplifying feature of the uniform background. In applications to dense crystalline matter such as metals it would be desirable to generalize the model by replacing the uniform background by a suitable static periodic potential.

In applications to systems where the positive ions do not form a regular lattice, as in white dwarfs, it would be desirable to take into account the fluctuating electric fields due to the random motion of the positive ions.[13] ft should be mentioned also that at the high densities sound in white dwarfs, relativistic corrections are Iometimes appreciable, making a relativistic generalization of the model desirable.[13]

There are several physical processes which are directly sensitive to the single-particle energies, lifetimes, and wave functions discussed in this paper.

One example is the x-ray emission or absorption spectrum of atoms in metals for bound hole to hole transitions. The transition energy should be given by the difference of the corresponding single-particle energies. Because of the relatively small or moderate coupling of the electron system to the radiation (and phonon) fields, one expects that an appreciable fraction of the linewidth of this radiation is determined by interelectronic processes.

Another example is that of orbital electron capture by a nucleus in a dense medium. One can picture this process as resulting in a bound-hole excitation of the electron gas. One expects then that the single-particle energies (in addition to determining the accompanying x-ray radiation spectrum) contribute additively to the energy of the emitted monoenergetic neutrinos. Moreover, the capture rate should be proportional to the square of the single-particle wave function at the nucleus.[63,64]

In principle, many details of the decay process of the bound hole, as implied by the estimates of Table I or by the general level-width formulas, are subject to direct experimental verification. We mention, in particular, the angular correlation of the decay products and the branching ratio for plasmon emission.

A specific prediction following from the numerical estimates given here is that for "good" metals (defined, of course, as those to which the present theory is applicable) x-ray emission or absorption lines involving transitions to or from a bound state with binding energy lying in the single, unaccompanied plasmon emission range should be considerably broadened or, preferably, missing entirely.

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APPENDIX

Lowest Order Evaluation of Level Width Γ

We wish to evaluate the expectation values

$$\Gamma_i=\beta^2\,\mathrm{Im}\langle M_i(w)\rangle, \tag{A1}$$

in the limit $\beta\to 0$, with γ fixed at a value greater than that needed for binding, for diagrams M_d and M_e of Fig. 5.

The expectation values are, with respect to the "unperturbed" bound-state wave functions ψ, solutions of (43). A factor of β^2 is separated off for convenience in order that the expectation value be non-vanishing in the limit $\beta\to 0$.

If M_i is diagonal in a momentum representation, which is true of diagrams M_d and M_e, (A1) can be written in the form

$$\Gamma_i=\beta^2\,\mathrm{Im}\int d^4p\;|\langle\psi|\,p\rangle|^2 M_i(p,w), \tag{A2}$$

where $M_i(p^2,w)$ is the diagonal element of $M_i(w)$.

Performing now the transformation $p\to(\gamma\beta)^{1/2}p$,

[62] In both cases the system as a whole is electrically neutral and the potential at the origin goes like Z/r. I wish to thank Dr. W. Lakin for a helpful discussion of this point.

[63] H. Brysk and M. E. Rose, Rev. Mod. Phys. **30**, 1169 (1958).

[64] J. Bahcall, Phys. Rev. **26**, 1143 (1962). I wish to thank Dr. Bahcall for sending me a preprint of this article.

we obtain

$$\Gamma_i=\beta^2\,\mathrm{Im}\int d^3p\;|\langle\psi_s|p\rangle|^2 M_i(\gamma\beta p^2;\gamma\beta w_s), \quad \text{(A3)}$$

where ψ_s is a normalized scaled wave function, which, in the limit $\beta\to 0$, is a solution of (55), and w_s is the corresponding discrete eigenvalue.

As β approaches zero with γ fixed, *provided that* $M_i(0,0)$ *exists*, we obtain from (A3)

$$\Gamma_i(\beta=0)=\beta^2\,\mathrm{Im}M_i(0,0). \quad \text{(A4)}$$

This is the same expression that we would obtain for the level width (inverse lifetime) of a source-free hole excitation of zero momentum and energy.

It turns out that $\mathrm{Im}M(0,0)$ does exist for diagram M_e but is logarithmically infinite as $\beta\to 0$ for M_d. This requires one to use the more general formula (A3) for M_d.

Diagrams of The Type M_d

We consider first the totality of diagrams of the type M_d with an arbitrary number of inertions in the dotted line.

For reasons given in the text, the plasmon contribution to Γ_d is technically of higher order in β than the pair portion and, therefore, we consider here only the pair portion. We take as a starting point the closed expression (70):

$$M_d(p^2,w)=\frac{2}{\pi}\int d^3q\,\frac{\mathrm{Im}Q_0(q,\Delta)}{|q^2+4\pi\beta Q_0(q,\Delta)|^2}\theta(1-|p-q|). \quad \text{(A5)}$$

According to (A3), in calculating the corresponding value of Γ_i we have also to make the replacement

$$p\to(\beta\gamma)^{1/2}p, \quad w\to(\beta\gamma)w_s. \quad \text{(A6)}$$

The real and imaginary parts of Q_0 are given in (32) and (33). An examination of these expressions, taking into account (A6), shows that in lowest order in β we can make the following replacements in (A5):

$$\theta(1-|p-q|)\to\theta(1-q), \quad \text{(A7)}$$

$$q^2+4\pi\beta Q_0(q,\Delta E)\to q^2+4\beta/\pi, \quad \text{(A8)}$$

$$\mathrm{Im}Q_0(q,\Delta E)\to\frac{1}{2\pi}\{\gamma\beta|w_s|/q+\gamma\beta p^2/2q+q/2\}. \quad \text{(A9)}$$

Thus,

$$M(\gamma\beta p^2,\gamma\beta w)=\frac{1}{2\pi}\frac{2\beta^2}{\pi}\int d^3q \times\frac{(\gamma\beta|w_s|/q+\gamma\beta p^2/2q+q/2)}{(q^2+4\beta/\pi)^2}\theta(1-q). \quad \text{(A10)}$$

The term $q/2$ in the numerator leads to $a\ln\beta$ contribution to Γ. The other terms are finite in the limit $\beta\to 0$. The integrations in (A10) are elementary and one obtains for Γ, using (A3):

$$\Gamma_d=\beta^2-\frac{1}{\pi}[\ln(\pi/4\beta)-1+(\pi/2)\gamma[|w_s|+\langle p^2\rangle_\gamma/2]], \quad \text{(A11)}$$

where the symbol $\langle\ \rangle_\gamma$ denotes an expectation value with respect to scaled wave functions, solutions of (54) with eigenvalue w_s, for fixed γ.

Diagram M_e

In this case we are interested only in the limit $\mathrm{Im}M(0,0)$ which turns out to exist, of the imaginary part of matrix element $M(p^2,w)$ of (A2) for diagram M_e.

The simplest way to calculate Γ_e to lowest order is to use the expressions (60) and (61) to compare the value of $\mathrm{Im}\Gamma_e$ for zero momentum excitations to the coefficient of $\ln(1/\beta)$ for Γ_d.

Modifying these formulas for application to the particular case of the decay of a zero momentum and energy hole excitation one obtains the following expressions, disregarding a common constant of proportionality

$$\mathrm{Im}\Gamma_d=\int_0^1 d^3q\int_{p_1<1<|p_1+q|} d^3p_1\,g^2(p,q)\delta(q\cdot p_1) +\text{plasmon mode}, \quad \text{(A12)}$$

$$\mathrm{Im}\Gamma_e=-\tfrac{1}{2}\int_0^1 d^3q\int_{p_1<1<|p_1+q|} d^3p_1 \times g(p,q)g(p,\bar{q})\delta(q\cdot p_1). \quad \text{(A13)}$$

The factor of $-\frac{1}{2}$ for the exchange interference diagram M_e is due to the Pauli principle.

Note that because of conservation of energy and momentum the two holes in the final state come off at right angles to each other.

In (A13), $\bar{q}$ is the "exchange momentum transfer" which in our case is

$$\bar{q}=p_1-p\to p_1. \quad \text{(A14)}$$

The coupling constants g to lowest order in β are given by

$$g(p,q)=\mathrm{const}[\beta/(q^2+4\beta/\pi)]. \quad \text{(A15)}$$

To lowest order in β we have then from (A15), (A14), (A13), and (A12), dropping the plasmon mode and common constants of proportionality,

$$\Gamma_d=\beta^2\int\frac{d^3q}{q^4}\int_{p_1<1<|p_1+q|} d^3p_1\,\delta(q\cdot p_1), \quad \text{(A16)}$$

$$\Gamma_e=-\tfrac{1}{2}\beta^2\int_0^1\frac{d^3q}{q^2}\int_{p_1<1<|p_1+q|}\frac{d^3p_1}{|p_1|^2}\delta(q\cdot p_1). \quad \text{(A17)}$$

In evaluating the above expressions we are concerned with integrals of the form

$$I(q)=\int d^3p\, f(p^2)\theta(|p+q|-1)\theta(1-p)\delta(q\cdot p). \quad \text{(A18)}$$

Integrals of this type are easily evaluated in the following way (we again neglect constants of proportionality).

First of all, the angular average of $\delta(q\cdot p)$ is given by

$$\langle\delta(q\cdot p)\rangle=\frac{1}{qp}\frac{1}{2}\int\delta(x)dx=\frac{1}{2}\frac{1}{qp}, \quad \text{(A19)}$$

where x is the cosine of the angle between q and p. In the remaining factors of (A18), we can assume that p and q are perpendicular and we obtain

$$I(q)\sim\frac{1}{}\int_0^1 pdp\, f(p^2)\theta(p^2+q^2-1)\theta(1-p^2). \quad \text{(A20)}$$

Next we perform the change of variables

$$s=p^2, \quad t=q^2. \quad \text{(A21)}$$

Substituting this into (A20), we obtain

$$I(t)\sim t^{-1/2}\int_0^1 ds\, f(s)\theta(s+t-1)\theta(1-s). \quad \text{(A22)}$$

We employ now the partial integration formula

$$\theta(s+t-1)=\theta(s-1)+\int_0^t dy\,\delta(y+s-1). \quad \text{(A23)}$$

If we substitute this into (A22), only the second term contributes and for this term the s integration can be carried out immediately, yielding

$$I(t)\sim t^{-1/2}\int_0^t dy\, f(1-y)\theta(y). \quad \text{(A24)}$$

Since t is less than unity the θ function may be dropped and we obtain the final result

$$I(t)\sim t^{-1/2}\int_0^t dy\, f(1-y). \quad \text{(A25)}$$

For M_d, f is unity while for M_e, $f(x)=1/x$. For M_d then $I(t)\sim t^{1/2}=q$ and we verify from (A16) that Γ_d diverges like $\ln\beta$ in the limit $\beta\to 0$.

From the preceding work we obtain for the ratio Γ_e/Γ_d in the limit $\beta\to 0$:

$$\left(\frac{\Gamma_e}{\Gamma_d}\right)\ln(1/\beta)=-\tfrac{1}{2}\int_0^1 qdq\, r(q), \quad \text{(A26)}$$

where the ratio $r(q)$ is given by

$$r(q)=\int_0^t\frac{dy}{1-y}\Big/\int_0^t dy=\frac{-\ln(1-t)}{t}=\frac{-\ln(1-q^2)}{q^2}. \quad \text{(A27)}$$

Thus

$$\left(\frac{\Gamma_e}{\Gamma_d}\right)\ln(1/\beta)=-\tfrac{1}{4}\int_0^1\frac{dt}{t}[-\ln(1-t)]=-\tfrac{1}{4}\left(\frac{\pi^2}{6}\right). \quad \text{(A28)}$$

Since, from (A11), the coefficient of $\ln(1/\beta)$ for Γ_d is β^2/π we obtain from (A28) the final result

$$\Gamma_e=(\beta^2/\pi)(-\tfrac{1}{4})(\pi^2/6). \quad \text{(A29)}$$