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**Positronium Formation in Interacting Electron Gas**

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A two-body bound state equation for a positron and an electron in an interacting electron gas is rederived, using a Green's function decoupling scheme and various approximations required to define a bound state are explained. The equation has some new features not discussed before, and the solution rules out the formation of positronium-like state at metallic densities. But the critical \( r_s \)-value where the bound state formation starts is found to be higher than previously reported.

§ 1. Introduction

The question whether a positronium-like two-body bound state forms when positrons are injected into metals is often discussed in the literature.\(^1\)\(^{-3}\) In this work we re-examine the criterion of the bound state formation and show that the \( r_s \)-values quoted are too low. \( r_s \) is the usual electron gas parameter connected to the density of electrons per c.c., \( n \), by

\[
\frac{1}{n} = \frac{4\pi}{3} a_0^3 r_s^3.
\]  

(1.1)

Callaway\(^1\) argued that the two-body binding energy must be at least equal to the Fermi energy \( E_F \) before a positron could capture an electron. He arbitrarily took \( E_F = 0.2 \) ryd, which is lower than the Fermi energy of most metals, and looked for a bound state of that energy when the electron-positron interaction was represented by a simple Yukawa potential. He concluded \( r_s \geq 11.2 \) so that the bound state formation could occur. Held and Kahana\(^2\) pointed out that exclusion principle restrictions should be taken into account. They started from a two-body equation of the Bethe-Goldstone type with exclusion principle taken care of and the interaction properly screened. They sought a zero energy bound state and ignored Callaway's argument that the binding energy should be equal to the Fermi energy. According to their calculation, the bound state formation occurred for \( r_s \geq 8.5 \). Kanazawa et al.\(^3\) discussed a similar equation, but their interaction was of pure Coulomb type \( (V_{\alpha} \sim 4\pi e^3/q^2) \) when the momentum transfer \( q \) exceeds the plasma cutoff \( k_e \). They obtained the critical \( r_s = 4.521 \) for \( k_e = 0 \), but for finite \( k_e \), positronium did not form below \( r_s = 7.54 \), the value up to which they extended their investigation. Bergersen\(^4\) has used a different defini-

\(^{(*)}\) This is a sequel to the previous paper containing general formal theory besides a general derivation of an equation for positronium formation.

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We shall here derive a bound state equation in which the interaction and Pauli principle restriction are similar to those used by Held and Kahana, but the binding energy must be at least the Fermi energy of the electron gas before the bound state formation occurs. The equation is non-linear in \( r_3 \) and its solution shows that the critical \( r_3 \) is higher than hitherto found. (See however footnote to Eq. (2·20).) In the preceding paper a formal derivation of the linear equation for the two-particle Green's function is given. Several approximations were then made to reduce it to a "Bethe-Goldstone type" equation. Here we give an alternative derivation of the same equation and it is hoped that such a derivation brings out an alternative interpretation of the various interaction terms.

Before we derive the equation it is necessary to clarify the meaning of the bound state and binding energy of an electron and a positron in the environment of the electron gas. Clearly these concepts have no precise definition just as in the general question of bound states in a Fermi gas. However, in an approximate way, at low densities the two-particle bound state can be discussed. An isolated bound state of a positron and an electron in a high density electron gas is physically implausible. At the other extreme of zero density, the positronium is well known, and the binding energy in the centre of mass system is well defined. Starting from this limit, we introduce more and more electrons. Two things will happen. First, the centre-of-mass system of any one pair becomes ill-defined because of the identity of electrons. Nevertheless one can make a low density approximation, say the ladder approximation (or equivalently, factorize all three and higher order Green function into one- and two-particle Green's functions), and obtain a meaningful two-particle equation, with recognizable binding energy term. Secondly, the bare Coulomb interaction between the electron-positron pair becomes dynamically screened by a frequency and wave-vector dependent dielectric function. With such an interaction, the conventional definition of the bound state does not hold. One then makes the static approximation, and obtains an ordinary time-independent potential. To rule out the formation of bound states in metals, it is enough to show that no bound state exists in this static limit; for then, a bound state in the usual sense certainly cannot exist when the potential becomes time dependent.

§2. Derivation of the bound state equation

The Hamiltonian for the electron-positron system is

\[
\begin{align*}
H &= \sum_{k,\sigma} \epsilon_k^{-} b_{k\sigma}^d b_{k\sigma}^\dagger + \sum_{k,\sigma} \epsilon_k^{+} d_{k\sigma}^d d_{k\sigma}^\dagger \\
&+ \frac{1}{2} \sum_{k_1k_2q, \sigma_1\sigma_2} V_{\sigma_1\sigma_2}^{ee} b_{k_1+q\sigma_1}^d b_{k_1-q\sigma_1}^\dagger b_{k_2\sigma_2}^d b_{k_2\sigma_2}^\dagger + \sum_{k_1k_2q, \sigma_1\sigma_2} V_{\sigma_1\sigma_2}^{pp} d_{k_1+q\sigma_1}^d d_{k_1-q\sigma_1}^\dagger b_{k_2\sigma_2}^d b_{k_2\sigma_2}^\dagger \\
&\quad \quad + \sum_{k_1k_2q, \sigma_1\sigma_2} V_{\sigma_1\sigma_2}^{ep} b_{k_1+q\sigma_1}^d d_{k_1-q\sigma_1}^\dagger b_{k_2\sigma_2}^d d_{k_2\sigma_2}^\dagger.
\end{align*}
\]  

(2·1)
Here $b_{ks}, d_{ks}$ are the electron and positron annihilation operators respectively. We measure the energies from the chemical potentials.

\[
\begin{align*}
\epsilon_k^- &= \epsilon_k - \mu_e, & \epsilon_k^+ &= k^2/2m, \\
\end{align*}
\]

(2.2)

Since the positron density is very low, we have left out the positron-positron interaction term. In the summations the $q=0$ term has to be left out. We also have

\[
\begin{align*}
V_e^{ee} &= 4\pi\alpha^3/v_q^4, & V_e^{ep} &= -4\pi\alpha^3/v_q^2.
\end{align*}
\]

(2.3)

The definitions of the Green's functions are:

\[
\begin{align*}
G_{t\sigma}^e(k_1, k_2) &= (-i) \left< T(b_{k_1}(t_1) b_{k_2}(t_2)) \right>, \\
G_{t\sigma}^p(k_1, k_2) &= (-i) \left< T(d_{k_1}(t_1) d_{k_2}(t_2)) \right>, \\
G_{k\sigma',\epsilon_k}^{ep}(K-p', K+p'; K-p', K+p') &= (-i)^2 \left< T(b_{K-p',\sigma_1}^\dagger(t_1) d_{K+p',\sigma_1}(t_1') b_{K-p',\sigma_2}^\dagger(t_1') d_{K+p',\sigma_2}(t_1')) \right>, \\
G_{k\sigma',\epsilon_k}^{ep}(K-p', K+p'; K-p', K+p') &= (-i)^2 \left< T(b_{K-p',\sigma_1}^\dagger(t_1) b_{K+p',\sigma_1}(t_1') b_{K+p',\sigma_2}^\dagger(t_1') b_{K-p',\sigma_2}(t_1')) \right>. \\
\end{align*}
\]

(2.4)

$T$ is the usual chronological operator and $\langle \rangle$ denotes the thermodynamic average.

The equations of motion satisfied by these Green's functions are

\[
\begin{align*}
\left(i \frac{\partial}{\partial t_1} - \epsilon^-_k\right) G_{t\sigma}^e(k_1, k_1') + i \sum_{k', q, \sigma'} V_q^{ee} G_{k\sigma'}^{ee}(k+q, k; k', k'+q+1) &+ i \sum_{k', q, \sigma'} V_q^{ep} G_{k\sigma'}^{ep}(k+q, k; k', k'+q+1) = \delta(11'), \\
\left(i \frac{\partial}{\partial t_1} - \epsilon^+_k\right) G_{t\sigma}^p(k_1, k_1') + i \sum_{k', q, \sigma'} V_q^{ep} G_{k\sigma'}^{ep}(k, k+q; k', k'+q+1, k_1') &+ i \sum_{k', q, \sigma'} V_q^{ep} G_{k\sigma'}^{ep}(k, k+q; k', k'+q+1, k_1') = \delta(11').
\end{align*}
\]

(2.5)

If one neglected the interactions, one gets the equations for the unperturbed Green's function:

\[
\begin{align*}
\left(i \frac{\partial}{\partial t_1} - \epsilon^-_k\right) G_{t\sigma}^{e(0)}(k_1, k_1') &\delta(11'), \\
\left(i \frac{\partial}{\partial t_1} - \epsilon^+_k\right) G_{t\sigma}^{p(0)}(k_1, k_1') &\delta(11').
\end{align*}
\]

(2.7)

(2.8)

The equation for $G^{ep}$ requires higher order Green's functions:

\[
\begin{align*}
\left(i \frac{\partial}{\partial t_1} - \epsilon_{K-p}\right) G_{k\sigma',\epsilon_k}^{ep}(K-p', k'; K-p', K+p') &+ i \sum_{k', q, \sigma'} V_q^{ee} G_{k\sigma'}^{ee}(K-p+q, k'; K+p; K-p', k'+q+1, K+p') \\
+ i \sum_{k', q, \sigma'} V_q^{ep} G_{k\sigma'}^{ep}(K-p+q, k'; K+p; K-p', k'+q+1, K+p') &\delta(11').
\end{align*}
\]

(2.9)
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\[ +i \sum_{k', q', \sigma'} V_q^{\sigma'} G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, k', K+p_2; K-p'1', k'+q_1^+, K+p'2') \]
\[ = \delta (11') \delta (p-p') G_{d_{q}, \varepsilon_{s}}^{\text{ep}} (K+p_2, K+p_2'), \] (2.9)

where

\[ G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, k', K+p_2; K-p'1', k'+q_1^+, K+p'2') \]
\[ = (-i)^{\langle T (b_{K-p+q_1} (t_1) b_{K-p+q_1}^+(t_1) d_{K+p_2} (t_2) d_{K+p_2}^+(t_2') b_{k'+q_1^+}^+(t_1') \delta_{K-p+q_1} (t_1')) \rangle}. \] (2.10)

The definition of \( G_{d_{q}}^{\text{ep}} \) can be easily inferred. We now multiply (2.5) by \( G_{d_{q}, \varepsilon_{s}}^{\text{ep}} (K+p_2, K+p_2') \) and subtract from (2.9) to get rid of the inhomogeneous term

\[ \begin{align*}
&\left( i \frac{\partial}{\partial t_1} - \epsilon_{K-p} \right) [G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p_1, K+p_2; K-p'1', K+p'2') ] \\
&- \delta (p-p') G_{d_{q}, \sigma}^{\varepsilon_{s}} (K-p_1, K-p'1') G_{d_{q}, \varepsilon_{s}}^{\text{ep}} (K+p_2, K+p_2') \\
&+ i \sum_{k', q', \sigma'} V_q^{\sigma'} [G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, k', K+p_2; K-p'1', k'+q_1^+, K+p'2') ] \\
&- G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, k'; K-p_1', k'+q_1^+, K+p') \\
&+ i \sum_{k', q', \sigma'} V_q^{\sigma'} [G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, k', K+p_2; K-p'1', k'+q_1^+, K+p'2') ] \\
&- G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, k; K-p'1', k'+q_1^+, K+p') \\
&= 0.
\end{align*} \] (2.11)

Now operate with \( (i \frac{\partial}{\partial t_2} - \epsilon_{K+p}') \). The only term which requires careful handling is \( G_{d_{q}}^{\text{ep}} \); there are two inhomogeneous terms, one coming from \( t_3 = t_2' \) and another from \( t_3 = t_1^+ \). We write down the final result:

\[ \begin{align*}
&\left( i \frac{\partial}{\partial t_3} - \epsilon_{K+p} \right) \left( i \frac{\partial}{\partial t_1} - \epsilon_{K-p} \right) [G_{d_{q}, \sigma, \varepsilon_{s}}^{\text{ep}} (K-p_1, K+p_2; K-p'1', K+p'2') ] \\
&- G_{d_{q}, \sigma}^{\varepsilon_{s}} (K-p_1, K-p'1') G_{d_{q}, \varepsilon_{s}}^{\text{ep}} (K+p_2, K+p_2') \delta (p-p') \]
\[ - i \sum_{q} V_q^{\sigma'} \delta (21^+) G_{d_{q}, \sigma', \varepsilon_{s}}^{\text{ep}} (K-p+q_1, K+p-q_2; K-p'1', K+p'2') \]
\[ = - \sum_{k', q', \sigma'} \sum_{k'', q'', \sigma''} V_q^{\sigma'} V_{q''}^{\sigma''} \left\{ G_{d_{q}, \sigma', \sigma''}^{\text{ep}} (K-p+q_1, k', \sigma''; K-p'1', \sigma''; k''; K+p+q_2; K-p'1', k''+q_2', K+p'2') \right\} \]
\[ - G_{d_{q}, \sigma'}^{\varepsilon_{s}} (K-p+q_1, k_1', K-p_1', k_1'+q_1^+) \times G_{d_{q}, \sigma}^{\varepsilon_{s}} (k_2', K+p+q_2'; k_2''+q_2', K+p_2') \}
\[ + \{ G_{d_{q}, \sigma', \sigma''}^{\text{ep}} (K-p+q_1, k', k_1; K+p+q_2; K-p'1', k''+q_2', K+p') \}
\[ - G_{d_{q}, \sigma'}^{\varepsilon_{s}} (K-p+q_1, k; K-p_1', k'+q_1^+) \}
\]
This is an exact equation. The definition of $G_4$ is obvious. If we neglect all the terms on the right-hand side, we get

\[
\left( i \frac{\partial}{\partial t_1} - \epsilon_{K+p} \right) \left( i \frac{\partial}{\partial t_1} - \epsilon_{K-p} \right) \left[ G_{s_1,s_2}^{ep} (K-p1, K+p2; K-p'1', K+p'2') \right] 
- \delta (p-p') G_{s_1,s_2}^e (K-p1, K-p1') G_{s_1,s_2}^p (K+p2, K+p2') 
- i \sum_q V_{q}^{ep} \delta (21^+) G_{s_1,s_2}^{ep} (K-p+q1, K+p-q1; K-p'1', K+p'2') = 0 .
\]

\[ (2.13) \]

Majumdar derived an equation of the same form except that $V_{q}^{ep}$ was a short range potential. As a starting point he had neglected $V_{q}^{ee}$ in (2.1) but assumed that $V_{q}^{ep}$ would be a static short-ranged potential. To obtain (2.13), he factorized $G_3^{ep}$ of Eq. (2.9) (with $V_{q}^{ee}=0$) into $G_{s_1,s_2}^e G_{s_1,s_2}^p - G_{s_1,s_2}^{ep} G_{s_1,s_2}^{p}$. It is clear therefore that the primary effect of the right-hand side of (2.12) is to screen the bare interaction $V_{q}^{ep}$ of (2.13).

We shall factorize $G_4$ with two approximations. First, the low density of positrons enables us to disregard any two-positron correlation. Secondly, we shall use the RPA, that is $V_{q}^{ep}$ and $V_{q}^{ee}$ on the right will carry the same momentum transfers $|q|$. Then

\[
G_{4}^{eeep} - G_{3}^{eeep} G_{3}^{ep} \approx \delta (q + q''') \delta (k' + q'' - k'') 
\times G_{s_1,s_2}^{ep} (K-p+q1, K+p-q2; K-p'1', K+p'2') 
\times G_{s_1,s_2}^e (k', k'' - q2) G_{s_1,s_2}^p (k''2, k' + q1^+),
\]

\[ (2.14) \]

Now the right-hand side of (2.12) becomes

\[
- \sum_q V_{q}^{ep} G_{s_1,s_2}^{ep} (K-p+q1, K+p-q2; K-p'1', K+p'2') 
\times \left\{ \sum_{k',q'} V_{q'}^{ee} G_{s_1,s_2}^e (k', k'2) G_{s_1,s_2}^{p} (k' + q2, k' + q1^+) \right\} .
\]

\[ (2.15) \]

But it is well known that the dielectric function $\varepsilon_{RPA}$ of the electron gas in the RPA is given by

\[
\frac{1}{\varepsilon_{RPA} (q, 12)} = i \sum_{k',q'} V_{q'}^{ee} G_{s_1,s_2}^e (k', k'2) G_{s_1,s_2}^{p} (k' + q2, k' + q1^+) .
\]

\[ (2.16) \]

The dielectric function is time dependent. To obtain a bound state equation in the conventional sense we make the static approximation*)

*) The equation including frequency dependent dielectric function requires a more detailed discussion. The restriction to the subspace of two equal-time indices in (2.26) is no longer possible.
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\[
\frac{1}{\varepsilon_{\text{RPA}}} - \delta(12) = \left( \frac{1}{\varepsilon_{\text{RPA}}(q, \omega = 0)} - 1 \right) \delta(12). \tag{2.17}
\]

So (2.15) simplifies to

\[
i \sum_q V_q^{ep} \delta(12) \left( \frac{1}{\varepsilon_{\text{RPA}}(q, \omega = 0)} - 1 \right) 
\times G^{ep}_{\varepsilon, \varepsilon_t}(K - p + q1, K + p - q2; K - p', K + p'2'). \tag{2.18}
\]

From (2.12) we thus obtain an equation

\[
\left( i \frac{\partial}{\partial t_2} - e \frac{\delta}{\delta K_p} \right) \left( i \frac{\partial}{\partial t_1} - e \frac{\delta}{\delta K_p} \right) G^{ep}_{\varepsilon, \varepsilon_t}(K - p1, K + p2; K - p'1, K + p'2') 
\times \delta(p - p') G_{\varepsilon, \varepsilon_t}(K - p1, K - p1') G^{ep}_{\varepsilon, \varepsilon_t}(K + p2, K + p2') \]

\[-i \sum_q V_q^{ep} \frac{1}{\varepsilon_{\text{RPA}}(q, \omega = 0)} \delta(12) \times G^{ep}_{\varepsilon, \varepsilon_t}(K - p + q1, K + p - q2; K - p'1, K + p'2') = 0. \tag{2.19}
\]

Using (2.7) and (2.8), we can write this as

\[
G_2^{ep} = G_1^{ep} + i G_1^{ep} G_1^{p(0)} \bar{V} G_1^{ep} \tag{2.20}^*)
\]

where for brevity we omit the momentum indices and

\[
\bar{V} = V_q^{ep} \frac{1}{\varepsilon_{\text{RPA}}(q, \omega = 0)} \delta(12). \tag{2.21}
\]

Now define an operator \( \mathcal{Q} \) such that

\[
G_2^{ep} = \mathcal{Q} G_1^{ep}; \tag{2.22}
\]

the equation for \( \mathcal{Q} \) is

\[
\mathcal{Q} = 1 + i G_1^{p(0)} G_1^{p(0)} \bar{V} \mathcal{Q}. \tag{2.23}
\]

The existence of the delta function in time in (2.21) enables us to restrict ourselves to the subspace where the left time indices are equal in \( \mathcal{Q} \). As Martin and Schwinger\(^7\) show, we should now write

\[
G_1^{p(0)} G_1^{p(0)} = \left[ (G_1^{p(0)})^{-1} + (G_1^{p(0)})^{-1} \right]^{-1} \left[ G_1^{p(0)} + G_1^{p(0)} \right], \tag{2.24}
\]

\[
(G_1^{p(0)})^{-1} + (G_1^{p(0)})^{-1} = \left( i \frac{\partial}{\partial t_1} + i \frac{\partial}{\partial t_2} - \epsilon^+ - \epsilon^- \right). \tag{2.25}
\]

Clearly (2.25) translates the total time, but does not alter the relative times. \( G_1^{p(0)} + G_1^{p(0)} \) changes either of the times but not both, and to keep the pair of

* A slightly more rigorous derivation employing functional derivatives and vertex functions can be given.\(^{10}\) The \( G_{1}^{p(0)} \) and \( G_{1}^{p(0)} \) are then replaced by \( G_{1}^{e} \) and \( G_{1}^{p} \) also. The complete solution of (2.20) requires self-consistent calculation of \( G_{1}^{s} \) as well. We shall, however, restrict ourselves to the simpler form (2.20).
time indices equal. Hence only the combination $[G_{\ell}^{(0)} + G_{\ell}^{(r)}]$ at vanishing time difference occurs. Now write

$$\Omega(11; 1'2') = \frac{1}{\tau} \sum_{\ell} \Omega(\nu_{1}, \nu_{2}) \exp \left[ -\frac{\pi}{\tau} (t_{1} - t_{1}') - \frac{\pi}{\tau} (t_{1} - t_{2}') \right],$$

$$G_{\ell}^{(0)}(12) = \frac{1}{\tau} \sum_{\ell} \left( \frac{\pi}{\tau} - \epsilon_{k} - \mu \right)^{-1} \exp \left[ -\frac{\pi}{\tau} (t_{1} - t_{3}) \right].$$

Here $\nu_{1}, \nu_{2}$ are odd integers and $\tau = -i\beta$. Substitute (2.26), (2.27) in (2.23) and use the fact that at vanishing time difference,

$$G_{\ell}^{(0)}(k1, k1) = \frac{1}{2i} \tanh \frac{1}{2} \beta \epsilon_{k}^-, \quad G_{\ell}^{(r)}(k1, k1) = \frac{1}{2i} \tanh \frac{1}{2} \beta \epsilon_{k}^+. \quad (2.28)$$

We get

$$\langle K-k, K+k \mid \Omega(v) \mid K-p, K+p \rangle = \delta(k-p)$$

$$+ F(K, k; \nu) \sum_{q} \hat{V}_{q} \langle K-k+q, K+k-q \mid \Omega(v) \mid K-p, K+p \rangle,$$

with

$$F(K, k; \nu) = \frac{1}{2} \left[ \tanh \frac{1}{2} \beta \epsilon_{K-k}^+ + \tanh \frac{1}{2} \beta \epsilon_{K+k}^- \right]. \quad (2.30)$$

We have put $\nu_{1} + \nu_{2} = 2\nu$.

The solutions of the homogeneous equation

$$\psi(K, k; \nu) = F(K, k; \nu) \sum_{P} \hat{V}_{|k-p|} \psi(K, p; \nu) \quad (2.31)$$

will now be discussed. Take the zero temperature limit $\beta \to \infty$, $2\pi i \nu / \beta \to E$, and, as the density of positrons is very low, we need keep only particle-particle correlations:

$$\lim_{\beta \to \infty} \left[ \tanh \frac{1}{2} \beta \epsilon_{K-k}^+ + \tanh \frac{1}{2} \beta \epsilon_{K+k}^- \right] = \theta^+(\epsilon_{K-k}^+) \theta^+(\epsilon_{K+k}^-), \quad (2.32)$$

where $\theta^+(x) = 1$ if $x \geq 0$, zero otherwise. Therefore (2.31) becomes

$$(E - \epsilon_{K-k}^+ - \epsilon_{K+k}^-) \psi(K, k; E) = \sum_{|k-p| \geq \epsilon_E, \epsilon_K, \epsilon_p \geq \epsilon_F} \hat{V}_{|k-p|} \psi(K, p; E). \quad (2.33)$$

In the centre of mass system $K=0$ and $-E = E_B$, the binding energy. We also have $\mu_{e}^0 = k_{F}^2 / 2m$, $\mu_{p}^0 = (k_{F}^+)^2 / 2m$ and $k_{F} \gg k_{F}^+$. So we get

$$(E_{B} + 2\epsilon_{k} - \mu_{e}^0 - \mu_{p}^0) \psi(k, E_{B}) = \sum_{|k-p| \geq k_{F}} \hat{V}_{|k-p|} \psi(p, E_{B}). \quad (2.34)$$

This is the bound state equation. (Compare our other derivation given in the preceding paper.) By putting $\hat{V} = V$, and neglecting $\mu_{e}^0$, $\mu_{p}^0$ and the exclusion principle, one gets the equation for positronium. The solution for this limiting case is well known from the solution of the hydrogen atom in the momentum
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There are three distinct manifestations of the many-body problem. The binding energy is measured with reference to the chemical potential \( \mu_0 \) (we shall neglect the small \( \mu_p \)); there is a screening of the potential, and the Fermi distribution makes certain momentum states unavailable. Clearly we have three possibilities: (i) the extreme low density case, when \( \mu_0 \) is small, and a positronium-like state may exist with \( \mu_0 \ll E_B \); (ii) the unphysical situation \( E_B < \mu_0 \), where auto-ionization will prevent any bound state formation, and (iii) the critical density case \( E_B = \mu_0 \). It is the last we have to consider in detail.

§ 3. Solution of the bound state equation

To obtain explicit answers, we shall first use the Thomas-Fermi dielectric function, so that the interaction term can be written as

\[
\tilde{V}_{k-p} = -4\pi e^2/\nu \left[ |k-p|^2 + k_s^2 \right],
\]

where \( \nu \) is the volume of the system, and

\[
k_s = 0.82 r_s^{-1/3} k_F.
\]

Equation (2·34) now becomes

\[
k^2 \phi(k) = \frac{me^2}{2\pi^2} \int_{|p| \geq k_F} \frac{d^3p \phi(p)}{|k-p|^2 + k_s^2}.
\]

We will look for only spherically symmetric solutions, so that \( \phi(k) \) is a function of \( |k| \) only. The angular integration can then be done. Introducing the variable transformations

\[
k = k_F/x, \quad p = k_F/y, \quad \phi(k) k^3 = u(x), \quad \phi(p) p^3 = u(y),
\]

we get

\[
u(x) = \lambda \int_1^y dx \ln \frac{(x+y)^2 + \nu^2 x^2 y^2}{(x-y)^2 + \nu^2 x^2 y^2},
\]

where

\[
\lambda = \frac{me^2}{2\pi k_F} = \alpha r_s/2\pi,
\]

\[
\nu = k_s/k_F = 0.82 r_s^{-1/3},
\]

\[
\alpha = \left(4/9\pi\right)^{1/3}.
\]

Note that for any fixed \( r_s \), \( \nu \) is known and the kernel is a simple Fredholm kernel. The eigenvalue \( \lambda \) is however, itself a function of \( r_s \), so that (3·5) is really a non-linear equation for \( r_s \).

The non-linearity disappears if \( \nu = 0 \), that is, if we take purely Coulomb interaction between the particles, maintaining however the Pauli principle restric-
tions on the scattering. This kind of interaction is used by Kanazawa et al., and they found a bound state at $r_s = 4.521$ for their equation. In our case an exact solution is possible in this $\nu = 0$ case. Note $u(x)$ is odd in $x$, and we can write

$$u(x) = \lambda \int_{-1}^{1} dy u(y) \ln \left| \frac{x+y}{x-y} \right|.$$ (3.7)

Make the transformation

$$x = \cos \theta, \quad y = \cos \phi, \quad u(\cos \theta) = V(\theta), \quad u(\cos \phi) = V(\phi)$$ (3.8)

and use the identity

$$\ln \left| \frac{\cos \theta + \cos \phi}{\cos \theta - \cos \phi} \right| = \sum_{n=0}^{\infty} \frac{4}{2n+1} \cos(2n+1)\theta \cos(2n+1)\phi.$$ (3.9)

The solution is

$$V(\theta) = 4\lambda \sum_{n=0}^{\infty} \frac{\cos(2n+1)\theta}{2n+1} C_{2n+1},$$ (3.10)

with

$$C_{2n+1} = \int_{0}^{\pi} V(\phi) \cos(2n+1)\phi \sin \phi d\phi.$$ (3.11)

This leads to the equations

$$C_{2m+1} = 4\lambda \sum_{n=0}^{\infty} \frac{1}{2n+1} A(m, n) C_{2n+1},$$ (3.12)

with

$$A(m, n) = -2 \left[ \frac{(2m+1)^2 + (2n+1)^2 - 1}{(2m+2n+3)(2m+2n+1)} \right].$$ (3.13)

The eigenvalues are given by the infinite determinant

$$\det \left| \frac{1}{\lambda} \delta_{mn} - \frac{4}{(2m+1)^{1/2}(2n+1)^{1/2}} A(m, n) \right| = 0.$$ (3.14)

The largest eigenvalue is sufficient for our purpose, and can be calculated on the computer by progressively increasing the size of the determinant. The largest eigenvalue comes out to be $1/\lambda = 3.132$ for a $8 \times 8$ determinant, and does not change on increasing the size of the determinant to $40 \times 40$. Hence, the bound state formation starts at

$$r_s = \frac{2\pi}{\alpha \cdot \frac{1}{3.132}} = 3.85$$ (3.15)

and is possible for lower density (larger $r_s$).

Since (3.7) is a Fredholm type equation, a simple variational attack is pos-
sible, and this works for finite \( \nu \) as well. Consider a variational solution
\[
\phi(x) = \sqrt{3}x. \tag{3.16}
\]
This is properly normalized and goes to zero at \( x = 0 \). Then the critical value of \( r_e \), denoted by \( r_{sc} \), satisfies the inequality
\[
\left( \frac{\alpha r_{sc}}{2\pi} \right)^{-1} = \frac{1}{\lambda_0} \geq 3 \int_0^1 dx \int_0^1 dy 2xy \ln \left| \frac{x+y}{x-y} \right| = 3
\]
so that
\[
r_{sc} \leq 4.019. \tag{3.17}
\]
For the more general case of fixed but finite \( \nu \), we can obtain the upper and lower bounds of the lowest eigenvalue \( \lambda_0 \). Note that the kernel
\[
K(x, y; \nu) = \ln \frac{(x+y)^2 + \nu^2 x^2 y^2}{(x-y)^2 + \nu^2 x^2 y^2} \tag{3.18}
\]
vanishes at \( x = 0 \), so that \( u(0) = 0 \). We use (3.16) again to obtain the upper bound of \( r_{sc} \).
\[
\left( \frac{\alpha r_{sc}}{2\pi} \right)^{-1} = \frac{1}{\lambda_0} \geq 1 \int_0^1 dx \int_0^1 dy \phi(x) K(x, y; \nu) \phi(y). \tag{3.19}
\]
The upper bound for a fixed \( \nu \) is numerically calculated and plotted in Fig. 1. It is easily proved that \( K(x, y; \nu) \) is monotonically decreasing function of \( \nu \). By the Weyl-Courant lemma the eigenvalue \( \lambda_0(\nu) \) will be a monotonically increasing function, so that the exact \( r_{sc} \) value increases with \( \nu \).

To obtain the lower bound of the lowest eigenvalue \( \lambda_0 \), notice that the sum of the reciprocals of the eigenvalues is finite for finite \( \nu \). This is simply the statement about the trace of the kernel
\[
S = \sum_{n=0}^{\infty} \frac{1}{\lambda_n} = \int_0^1 K(x, x; \nu) dx
\]
\[
= \ln(4 + \nu^2) - 2 \ln \nu + \frac{4}{\nu} \tan^{-1} \frac{\nu}{2}. \tag{3.20}
\]
As \( \nu \to 0 \), the sum \( S \) diverges logarithmically. Even in the limit \( \nu = 0 \), we have a Fredholm type equation (3.7), so this divergence is not due to any particular eigen-
value approaching zero, but is a property of the sum. As the kernel is positive definite, we must have

\[ S = \sum_{n=0}^{\infty} \frac{1}{k_n} \geq 1 \quad \text{or} \quad \frac{\alpha r_{sc}}{2\pi} \geq 1. \]  

(3·21)

This lower bound is also plotted in Fig. 1.

The equation (3·5) may, of course, be replaced by a set of linear equations, and the eigenvalue sought from the zeros of the secular determinant evaluated on a CDC 3600 computer. For \( \nu = 1 \) and 1.5 these exact eigenvalues thus derived are also shown on Fig. 1. The size of the final determinant is 40 \( \times \) 40. For \( \nu = 2 \), even an increase of the determinant size to 60 \( \times \) 60 did not produce a value better than the upper bound, which is probably very close to the exact value here.

The solution \( r_s \) of the non-linear equation (3·5) may now be obtained as follows. Since \( \nu \) is a function of \( r_s \), we require a self-consistent solution. Starting from any \( r_s \), we fix \( \nu \), and the final eigenvalue \( r_s \) must be equal to the starting value. If we now plot \( \nu \) given by (3·6) in Fig. 1, the intersection of this curve with the exact eigenvalue curve must give the self-consistent solutions. The figure clearly shows that there are no intersections of the Thomas-Fermi screening curve with the exact curve in the metallic region of \( r_s \), in fact certainly none below \( r_s \approx 15 \). In most of the metallic region, the screening curve is lower than the lower bound.

The result is, however, quite sensitive to the exact form of screening. For instance if we use the Sawada-Brout cutoff wave vector \( k_c = 0.47r_1^{1/3}k_F \) as the screening wave vector, the limiting value is \( r_s \approx 12 \) (see Fig. 1); again there is no solution in the metallic region.

In (3·1), we could have used the complete static dielectric function of the electron gas. Corresponding to (3·3), we obtain an integral equation with a rather complicated kernel. One can verify that the kernel is still of Fredholm type, but an explicit solution is rather difficult. Held and Kahana solved the problem variationally to get the binding energy as a function of \( r_s \). We can use their result to estimate the critical \( r_{sc} \) with static dielectric function. The binding energy has to be made equal to \( E_B = k_e^2/2m = (1/2\alpha^2 r_s^2) \cdot (e^2/\alpha_0) \) where \( \alpha = (4/9\pi)^{1/3} \). We look for the value of \( r_s \) where the curve for \( E_B \) as a function of \( r_s \) intersects their energy curve. The value of \( r_{sc} \) obtained in this way is \( r_{sc} = 9.8 \), higher than their old estimate 8.5. The result is physically plausible because the potential corresponding to the static dielectric constant has a much longer range than the potential (3·1) with Thomas-Fermi screening; this longer range helps in the binding of charge.

§ 4. Discussion

It is clear that a bound state of a positron and an electron does not form in a metal, and the electron gas theory gives \( r_{sc} \) higher than previously thought.
Experiments on metal ammonia solutions, where the free electron density can be varied to some extent, have been done to examine this question. However, as already recognized, the applicability of the electron gas theories to the metal ammonia solutions is doubtful. The value $r_{se}$ is in a region where the results of the electron gas theory are not reliable. Also the problem of positrons in metal ammonia solutions is complicated by formation of polarized atomic clusters around the positronium.

One can also show that the bound state formation is not helped by phonons. If electron-phonon and positron-phonon interactions are included, the static limit of (2.21) cannot be obtained. The subsequent analysis has to be replaced by the more complete analysis of the equation with frequency dependent dielectric function (cf. footnote on page 9). Passage into the superconducting state does not have any effect because one can show that the kernel becomes repulsive, rather than attractive, in this state. (See Rajagopal and Majumdar.)

References