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APPLICATION OF THE VARIATIONAL PRINCIPLE FOR THE DETERMINATION OF THE BINDING ENERGY OF A PROTON-ELECTRON-POSITRON SYSTEM

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The energy of a system of three particles, proton, electron, and positron, has been determined by the variational method. It is found to be $E \leq 0.563$ Ry. The system can only dissociate into a proton and a positronium atom, with the dissociation energy $|\epsilon| \geq 0.063$ Ry.

1. FORMULATION OF THE PROBLEM

WE consider the problem of the determination of the ground state of a system consisting of a fixed (at the origin) proton and two particles, an electron and a positron, moving in the field of the proton.

Let r_1 be the distance between the proton and the electron, r_2, that between the proton and the positron, and r_{12}, the distance between the electron and the positron. The potential energy of the system is

$$U_1 = e^2/r_2 - e^2/r_1 - e^2/r_{12}. \tag{1}$$

It was shown by Hylleraas[1] and Breit[2] that it is possible to separate the variables in the wave function of two particles moving in a Coulomb field. The equation in six variables is thus reduced to an equation in three variables, r_1, r_2, and the angle θ between r_1 and r_2, which determine the relative position of the particles. The three remaining variables determine the total angular momentum L of the whole system. This method leads to the following Schrödinger equation for the ground state ($L = 0$):

$$\frac{1}{r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial\psi}{\partial r_1}\right)+\frac{1}{r_2^2}\frac{\partial}{\partial r_2}\left(r_2^2\frac{\partial\psi}{\partial r_2}\right) + \left(\frac{1}{r_1}+\frac{1}{r_2}\right)\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\psi}{\partial\theta}\right)\right] + \frac{2m}{\hbar^2}(E-U_1)\psi = 0. \tag{2}$$

In solving the analogous problem of the helium atom one chooses as a first approximation that solution in which the interaction between the electrons is neglected. In our case this is not possible, since our system would not even exist without the attraction between the electron and the positron. A separation of variables in Eq. (2) is therefore impossible.

We find the solution to Eq. (2) by the variational method. In choosing a trial function we must use those methods of solution of the problem of the helium atom in which the variables are not separated. The solutions of Hylleraas[3] and Slater[4] are of this kind. We must also consider the physical characteristics of the system; we note that it is analogous to the ionized hydrogen molecule consisting of two protons and one electron. In deciding what should be the form of the solution of Eq. (2) we must therefore pay attention to the following facts. It is known that the problem of the hydrogen ion reduces mathematically to the problem of two centers: find the stationary states of the electron in the field of two fixed positive charges with the relative distance R. The solution can be found using the methods of Born and Oppenheimer,[5] who made a general study of the system consisting of several protons and electrons. These authors show that the wave functions of the protons can generally be regarded as solutions of the equation of motion of particles in a potential well given by the electrons moving in the field of the protons. Let ξ be the set of electron coordinates relative to the protons, and x the set of relative proton coordinates. The wave function can then be written in the form

$$\psi(x, \xi) = \Phi_0(x)F_0(x, \xi) + \Phi_1(x)F_1(x, \xi) + \cdots.$$

Here $F_0(x, \xi)$, as a function of the coordinates ξ, is the wave function of the ground state of the electrons in the field of the fixed protons. It depends on the proton coordinates x parametrically. The energy of the system of electrons, $V(x)$, is then also a function of the parameters x. The function $\Phi_0(x)$ is the wave function of the system of protons in the first approximation. The quantity

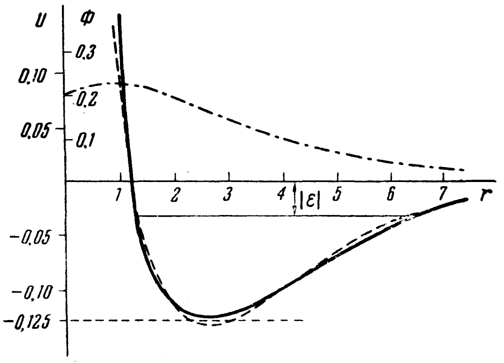
V (x) appears as the potential energy of the coupling of the system of protons:

$$\nabla_x^2\Phi_0(x) + (2M/\hbar^2)(E_p - V(x))\,\Phi_0(x) = 0,$$

where M is the mass of the proton. The potential V (x) is no other than the potential of the exchange forces which couple the heavy nuclei of the molecules.

These results not only suggest the choice of the trial function, but also play a decisive role in the analysis of the solution and of the character of the forces binding our system. It should be recalled at this point that the potential V (x) for the ionized hydrogen molecule has the form of a well similar to the one shown in the figure (see below), where x stands for the distance between the protons, r. The minimum of 0.1025 atomic units is located at the distance $r_m = 2a_0$ (a_0 is the Bohr radius) between the protons; as the protons come closer to each other the potential increases according to the Coulomb law e^2/r, while it goes to zero as $-\frac{4}{3}re^{-r}$ at large relative proton distances.

The Born-Oppenheimer method is based on the fact that the ratio of the electron mass m to the proton mass M is small, so that the wave function can be expanded in powers of m/M. In our case the proton is replaced by the positron, which has a mass equal to that of the electron. However, a method of solution analogous to that of Born can be found even for this system. This was done by Slater[4] in the solution of the problem of the helium atom. He regarded one electron as fixed at the distance r_1, and determined the motion of the other electron in the field of the two centers (+e) and (−e). Slater first found the energy of the second electron, $V(r_1)$, as a function of the distance r_1 between the nucleus and the first electron (which enters as a parameter), and then regarded this energy as a field of conservative forces imposed on the first electron by the remaining part of the system. This is equivalent to the Born method. Slater pointed out the great accuracy of this method, which allowed him to restrict himself to the first approximation. Hylleraas[3] also remarks on the accuracy of the Slater method.



Solid curve: potential U of formula (23) in atomic units, counted from (−1/4) as the zero point; dotted curve: the function (24); dash-dotted curve: the wave function Φ(r).

In our problem we denote the position of the proton by the point a, and put the positron at the fixed point b. The coordinate of the positron, $r_2 = R$, will then be a constant parameter in Eq. (2). This leads us to the problem of two centers. Its solution is given by a system of wave functions of the hydrogen ion which depend on the distance $r_2 = R$ as on a parameter. This system of functions is found in a known fashion by separating the variables in elliptic coordinates:

$$\xi_0 = (r_1 + r_{12})/R, \qquad \eta_0 = (r_1 - r_{12})/R \tag{3}$$

The functions can be written in the form

$$F_{nlm}(R;\ \xi_0,\ \eta_0) = X_n(R,\ \xi_0)\,Y_{lm}(R,\ \eta_0). \tag{4}$$

We shall seek the solution of the equation in the form of an expansion in terms of the normalized eigenfunctions of the problem of two centers, $F_{nlm}(r_2;\ r_1,\ r_2)$:

$$\psi = \Phi_0(r_2)\,F_{00\sigma}(r_2;\ r_1,\ r_{12}) + \Phi_1(r_2)\,F_{10\sigma}(r_2;\ r_1,\ r_2) + \cdots$$

We note that the expansion includes only functions $F_{nl\sigma}$ with the index σ, which corresponds to the vanishing of the projection of the angular momentum on the proton-positron axis. In the present paper we restrict ourselves to the first term in the expansion only. As we are using the variational principle, the corrections to the wave function can only lower the energy level. According to Slater and Born, Φ_0 must be the first approximation to the positron wave function. However, this function is somewhat more complicated than in the aforementioned papers.

2. THE LAGRANGE FUNCTION AND THE WAVE FUNCTION

We introduce the variables

$$r = r_2, \qquad \xi = r_1 + r_{12}; \qquad \eta = r_1 - r_{12}. \tag{5}$$

Fixing the positron coordinate r, we obtain the elliptic coordinates (3) of the electron: $\xi_0 = \xi/r$, $\eta_0 = \eta/r$. Let $F(r;\ \xi,\ \eta)$ be the wave function (4) of the ground state of the electron in the field of the positive charges fixed at the distance r. For the trial function we take

$$\psi(r,\ \xi,\ \eta) = \Phi(r)\,F(r;\ \xi,\ \eta), \tag{6}$$

in analogy to Slater's solution of the problem of the helium atom.[4] Following Slater, we must regard $F(r;\ \xi, \eta)$ as a wave function in the variables ξ_0 and η_0, normalized to unity. The normalization factor $A(r)$ is a function of the parameter r:

$$F(r;\ \xi,\ \eta) = A(r) f(r;\ \xi,\ \eta). \tag{7}$$

Knowing the volume element and the normalization condition in elliptic coordinates, we can write this condition also in the coordinates (5):

$$\frac{1}{r}\frac{\pi}{4}\int_{r}^{\infty} d\xi \int_{-r}^{+r} d\eta\,(\xi^2-\eta^2)\,F^2(r;\ \xi,\ \eta) = 1. \tag{8}$$

Substituting in this formula the expression (7) for F, we obtain the following relation:

$$\frac{\pi}{4}A^2(r)\,J(r) = 1,$$

$$J(r) = \frac{1}{r}\iint f^2(r;\ \xi,\ \eta)\,(\xi^2-\eta^2)\,d\xi d\eta. \tag{9}$$

The quantity J (r) can be used to simplify the later calculations. According to Slater, the function $\Phi(r)$ is the wave function for the motion of a particle in some spherically symmetric potential well, normalized to unity. However, the simple method for finding this function which Slater employed in the helium problem cannot be applied in the present case.

We solve the problem in the following fashion. The wave function (6) and the lowest energy level E are determined by the minimum condition for the functional

$$E = \iiint L(r,\ \xi,\ \eta,\ \partial\psi/\partial r,\ \partial\psi/\partial\xi,\ \partial\psi/\partial\eta,\ \psi)\,d\tau. \tag{10}$$

Here L is the Lagrange function for the proton-electron-positron system in the coordinates (5). It is known that the integral (10) is equal to the energy of the system if ψ is the solution of Eq. (2), normalized to unity. We find the volume element $d\tau$ and the normalization condition in terms of the coordinates (5) from the analogous formulas in terms of the coordinates r_1, r_2, and r_{12}:[3]

$$\iiint \psi^2 d\tau = \pi^2 \int_0^{\infty} r dr \int_r^{\infty} d\xi \int_{-r}^{+r} d\eta\,(\xi^2-\eta^2)\,\psi^2 = 1. \tag{11}$$

With condition (8), this leads to the following normalization for the function $\Phi(r)$:

$$4\pi\int_0^{\infty}\Phi^2 r^2 dr = 1.$$

For the determination of the Lagrange function it is convenient to use the analogous function for the helium atom, derived by Hylleraas[3] in terms of the coordinates r_1, r_2, and r_{12}, but to define the potential according to formula (1). We note that the transformation (5) is reminiscent of the transformation used by Hylleraas in the paper just mentioned. Making use of this analogy, we find the Lagrange function for the proton-electron-positron system in terms of the coordinates (5):

$$\begin{aligned} L d\tau = \pi^2 e^2 r \Big\{ a_0 \Big[& \frac{5\xi^2-\eta^2-4r^2}{2}\left(\frac{\partial\psi}{\partial\xi}\right)^2 \\ & + \frac{\xi^2-5\eta^2+4r^2}{2}\left(\frac{\partial\psi}{\partial\eta}\right)^2 + \frac{\xi^2-\eta^2}{2}\left(\frac{\partial\psi}{\partial r}\right)^2 \\ & - (\xi^2-\eta^2)\frac{\partial\psi}{\partial\eta}\frac{\partial\psi}{\partial\xi} + \frac{r^2-\xi\eta}{r}(\xi+\eta)\frac{\partial\psi}{\partial r}\left(\frac{\partial\psi}{\partial\xi}-\frac{\partial\psi}{\partial\eta}\right)\Big] \\ & + \left(\frac{\xi^2-\eta^2}{r} - 4\xi\right)\psi^2\Big\} dr d\xi d\eta. \end{aligned} \tag{12}$$

In the following we shall use atomic units (the energy unit in this system is twice the energy of the hydrogen atom, i.e., 2 Ry). In going over to this system we must set $a_0 = 1$ and $e = 1$ in the Lagrangian (12).

We must now write down the explicit expression for the wave function of the ground state of the hydrogen ion (4): $n = 0$, $l = 0$, and $m = \sigma$. At this point we note the following peculiarity. The system of functions (4) was obtained by separating the variables in elliptic coordinates (3). For each value of the distance R between the positive charges we separately determine a set of eigenvalues and eigenfunctions. The function F, therefore, depends on R as on a parameter, but there is no analytic expression for this dependence. As for the analytic dependence on ξ_0 and η_0, it is natural to refer to that form of the wave function (4) which was found by the variational method. Teller[6] has used the variational principle to calculate those functions $X_n(R, \xi_0)$ of the system (4) which have no nodes. He found the following approximate expression for the ground state:

$$X_0(R,\ \xi_0) = C\exp(-\sqrt{\gamma_0}\,\xi_0), \tag{13}$$

where γ_n is the eigenvalue in the equation for the function $X_n(R, \xi_0)$. The magnitude of this eigenvalue depends, first, on its number, but it is also a function of the distance R. Teller has given a table of the first few eigenvalues as a function of R. Guillemin and Zener[7] also determined the ground state wave function from the system (4) with great accuracy. Their choice was based on the following considerations.

It is known that, if the distance between the centers a and b is increased to infinity, then the elliptic coordinates (3) go over into parabolic coordinates with respect to that center which is at a finite distance from the electron. If, on the other hand, the charges a and b are brought together in the point O, the equations for X_n

and Y_{lm} go over into the equations of the Laguerre polynomials for the radial function of the helium atom and into the equations of the spherical functions, respectively. For large distances R between the centers a and b the wave functions (4) themselves go over into a symmetric combination of the wave functions of the hydrogen atom at the points a and b. If the charges are brought together at one point, these functions go over into the wave function of the helium atom:

$$\Psi_{R\to 0} = 2\sqrt{2/\pi}e^{-2r_0}, \qquad \Psi_{R\to\infty} = (e^{-r_a} + e^{-r_b})/\sqrt{2\pi}. \quad (14)$$

Guillemin and Zener therefore require that the wave function, firstly, satisfy the boundary conditions (14), and, secondly, that it can be expressed in the form of the product $X(\xi_0)Y(\eta_0)$. This function then has the form

$$\Psi(R;\ \xi_0,\ \eta_0) = Ce^{-\alpha R\xi/2}(e^{-\beta R\eta_0/2} + e^{+\beta R\eta_0/2}). \quad (15)$$

The normalization factor $C(R)$ and the quantities $\alpha(R)$ and $\beta(R)$ are continuous functions of the parameter R. In virtue of the foregoing properties of the elliptic coordinates (3), the function (15) satisfies the boundary conditions (14) if $\alpha(R)$, $\beta(R)$, and $C(R)$ satisfy the boundary conditions

$$\alpha(0) = 2, \qquad \beta(0) \text{ finite}, \qquad C(0) = 2/\sqrt{2\pi};$$
$$\alpha(\infty) = 1, \qquad \beta(\infty) = 1, \qquad C(\infty) = 1/\sqrt{2\pi}. \quad (16)$$

Guillemin and Zener find $\alpha(R)$ and $\beta(R)$ from the minimum conditions for the functional. They also give a table of these quantities for several values of R together with a derivation of the general formula. Teller's[6] tables for the function $\gamma(R)$ in formula (13) correspond to the quantity $2\sqrt{\gamma} = R\alpha$.

We therefore seek the wave function in the form (6). Here F is the ground state function for the problem of two centers, the parameter R becoming the independent variable r. In the coordinates (5) this function is written, according to (7) and (15),

$$F = Af, \qquad f = e^{-\alpha\xi/2}\cosh(\beta\eta/2). \quad (17)$$

$\alpha(R)$ and $\beta(R)$ are continuous functions determined from the tables of references 6 and 7 and the boundary conditions (16). The normalization factor $A(r)$ has, according to (16), the following values at the ends of the half axis $0 \le r < \infty$:

$$A(0) = 4/\sqrt{2\pi}, \qquad A(\infty) = 2/\sqrt{2\pi}. \quad (16a)$$

Integrating over ξ and η in (9), we can write the function $J(r)$ in the explicit form

$$J(r) = \frac{2e^{-\alpha r}}{\alpha}\left\{\frac{r^2}{3} + \frac{1}{\alpha}\left(r + \frac{1}{\alpha}\right)\left(1 + \frac{\sinh\beta r}{\beta r}\right)\right.$$
$$\left. + \frac{1}{\beta^2}\left(\cosh\beta r - \frac{\sinh\beta r}{\beta r}\right)\right\}. \quad (18)$$

Using the boundary conditions (16) for α and β, we can show that

$$J(0) = {}^1/_2, \qquad J(\infty) = 2. \quad (18a)$$

Substitution of the numerical values of references 7 and 6 shows that J is a monotonically increasing function of r. The normalization conditions (8) and (9) at the points $r = 0$ and $r \to \infty$ are automatically fulfilled by virtue of Eqs. (16a) and (18a). At intermediate points the factor $A(r)$ is determined by the first of the formulas (9) and formula (18).

3. SOLUTION OF THE PROBLEM

In solving the problem by the variational method we substitute the Lagrangian (12) in the integral (10) and integrate over the volume in the manner indicated in formula (11). The trial function (6) is conveniently written in the form

$$\psi = \Phi F = \varphi(r)f(r;\xi,\eta), \qquad \varphi(r) = \Phi(r)A(r). \quad (19)$$

The function $\varphi(r)$ is unknown. The integration over the variables ξ and η does not cause any basic difficulties but is very cumbersome. With the help of the function $J(r)$ the calculations can be somewhat simplified. Using Eq. (18), we can write the result in the form

$$E = \pi^2\int_0^\infty\left\{\frac{r^2}{2}\frac{d\varphi}{dr}\frac{d}{dr}(J\varphi) + r\chi(r)\varphi^2\right\}dr,$$
$$\pi^2\int_0^\infty \varphi^2 Jr^2 dr = 1. \quad (20)$$

Here $\chi(r)$ is a function of r, both explicitly and implicitly through $\alpha(r)$ and $\beta(r)$. After some simple calculations, using (9) and (19), we can replace the function $\varphi(r)$ in the integral (20) by the normalized function $\Phi(r)$. Then formulas (20) take the form

$$E = 4\pi\int_0^\infty\left\{\frac{1}{2}\left(\frac{d\Phi}{dr}\right)^2 + \left[\frac{\chi(r)}{rJ} - \frac{J_r^2}{8J^2}\right]\Phi^2\right\}r^2\,dr,$$
$$4\pi\int_0^\infty \Phi^2 r^2 dr = 1. \quad (21)$$

Here J_r is a total derivative:

$$J_r \equiv dJ/dr = \partial J/\partial r + \alpha_r\partial J/\partial\alpha + \beta_r\partial J/\partial\beta.$$

Equations (21) define the isoperimetric problem of variational calculus, which can be reduced to the problem of the absolute minimum of the functional

$$S^* = 4\pi \int_0^\infty L^* r^2 \, dr, \tag{21a}$$

where we take $L^* = L + \lambda\Phi^2$ for the new Lagrangian. It is known from quantum mechanics that the factor λ in the Lagrangian in this case determines the energy of the system: $\lambda = -E$. The Euler equation for the functional S^* gives

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) - 2\left[\left(\frac{\chi(r)}{rJ} - \frac{J_r^2}{8J^2}\right) + \lambda\right]\Phi^2 = 0.$$

This is the equation of motion of a particle in a spherically symmetric potential field,

$$\frac{1}{2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) - (U(r) - E)\,\Phi = 0 \tag{22}$$

with the potential energy (in atomic units)

$$U(r) = \chi / rJ - J_r^2 / 8J^2, \tag{23}$$

given by the explicit formula

$$\begin{aligned}U(r) = {} & \frac{1}{r} + \frac{5\beta^2}{8} + \frac{1}{8rJ}\left(\frac{\partial}{\partial r} + \alpha_r\frac{\partial}{\partial\alpha} + \beta_r\frac{\partial}{\partial\beta}\right)^2 (rJ) \\ & - \frac{J_r^2}{8J} + \frac{e^{-\alpha r}}{J\alpha}\left\{\left(r + \frac{1}{\alpha}\right)\left(\frac{5\alpha}{4} - \frac{5\beta^2}{4\alpha} - 4\right)\left(\frac{\sinh r\beta}{r\beta} + 1\right)\right. \\ & \left. - \beta^2\left(\frac{5r^2}{6} + \frac{r}{4\alpha} + \frac{1}{4\alpha^2}\right) + \left(\frac{1}{4}\cosh r\beta + \frac{\alpha}{\beta}\sinh r\beta + \alpha r + 1\right)\right\} \\ & + \frac{\alpha_r}{2}\left(1 + \frac{1}{\alpha r}\right) - \frac{\alpha_r}{2}\frac{e^{-\alpha r}}{J\alpha}\left(\frac{r}{\alpha} + \frac{1}{\alpha^2} + \frac{1}{r\alpha^3}\right)\left(\frac{\sinh r\beta}{r\beta} + 1\right) \\ & - \beta_r^2\frac{e^{-\alpha r}}{J\alpha}\frac{r^2}{12}\left(\frac{r^2}{5} + \frac{r}{\alpha} + \frac{1}{\alpha^2}\right) \\ & + \frac{\beta_r}{2\beta}\frac{e^{-\alpha r}}{J\alpha}\left\{\left(r + \frac{1}{\alpha}\right)\left[\frac{2}{\alpha r}\left(\cosh r\beta - \frac{\sinh r\beta}{r\beta}\right) - \frac{r\beta^2}{3\alpha}\right]\right. \\ & \left. + \frac{3}{r\beta^2}\left(\cosh r\beta - \frac{\sinh r\beta}{r\beta}\right) - \frac{\sinh r\beta}{\beta}\right\}.\end{aligned} \tag{23a}$$

For $r \to 0$ the potential increases according to the Coulomb law:

$$U_{r\to 0} \approx 0.63 / r.$$

As the proton and the positron come close to each other there should be a repulsion given by the potential $(1/r)$. Hence we have here a screening effect. The behavior of the potential at infinity is determined by the boundary conditions (16) and (18a):

$$\lim U_{r\to\infty} = -\frac{1}{4} \text{ at. units}.$$

The first (Coulomb) term in formula (23a) cancels out, and the potential decreases exponentially as $r \cdot \exp(-0.49\,r)$. The intermediate points were calculated with the help of the tables of references 7 and 6. The resulting curve is shown in the figure (solid curve). It has the same behavior for $r \to 0$ and $r \to \infty$ as the potential for the ionized hydrogen molecule. Its minimum (0.375 at. un.) lies at $r_m = 2.5$. The limit at infinity of this quantity is the energy of the positronium atom $(-1/4)$. Thus the "free energy" amounts to only 0.125 at. un. of the total depth of the potential well (0.375 at. un.), while the remaining 0.25 at. un. represent the "bound" (internal) energy of positronium. The quantity $U(r)$ and the potential of the hydrogen ion are therefore comparable with each other: the minimum of $U(r)$ is somewhat lower and is located further away from the proton than is the case for the hydrogen atom.

The potential (23), therefore, has the same properties as the potential of the molecular forces binding the atomic nuclei in a homeopolar molecule. Hence the forces binding the positron have a quantum nature. They arise from the fact that the electron may be observed near the proton as well as near the positron, i.e., it belongs to both these particles simultaneously. This circumstance is incorporated in the choice of the form of the trial function (5). It was proposed by Ferrell[8] that the forces coupling the positron to the molecules of the medium have a potential of the same form as the $U(r)$ shown in the figure. In the calculation of the potential of the hydrogen molecule Hylleraas[9] assumed 50% screening of the nuclei, since a screening of this magnitude leads to good agreement with experiment. In our case the screening is also close to 50%.

We now compute the ground energy level in Eq. (22). We use the following approximate formula for the potential (23):

$$\begin{aligned}U = U_0 + U_q = {} & 0.13\,[\exp(-0.96x) - 2\exp(-0.48x)] \\ & + (2r)^{-1}\exp(-2r)\end{aligned} \tag{24}$$

(in atomic units), where $x = r - 2.5$. This potential has the level $-1/4$ as zero point. Accordingly we introduce $\epsilon = E + 1/4$ instead of the energy E. The dotted curve representing the potential (24) in the figure runs very close to the curve representing the potential (23). The main term in formula (24), U_0, is the well-known Morse potential.[10] The other term in (24) vanishes everywhere except near the origin of the coordinate system. We can obtain an exact solution of Eq. (22) by taking U_0 instead of U. For this purpose we make use of the method given in the book of Schiff.[11] After the substitution $\Phi(r) = v(r)/r$ Eq. (22) goes over into

$$v''(r) = (U_0 - \varepsilon_0)\,v(r) = 0$$

According to Schiff we must find a solution $v(r)$ which is zero at $r = 0$ and $r = \infty$. We solve the abovementioned equation by the method outlined in the book of Landau and Lifshitz.[10] After the substitution

$$z = (2\sqrt{0.13}/0.48)\, e^{-0.48x}, \qquad s = \sqrt{-\varepsilon_0}/0.48,$$
$$n = \sqrt{0.13}/0.48 - (s + 1/2), \qquad v(z) = e^{-z/2} z^s w(z),$$

we obtain the hypergeometric equation

$$zw'' + (2s + 1 - z)\, w' + nw = 0.$$

The characteristic equations for its roots are $\rho_1 = 0$ and $\rho_2 = -2s$. Since $z \rightarrow 0$ for $x \rightarrow \infty$, the only solution is the first hypergeometric function $w(z) = {}_1F_1(-n, 2s+1, z)$. The energy ϵ_0 is determined by the second boundary condition

$$\varepsilon_0 = -0.035. \tag{25}$$

We now turn to the potential (23), which is counted from the level -0.5. Equation (22) has the following form near the origin:

$$\nabla_r^2 \Phi - (1.25/r - \varepsilon)\, \Phi = 0.$$

Its characteristic roots are $\rho_1 = 0$ and $\rho_2 = -1$. The first solution therefore does not vanish at the origin. The second solution has there either a pole or a logarithmic divergence and must be discarded. Since the wave function of the ground state has no nodes, we may conclude, after integrating this equation once, that the derivative $\Phi'(r)$ is positive for small r. Assuming that the potential (23) has for large r the form $-k \exp(-\alpha r)$, we transform Eq. (22) to Bessel's equation by the substitution $y = \exp(-\alpha r/2)$. This problem was proposed in the book of Schiff.[11] Its solution is

$$\Phi(r) = J_\nu(by)/r = \frac{1}{r} e^{-\nu\alpha r/2} (B_0 + B_1 e^{-\alpha r/2} + \ldots). \tag{26}$$

The wave function has the form shown in the figure.

We shall solve Eq. (22) by the variational method:

$$\varepsilon = \frac{1}{2} \int_0^\infty (d\Phi/dr)^2 r^2\, dr + \int_0^\infty U(r)\, r^2\, dr, \qquad \int_0^\infty \Phi^2 r^2 dr = 1, \tag{27}$$

where $U = U_0 + U_q$ is the potential (24). Substituting the function

$$\Phi_i(r) = e^{-0.26r} (1 + 0.12\, re^{-0.1r}) / 4.82 \tag{28}$$

in the integral (27), we find the energy value

$$\varepsilon_i = \varepsilon_{0i} + \varepsilon_{qi} = -0.028 + 0.004 = -0.024.$$

Here ϵ_{qi} is the "Coulomb" part of the energy arising from the integral over U_q. The solution of Eq. (22) must have the asymptotic behavior (26). The value of ϵ_i is therefore higher than the actual level. From the minimizing sequence of functions Φ_i we can find the sequence of energies ϵ_i. The calculations show that the absolute value of ϵ_{qi} decreases as the absolute value of the energy ϵ_i increases with the number i. We can therefore assume that the energy $\epsilon_i = \epsilon_{0i} + \epsilon_{qi}$ approaches the limit ϵ_0, corresponding to the solution of Eq. (27) with the potential U_0, plus a correction ϵ_q which does not exceed 0.004. The sequence of ϵ_{0i}, however, has an exact lower limit, namely the solution (25). We can therefore regard

$$\varepsilon = -0.032 \text{ at. units}$$

as the solution of Eq. (22).

4. DISCUSSION

By this method the solution of the variational problem (10) with the boundary conditions (14) to (16) gives in first approximation the value $E = -0.282$ at. un. for the energy of the system. The ionization energy is equal to 0.032, i.e., about one third of that of the hydrogen ion. The system can only disintegrate into a proton and a positronium atom. Since we have used the variational method, the ionization energy found is lower than the actual one. With an appropriate choice of the functions $\alpha(r)$ and $\beta(r)$ (with the same boundary conditions) the potential well (23) can be made deeper. From a theoretical point of view this corresponds to solving the following variational problem: find those functions α and β, satisfying the boundary conditions (14) to (16), which lead to a minimum of the functional (21a). This variation leaves the limit $(-1/4)$ unchanged, since the latter depends only on the boundary conditions (14) to (16).

In comparing these results with those of other authors, we should recall that Simons[12] has made calculations for the "positronium chloride" molecule. He used the electrostatic field due to the negative chlorine ion. This field has been calculated by Hartree by the method of the self-consistent field in order to determine the energy of, for example, a sodium ion located in it. Simons developed a method to solve the problem of the motion of a positron in the field of the chlorine ion and found that the potential well of this ion is sufficiently deep to bind the positron. He obtained a heteropolar molecule analogous to sodium chloride.

By the method given in the present paper we can compute the forces of attraction between a positron (or positronium) and neutral atoms.

The method can also be applied to the helium atom. The calculations would probably confirm the assertion of Ferrell[8,13] that two counter-acting forces act between the positronium and the helium atom: the attractive Van-der-Waals forces and the repulsive forces arising from the fact that the two electrons of the helium atom form a closed shell. These repulsive forces should be the main reason for the formation of the long-lived component in liquid helium, but the Van-der-Waals forces work against this effect. The solution of an equation analogous to equation (2) for the helium-positronium system would lead to results which could be compared with presently available experimental data on positronium in liquid helium.[14] In another article,[15] published recently, Ferrell casts some doubt on the existing belief that the quenching of positronium atoms in gases by adding NO is caused by the exchange of electrons with opposite spins. He assumes that the annihilation is caused by the exchange interaction between the electron of the positronium and the valence electrons of the molecule. After an analysis of the experimental work on the quenching of positronium by DPH (diphenyl picryl hydrazyl) in benzene, Ferrell asserts the following: the annihilation of positronium is due to the capture of the whole positronium atom by the DPH molecule under the action of the covalent coupling between the electron of the positronium and the valence electrons of DPH. Further calculations based on the methods presented in the present paper could, perhaps, help in the resolution of the abovementioned questions.

In conclusion the author expresses his deep gratitude to his adviser, Prof. A. A. Sokolov.

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Translated by R. Lipperheide
83

ERRATA TO VOLUME 9

On page 868, column 1, item (e) should read:

(e). Ferromagnetic weak solid solutions. By way of an example, we consider the system Fe-Me with A2 lattice, where Me = Ti, V, Cr, Mn, Co, and Ni. For these the variation of the moment m with concentration c is

$$dm/dc = (N_d)_{Me} \mp 0.642 \ \{8 \ (2.478 - R_{Me}) + 6\,|2.861 - R_{Me}| \mp [\,8\,(2.478 - R_{\mathrm{Fe}}) + 6\,(2.861 - R_{\mathrm{Fe}})]\},$$

where the signs – and + pertain respectively to ferromagnetic and paramagnetic Me when in front of the curly brackets, and to metals of class 1 and 2 when in front of the square brackets. The first term and the square brackets are considered only for ferromagnetic Me. We then have dm/dc = –3 (–3.3) for Ti, –2.6 (–2.2) for V, –2.2 (–2.2) for Cr, –2 (–2) for Mn, 0.7 (0.6) for Ni, and 1.2 (1.2) for Co; the parentheses contain the experimental values.

ERRATA TO VOLUME 10

Page	Reads	Should Read
224, Ordinate of figure	10^{23}	10^{29}
228, Column 1, line 9 from top	3.6×10^{-2} mm/min	0.36 mm/min
228, Column 1, line 16 from top	0.5 mm/sec	0.05 mm/min
329, Third line of Eq. (23a)	+(1/4 cosh r +...	+1/4(cosh r +...
413, Table II, line 2 from bottom	–0.0924±	–1.0924±
413, Table II, line 3 from bottom	+1.8730±	+0.8370±
479, Fig. 7, right, 1st line	92 hr	9.2 hr
499, Second line of Eq. (1.8)	$+\tilde{k}\sin^2\alpha/\omega_N^2 + \langle c^2\tilde{k}^2 \ldots$	$+\left(\tilde{k}/\omega_H\right)^2 \sin^2\alpha \ \langle c^2\tilde{k}^2 \ldots$
648, Column 1, line 18 from top	18 × 80 mm	180 × 80 mm
804, First line of Eq. (17)	$-{}^1/_3\left(\alpha_x^2\alpha_y^2 + \ldots\right.$	$\ldots - 3\left(\alpha_x\alpha_y^2 + \ldots\right.$
967, Column 1, line 11 from top	$\sigma(N', \pi) \approx 46\,(N', N')$	$\sigma(N', \pi) > \sigma(N', N')$
976, First line of Eq. (10)	$= \frac{e^2}{3r^2c^4}$	$= \frac{e^2}{3\hbar^2c^2}$
978, First line of Eq. (23)	$\left[\frac{(2\gamma^2-1)^2}{(\gamma^2-1)\sin^4(\theta/2)}\right.$	$\left[\frac{(2\gamma^2-1)^2}{(\gamma^2-1)^2\sin^4(\theta/2)}\right.$