

The ground state of a particle under the influence of a uniformly charged sphere

H. X. Jiang and J. Y. Lin

Citation: *American Journal of Physics* **54**, 1046 (1986); doi: 10.1119/1.14823

View online: <http://dx.doi.org/10.1119/1.14823>

View Table of Contents: <http://scitation.aip.org/content/aapt/journal/ajp/54/11?ver=pdfcov>

Published by the American Association of Physics Teachers



Re-register for Table of Content Alerts

Create a profile.



Sign up today!



The ground state of a particle under the influence of a uniformly charged sphere

H. X. Jiang and J. Y. Lin

Department of Physics, Syracuse University, Syracuse, New York 13244

(Received 25 April 1985; accepted for publication 9 November 1985)

I. INTRODUCTION

In the study of the hydrogen atom in quantum mechanics, one assumes for simplicity that the proton is a point charge, thus leading to the familiar Coulomb interaction ($-e^2/r$) with the electron. We see from Shankar's book,¹ by using the perturbation theory, more accurate results can be obtained by assuming the proton is a uniformly dense charge distribution of radius R . The interaction becomes Coulombic at $r > R$, and harmonic-oscillator-like at $r < R$. The perturbation theory is a good approximation only for the problem with small R such as the hydrogen atom.

In this note, we have considered a system consisting of a particle with charge e and mass m under the attraction of a sphere of many uniformly distributed point charges with total charge Q and radius R (see Ref. 2 for classical treatment of this problem). If we allow the particle to penetrate into the sphere, the potential form of this system is exactly the same as the hydrogen atom with the proton being a uniformly dense charge distribution. The problem cannot be treated by using the perturbation theory if R becomes large. By using a variational approximation, we have calculated bound energies of the ground state of the particle as a function of R , the radius of the charged sphere. We have shown that the perturbation theory to the first order¹ is valid only within the region of $R < 0.1$ (in Coulomb units). The critical value of R , R_c , beyond which the hydrogenlike solution dominates over the harmonic oscillator solution, is given. When the radius of the charged sphere equals R_c , the most probable position of the particle is at the surface of the sphere.

II. CALCULATIONS

Consider the Schrödinger equation

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

and the potential of the charged particle,

$$\begin{aligned} v &= kr^2/2R^3 - 3k/2R, \quad r \leq R, \\ &= -k/r, \quad r > R, \end{aligned} \tag{2}$$

where $k = Qe$. The Hamiltonian is

$$H = -\hbar^2 \nabla^2 / 2m + kr^2/2R^3 - 3k/2R, \quad r \leq R, \tag{3}$$

$$= -\hbar^2 \nabla^2 / 2m - k/r, \quad r > R.$$

Noting that the wave function behaves like that of a hydro-

gen atom as $r \rightarrow \infty$ and like that of harmonic oscillator as $r \rightarrow 0$, so we may choose a trial wave function of the form

$$\psi(\mathbf{r}) = Ae^{-\alpha r^2}, \quad r \leq R, \tag{4}$$

$$= Be^{-\beta r}, \quad r > R.$$

Using the conditions of continuity of wave function and its derivative at $r = R$, we have $\alpha = \beta/2R$, $B = Ae^{\beta R/2}$, and from the normalization condition, we have

$$(4\pi A^2) \{ e^{-\beta R} (1 + 2\beta R) + (\pi R^3 \beta^3)^{1/2} \times \text{erf}[(\beta R)^{1/2}] \} = 4\beta^3, \tag{5}$$

where $\text{erf}(x)$ is the error function³ defined as

$$\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x e^{-t^2} dt.$$

Using the Coulomb units,⁴ where the units of mass, length, time, and energy are m , \hbar^2/mk , \hbar^2/mk^2 , and mk^2/\hbar^2 , respectively, all the parameters, in this paper, from now on are dimensionless. We get from Eqs. (4) and (5) that

$$E(\beta) = \langle \psi | H | \psi \rangle = (-1/4R) [F_1(\beta)/F_2(\beta)], \tag{6}$$

where

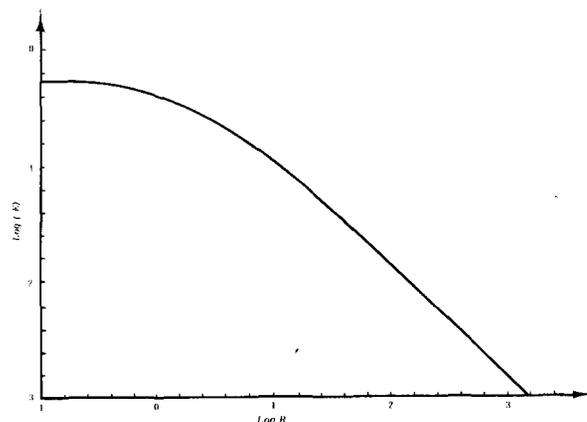


Fig. 1. The logarithmic plot of the ground state energy ($-E$) as a function of R .

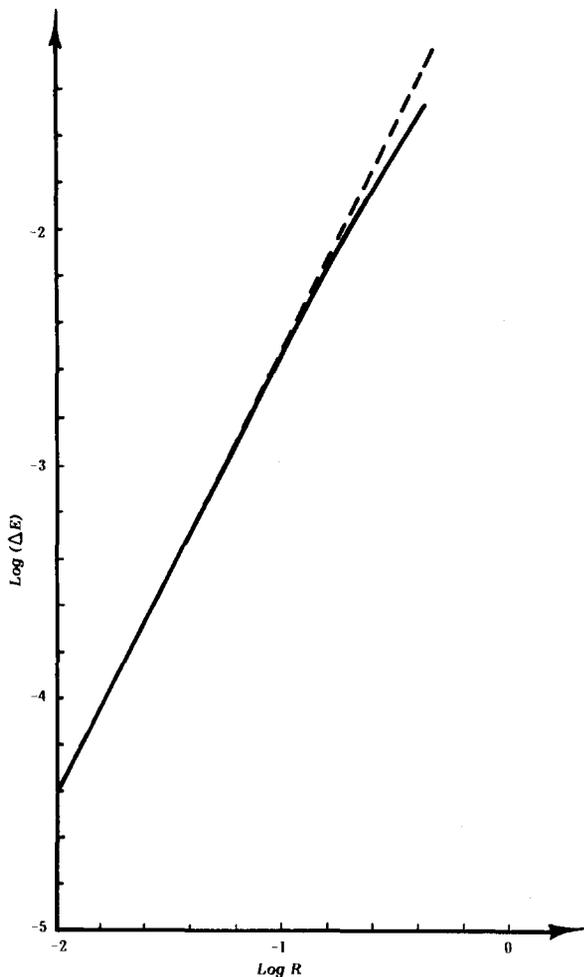


Fig. 2. The logarithmic plot of the $\Delta E = E - E_0$ as a function of R for small R . The dashed and solid lines are the results of the perturbation theory to the first order and of the variational method, respectively.

$$F_1(\beta) = 2\beta R(5 - \beta + \beta^2 R)e^{-\beta R} - (3 - 6\beta R + 3\beta^2 R)(\pi\beta R)^{1/2} \times \text{erf}[(\beta R)^{1/2}], \quad (7)$$

$$F_2(\beta) = (1 + 2\beta R)e^{-\beta R} + (\pi\beta^3 R^3)^{1/2} \text{erf}[(\beta R)^{1/2}].$$

The ground s -state energy can be obtained by taking the derivative of Eq. (6) with respect to β and setting it to zero. We find that

$$F_1'(\beta)F_2(\beta) = F_1(\beta)F_2'(\beta), \quad (8)$$

where $F_i'(\beta)$ ($i = 1, 2$) are the derivatives of F_i with respect to β . After simple calculations, we get

$$F_1'(\beta) = R(7 - 4\beta - 4\beta R + 5\beta^2 R - 2\beta^3 R^2)e^{-\beta R} - (1/2\beta)(3 - 18\beta R + 15\beta^2 R) \times (\pi\beta R)^{1/2} \text{erf}[(\beta R)^{1/2}], \quad (9)$$

$$F_2'(\beta) = R(1 - \beta R)e^{-\beta R} + (3R/2)(\pi\beta R)^{1/2} \text{erf}[(\beta R)^{1/2}].$$

For a given value of R , the value of β can be determined numerically from Eqs. (7)–(9). The wave function in Eq.

(4) and the ground s -state energy in Eq. (6) can subsequently be determined. The results are discussed in the following paragraphs.

III. DISCUSSION

The dependence of the ground-state energy E on the radius R is displayed in the plot of $\log(-E)$ vs $\log R$ in Fig. 1. As $R \rightarrow 0$, we get, from Fig. 1, that $E \rightarrow -1/2$, which is the ground state energy of a hydrogen atom (in Coulomb units). From Eq. (3), as R becomes larger, the term $-k/r$ can be considered as a perturbation; then the ground state energy is approximately

$$E = \omega/2 - 3/2R = 1/2R^{3/2} - 3/2R \rightarrow -3/2R, \quad (10)$$

where $\omega = R^{-3/2}$ is the frequency of the harmonic oscillator. The plot of $\log(-E)$ vs $\log R$ for large R should yield a straight line of slope -1 . This is clearly demonstrated in Fig. 1.

The plot of $\log(\Delta E)$ vs $\log R$ for small R is shown in Fig. 2 in which $\Delta E = E - E_0$, $E_0 = -1/2$ is the exact ground-state energy of a hydrogen atom, and E is the ground-state energy calculated from the variational approximation. From perturbation theory¹ the ground-state energy to the first order is

$$E = -1/2 + 2R^2/5$$

or

$$\Delta E = E - E_0 = 2R^2/5. \quad (11)$$

The dashed and solid lines are the results of the perturbation theory to the first order and of the variational method, respectively. Note that the straight line region only goes to about $R \sim 0.1$. This indicates that, for $R < 0.1$, the perturbation method to the first order is indeed a good approximation; beyond this region, it becomes poor or simply invalid. Next, we calculate the probability density function $P(r)$. From Eq. (4), we can write the wave function as

$$\psi(\mathbf{r}) = Ae^{-\beta r^2/2R}\theta(R-r) + Ae^{\beta R/2 - \beta r}\theta(r-R), \quad (12)$$

where $\theta(x)$ is the step function. Using Eqs. (5) and (12), we get

$$P(r) = [4\beta^3 r^2/F_2(\beta)][e^{-\beta r^2/2R}\theta(R-r) + e^{\beta R - 2\beta r}\theta(r-R)]. \quad (13)$$

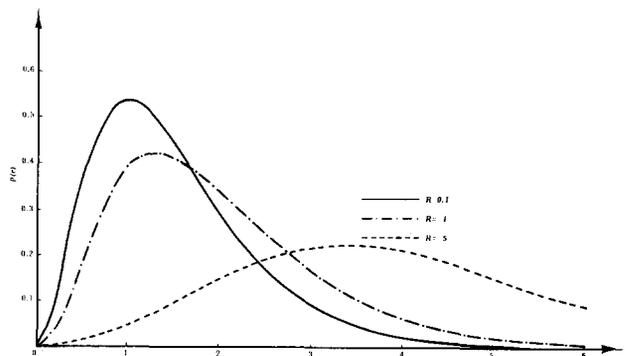


Fig. 3. The probability distribution function $P(r)$ vs r for three different values of R .

The plot of $P(r)$ vs r for three values of R ($R = 0.1, 1,$ and 5) is shown in Fig. 3. We see that when $R = 0.1$, $P(r)$ is very close to the probability density distribution of the s states of a hydrogen atom. For $R = 5$, we get almost the distribution corresponding to a Gaussian wave function, which is close to the distribution of the s state of the harmonic oscillator. For $R = 1$, the distribution is a composite of these two cases. We can also see from Fig. 3 that the most probable position of the particle r (P_{\max}) (written as r_{\max} from now on), increases if R increases. From Eq. (13), we can also calculate r_{\max} as a function of R . Differentiating Eq. (13) with respect to r and setting it equal to 0, we get

$$(1 - \beta r_{\max}^2/R)e^{-\beta r_{\max}^2/R}\theta(R - r_{\max}) + (1 - \beta r_{\max})e^{\beta R - 2\beta r_{\max}}\theta(r_{\max} - R) = 0. \quad (14)$$

Equation (14) can be analyzed for the following two cases:

(i) For $r_{\max} < R$, we have

$$r_{\max} = (R/\beta)^{1/2} \quad (\beta R > 1); \quad (15)$$

(ii) for $r_{\max} > R$, we have

$$r_{\max} = 1/\beta \quad (\beta R < 1). \quad (16)$$

For small R , $r_{\max} > R$, the particle has the highest probab-

ility of being found outside the sphere, which is hydrogen-like. For large R , $r_{\max} < R$, the particle can most likely be found in a region inside the sphere and we could call it harmonic-oscillator-like. Finally, the physical meaning of $r_{\max} = R$ ($\beta R = 1$) is that the particle has the highest probability moving around the surface of the sphere. From the condition of $\beta R = 1$ and Eq. (8), we get the critical value of R , $R_c = 1.425$ (in Coulomb units). We conclude from Eqs. (15) and (16) that, as R increases from $R < R_c$ to $R > R_c$, the wave function of the particle changes from hydrogen-like to harmonic-oscillator-like and the most probable position of the particle changes from outside of the sphere to inside of the sphere. For $Q = 1$, in normal units, $R_c = 1.425r_0$, where r_0 is the Bohr radius.

¹R. Shankar, *Principles of Quantum Mechanics* (Plenum, New York, 1982), p. 466.

²H. X. Jiang and J. Y. Lin, *Am. J. Phys.* **53**, 694 (1985).

³Milton Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions With Formulas, Graphs and Mathematical Tables*, National Bureau of Standards Applied Mathematics Series (National Bureau of Standards, Washington, DC, 1964), p. 297.

⁴L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Oxford, 1977), 3rd ed., p. 117.

On the relation between heat flux and temperature gradient

S. Simons

School of Mathematical Sciences, Queen Mary College, Mile End Road, London E1 4NS, United Kingdom

(Received 20 June 1985; accepted for publication 22 October 1985)

The energy conservation equation for heat flow takes the form

$$C \left(\frac{\partial T}{\partial t} \right) = -\text{div } \mathbf{J}, \quad (1)$$

where C and T are, respectively, the specific heat per unit volume and temperature of the medium, and \mathbf{J} is the heat flux. If this is then combined with the Fourier conduction equation

$$\mathbf{J} = -K \text{grad } T, \quad (2)$$

where K is the thermal conductivity, the familiar conduction equation for T :

$$\left(\frac{\partial T}{\partial t} \right) = (K/C) \nabla^2 T \quad (3)$$

is obtained. Now it was pointed out some years ago by Vernotte¹ that Eq. (3) cannot hold exactly, since, being parabolic, it predicts an infinite velocity of propagation whereas the true velocity cannot exceed that of the thermal carriers. Vernotte therefore suggested that Eq. (2) should be modified to

$$\mathbf{J} + \tau \left(\frac{\partial \mathbf{J}}{\partial t} \right) = -K \text{grad } T, \quad (4)$$

where τ is a relaxation time. The reasoning behind this modification is that on the one hand, Eq. (4), reduces to Eq. (2) if the changes in J are not too rapid, and on the other hand, Eqs. (1) and (4) yield

$$\frac{\partial T}{\partial t} + \tau \frac{\partial^2 T}{\partial t^2} = \left(\frac{K}{C} \right) \nabla^2 T, \quad (5)$$

which being a hyperbolic equation corresponds to a finite propagation velocity. Further, it may be shown² that if this propagation velocity is identified with that of the thermal carriers, then τ must be of the order of the relaxation time for the thermal carrier interaction. Subsequently further workers were involved in exploring the consequences of Eqs. (4) and (5) and in applying the same types of modification to other systems.³

It is clear, however, that despite the arguments given above, the basis for the inclusion of the terms $\tau(\partial \mathbf{J}/\partial t)$ in Eq. (4) is somewhat unsatisfactory, since other terms of a more complicated nature could also meet the objections leveled against Eq. (3). An alternative approach was therefore followed by Simons,⁴ who started with a microscopic description of the thermal carriers, and endeavored to obtain from this the relevant modifications of the macroscopic equations (2) and (3). This approach led however to somewhat lengthy calculations, the result of which were to give corrections to Eqs. (2) and (3) in the form of an infinite series of progressively higher derivatives of \mathbf{J} and T , of which the correction terms of lowest order gave Eqs. (4) and (5). The purpose of the present note is to point out that if a certain commonly used approximation is employed for the interaction term in the basic Boltzmann transport equation for the thermal carriers, then the required modification of Eq. (2) is obtained very simply, and it then takes exactly the form given by Eq. (4).

We begin by supposing that the heat is transported in an isotropic medium by particles whose state is specified by a wave number \mathbf{k} . These particles may be electrons or phonons, or indeed any other form of elementary excitation