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The hydrogen atom in a semi-infinite space limited by a conical boundary

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It is shown that the Schrödinger equation for the hydrogen atom in a semi-infinite space limited by a conical boundary, with the nucleus at the vertex, has an exact solution in spherical coordinates. The limit in which the conical boundary becomes a tight sheath around its own axis corresponds to a "one-dimensional" hydrogen atom with an infinitely degenerate ground state at the ionization threshold. This model of an atom in a semi-infinite space includes as a special case the pioneering plane-nodal-wave-function model used by Levine in 1965 to describe an isolated donor atom on the surface of a semiconductor.

I. INTRODUCTION

The hydrogen atom in semi-infinite spaces has been used as a model of impurity atoms or defects on and near the surface of solids.[1–9] It is more than a quarter of a century since Levine[1] formulated his plane-nodal-hydrogen-wave-function model to describe the behavior of an isolated donor atom right on the surface of a semiconductor. In the last decade, Liu and Lin[2] and Satpathy[3] studied the Wannier excitons near a semiconductor surface by considering an electron-hole coloumbic attraction inside the semiconductor and an impenetrable barrier outside its plane boundary; and Shan *et al.*[4–6] also studied surface effects on impurity states as a hydrogenic system in half-space. More recently, the hydrogen atom in semi-infinite spaces limited by paraboloidal[7,8] and hyperboloidal[9] boundaries, with the nucleus at a focus, have been investigated as models of atoms on the surface of solids. The boundaries simulate the confining effect on one atom due to its neighboring atoms in the solid, and the interest in Refs. 8 and 9 is the ionization of atoms in the solid subject to compression. While in the model of Ref. 8 the atom becomes ionized when the paraboloidal boundary gets close enough to the nucleus, in the model of Ref. 9 the low-lying bound states of the atom remain bound in the presence of hyperboloidal boundaries, even in the limit in which the latter become a tight sheath around the axis with the nucleus at the vertex.

In this paper, the study of the hydrogen atom in a semi-infinite space limited by a conical boundary, with the nucleus at the vertex, shows that the bound states of the system exhibit a qualitative behavior similar to the one found in Ref. 9. This quantum mechanics problem may be of interest to the readers of this Journal insofar as it has an exact solution, it illustrates the influence of the boundary condition in changing the energy spectrum of the atom, and its solutions are intrinsically interesting. In Sec. II, the Schrödinger equation for the hydrogen atom is written in spherical coordinates and its solutions are constructed subject to the condition that the wave function vanishes at the position of the conical boundary. The ionization threshold is analyzed, in particular, and it is found how the different states approach it as the conical boundary closes in around its own axis. When the cone becomes a tight sheath around the axis, the system has become a "one-dimensional" hydrogen atom with an infinitely degenerate ground state at the ionization threshold. In Sec. III, numerical and graphical results of the energy eigenvalues as functions of the conical-boundary half-angle are presented to illustrate the effect of the boundary on the states of the atom. We also discuss the connection of these results with those of some other models.

II. ENERGY EIGENVALUES AND EIGENFUNCTIONS

The Schrödinger equation for the hydrogen atom in spherical coordinates is found in every quantum-mechanics textbook,[10]

$$\left\{-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\right]-\frac{Ze^2}{r}\right\}\psi(r,\theta,\varphi)=E\psi(r,\theta,\varphi). \tag{1}$$

It is also known that it can be solved by the method of separation of variables admitting a factorizable solution,

$$\psi(r,\theta,\varphi)=R(r)\Theta(\theta)\Phi(\varphi), \tag{2}$$

in which each factor satisfies the respective ordinary differential equations

$$-\frac{d^2\Phi}{d\varphi^2}=m^2\Phi, \tag{3a}$$

$$\left(-\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}+\frac{m^2}{\sin^2\theta}\right)\Theta=\lambda(\lambda+1)\Theta, \tag{3b}$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{\hbar^2\lambda(\lambda+1)}{2\mu r^2}-\frac{Ze^2}{r}\right)R=ER. \tag{3c}$$

Equation (3a) corresponds to the eigenvalue equation of the square of the z component of the electron orbital angular momentum; its eigenvalues are quantized on account of the uniqueness condition on the values of the eigenfunction,

$$\Phi(\varphi)=e^{im\varphi}/\sqrt{2\pi}, \tag{4a}$$

$$m=0,\pm1,\pm2,..., \tag{4b}$$

when the azimuthal angular variable, $0\leqslant\varphi\leqslant2\pi$, changes by an integer multiple of 2π. Equation (3b) corresponds to the eigenvalue equation of the square of the electron orbital angular momentum; it is also the differential equation for the associated Legendre functions,[11,12]

$$\Theta(\theta)=P_\lambda^m(\cos\theta), \tag{5}$$

which are well behaved for $0\leqslant\theta\leqslant\pi$ and singular at $\theta=\pi$, in general. For any central force and when all the polar directions are available for the motion of the quantum system, $0\leqslant\theta\leqslant\pi$, the eigenvalues in Eq. (3b) are restricted to integer values of $\lambda=l=0,1,2,...$ and its eigenfunctions become the associated Legendre polynomials, $P_l^m(\cos\theta)$. This is the case for the ordinary hydrogen atom, but it is not for the hydrogen atom confined in the space defined by $0\leqslant\theta\leqslant\theta_0$, which is the system to be investigated in this work. Equation (3c) corresponds to the eigenvalue equation for the energy, and the second term on its left-hand side corresponds to the rotational kinetic energy contribution. It is also the differential equation for the associated Laguerre functions,[10,11]

$$R_{n_r\lambda}(r)=e^{-r/Za_0\nu}r^{\lambda}{}_1F_1\left(-n_r;2\lambda+2;\frac{2r}{Za_0\nu}\right), \tag{6a}$$

where $a_0=\hbar^2/\mu e^2$ is the Bohr radius, $\nu=n_r+\lambda+1$ is the energy parameter,

$$E=-\frac{Z^2e^2}{2a_0\nu^2}, \tag{6b}$$

and

$${}_1F_1(a;b;x)=\sum_{s=0}^{\infty}\frac{(a)_s x^s}{(b)_s s!}, \tag{7}$$

is the confluent hypergeometric function and $(a)_s=a(a+1)...(a+s-1)$, $(a)_0=1$. The asymptotic condition on the radial function $R(r\to\infty)\to 0$ imposed on Eq. (6a) can be satisfied only if $n_r=0,1,2,...$, in which case the confluent hypergeometric function becomes a polynomial, namely, an associated Laguerre polynomial of degree n_r. Correspondingly, for the ordinary hydrogen atom its energy parameter becomes the principal quantum number $\nu=n=n_r+l+1$.

The hydrogen atom in a semi-infinite space limited by the conical boundary $\theta=\theta_0$, with the nucleus at the vertex, is described by Eq. (1), or its equivalent Eqs. (3a,b,c), with the boundary conditions

$$\psi(r\to\infty,0\leqslant\theta\leqslant\theta_0,0\leqslant\varphi\leqslant 2\pi)=0, \tag{8a}$$

$$\psi(0\leqslant r<\infty,\theta=\theta_0,0\leqslant\varphi\leqslant 2\pi)=0. \tag{8b}$$

For the solutions of the type of Eq. (2) these boundary conditions become

$$R(r\to\infty)=0, \tag{9a}$$

$$\Theta(\theta=\theta_0)=0. \tag{9b}$$

The eigenfunctions can be constructed immediately from Eqs. (2), (4a), (5), and (6a),

$$\psi_{n_r\lambda m}(r,\theta,\varphi)=N_{n_r\lambda m}e^{-r/Za_0\nu}r^{\lambda}{}_1F_1\left(-n_r;2\lambda+2;\frac{2r}{Za_0\nu}\right)\times P_\lambda^m(\cos\theta)\frac{e^{im\varphi}}{\sqrt{2\pi}}, \tag{10}$$

where $Nn_{r\lambda m}$ is the normalization constant; $n_r=0,1,2,...$; λ is determined by the explicit form of the boundary condition of Eq. (9b), namely,

$$P_\lambda^m(\cos\theta_0)=0, \tag{11}$$

and the corresponding values of $\nu=n_r+\lambda+1$ determine the energy eigenvalues through Eq. (6b). Therefore, the solution of the eigenvalue problem requires the solution of Eq. (11). This is accomplished numerically by choosing the values of m and λ according to our convenience, and finding the zeros $\theta=\theta_0$ of the associated Legendre functions, using their hypergeometric function representation for $m\geqslant 0$,[11]

$$P_\lambda^m(\cos\theta)=(\sin\theta)^m\frac{(-\lambda)_m(\lambda+1)_m}{2^m(1)_m}\times{}_2F_1\left(-(\lambda-m),\lambda+m+1;m+1;\frac{1-\cos\theta}{2}\right), \tag{12}$$

where

$${}_2F_1(a,b;c;x)=\sum_{s=0}^{\infty}\frac{(a)_s(b)_s x^s}{(c)_s s!}. \tag{13}$$

It is not necessary to repeat the calculation for negative values of m, because P_λ^{-m} is proportional to P_λ^m. The states with the same magnitude of the magnetic quantum number but opposite signs, Eq. (4b), are doubly degenerate. For integer values of $\lambda=l$ the hypergeometric function of Eq. (12) becomes a polynomial of degree $l-m$. For noninteger values of λ the hypergeometric series is infinite, but for the purpose of finding its zeros, the series of Eq. (13) can be truncated taking a finite number of terms depending on the desired accuracy; the number of zeros in the interval $0<\theta<\pi$ is the nearest integer larger than $\lambda-m$. The zeros θ_0 of Eq. (11) obtained in this way determine the position of the conical boundaries for which the eigenvalue problem has been solved with the eigenfunctions of Eq. (10) and the eigenenergies of Eq. (6b).

At the ionization threshold $E\to 0$, and Eq. (6b) implies that $\nu\to\infty$ and in turn $\lambda\to\infty$ for finite values of n_r. In such a limit, the zeros of Eq. (11) tend to $\cos\theta_0\to 1$ or $\theta_0\to 0$. The way in which these limits are related can be established by making the following approximations $1+\cos\theta\approx 2$, $\lambda(\lambda+1)\approx\lambda^2$, and the change of variable,

$$x=\lambda\sqrt{2(1-\cos\theta)}, \tag{14}$$

in Eq. (3b), which is transformed into the ordinary Bessel equation,[11]

$$\left(x^2\frac{d^2}{dx^2}+x\frac{d}{dx}+(x^2-m^2)\right)\Theta=0. \tag{15}$$

Therefore, the position of the conical boundary and the orbital angular momentum eigenvalue parameter are related through the zeros, Eq. (9b), of the ordinary Bessel functions, $j_{m,s}$

$$\theta_0=\cos^{-1}\left(1-\frac{j_{m,s}^2}{2\lambda^2}\right)\xrightarrow[\text{finite } s]{\lambda\to\infty}\cos^{-1}(1)=0. \tag{16}$$

In the limit $\theta_0=0$ the conical boundary becomes a tight sheath around its axis and the hydrogen atom can be considered as "one dimensional." The ground state of such a system is infinitely degenerate at the ionization threshold.

It can also be recognized that the conical boundary becomes a plane for $\theta_0=\pi/2$, in which case our model is

Table I. Energy eigenvalues of hydrogen atom in different states and for different positions of conical boundary.

λ	$n_r=0,(n_\theta,m)$ $E[Z^2e^2/2a_0]$	(0,0) $\cos\theta_{0,1}$	(1,0) $\cos\theta_{0,2}$	(2,0) $\cos\theta_{0,3}$	(0,±1) $\cos\theta_{0,1}$	(1,±1) $\cos\theta_{0,2}$	(2,±1) $\cos\theta_{0,3}$	(0,±2) $\cos\theta_{0,1}$	(1,±2) $\cos\theta_{0,2}$	(2,±2) $\cos\theta_{0,3}$
0	−1	⋯								
1/2	−4/9	−0.65223								
1	−1/4	0.00000	⋯		⋯					
3/2	−4/25	0.37234	−0.90378		−0.41944					
2	−1/9	0.57735	−0.57735	⋯	0.00000	⋯		⋯		
5/2	−4/49	0.69827	−0.25547	−0.95636	0.26970	−0.73633		−0.33186		
3	−1/16	0.77460	0.00000	−0.77460	0.44721	−0.44721	⋯	0.00000	⋯	
7/2	−4/81	0.82555	0.19363	−0.55145	0.56859	−0.19968	−0.85057	0.22185	−0.63382	
4	−1/25	0.86114	0.33998	−0.33998	0.65464	0.00000	−0.65465	0.37796	−0.37796	⋯
9/2	−4/121	0.88692	0.45179	−0.15567	0.71766	0.15879	−0.46081	0.49184	−0.16937	−0.76782
5	−1/36	0.90618	0.53847	0.00000	0.76505	0.28523	−0.28523	0.57735	0.00000	−0.57735

reduced to that of Ref. 1. In such a case, the planar node condition of Eq. (11) requires $\lambda=l$ to be an integer and $l+m$ to be odd. Furthermore, for a given value of l, the corresponding magnetic states $m=\pm(l-1),\pm(l-3),\ldots,\pm1$(or 0), if l is even (or odd), have the same energy and are l degenerate. Consequently, $\nu=n$ is also an integer, and for a given value of n the degeneracy is of order $\Sigma_{l=0}^{n-1}l=n(n-1)/2$. These degeneracies are without taking the electron spin into account and are doubled if the spin degeneracy is included.

III. NUMERICAL RESULTS AND DISCUSSION

In this section, some numerical results are presented through Table I and Fig. 1(a)–(c), to illustrate the energy spectra of the hydrogen atom for different positions of the conical boundary. Each state is characterized by the set of numbers n_r, n_θ, m, where m takes the values of Eq. (4b), n_r the values described after Eq. (10), and n_θ is the number of nodes of $P_\lambda^m(\cos\theta)$ in the open interval $0<\theta<\theta_0$ or $\cos\theta_0<\cos\theta<1$. For each state, the choice of λ determines the position of the boundary, characterized by the value of $\cos\theta_0$, and the energy eigenvalue, in the way described after Eq. (11). The Table contains a sample of numerical data for the lowest lying states only, while the figures present a more global picture for those and some additional states.

The numerical data in Table I are restricted to the states without any radial excitation, $n_r=0$, and the three lowest excitations in both polar and azimuthal degrees of freedom, $n_\theta=0,1,2$ and $m=0,\pm1,\pm2$, respectively. The same entries for the orbital angular momentum parameter λ and the corresponding positions of the conical boundary $\cos\theta_{0,s}$ are valid for states with different radial excitations, $n_r=1,2,\ldots$, for which the energy entries are easily calculated using Eq. (6b). The ordinary hydrogen atom corresponds to $\theta_0=\pi$, when the entire space is available and the energy spectrum is given by Eq. (6b) with integer values of $\lambda=l$ and $\nu=n=n_r+l+1$; the corresponding energy levels have the dashed entries in Table I and are shown on the left sides of Fig. 1(a)–(c) for $\cos\theta_0=-1$. For integer values of $\lambda=l$, Eq. (11) has $l-|m|$ zeros, $\cos\theta_{0,s}$, symmetrically located relative to $\cos\theta_0=0$ and defining the position of the conical boundaries for which the atom in different states ($n_\theta=s-1=0,1,2,\ldots,l-|m|-1$) has the same energy. For the noninteger values of λ, the zeros of Eq. (11) are no longer symmetrically distributed and their number is the larger integer nearest to $\lambda-|m|$; it still holds valid that for given values of n_r and m, the different states ($n_\theta=s-1=0,1,2,\ldots$, larger integer nearest to $\lambda-|m|-1$) corresponding to the different conical boundaries $\cos\theta_{0,s}$ have the same energy, Eq. (6b) with $\nu=n_r+\lambda+1$. If we follow the energy of each state as the conical boundary decreases its half angle from $\theta_0=\pi$ to 0, or correspondingly its cosine goes from −1 to 1, we notice a monotonic increase. The well-known n^2 degeneracy of the ordinary hydrogen atom energy levels[10] is reduced, in general, by the presence of the conical boundaries to one for the $m=0$ states and to a double degeneracy for the other m states, as described after Eq. (13). In the particular case of the plane boundary, $\cos\theta_0=0$ or $\theta_0=\pi/2$, the degeneracy is $n(n-1)/2$ according to Levine[1] and the discussion at the end of Sec. II; this is illustrated by the states (0,0,0) with $n=2$, (1,0,0) and (0,0,±1) with $n=3$, (2,0,0), (0,1,0), (1,0,±1) and (0,0,±2) with $n=4$, etc. Figure 1(a)–(c) illustrates the crossings of energy levels for states differing in two or more quantum numbers, and no such crossings for states differing in one quantum number. The low-lying states, with finite values of n_r and n_θ, tend to become closer among themselves and to the ionization threshold as the boundary approaches its own axis, i.e., $E\to0$ as $\cos\theta_0\to1$; this general trend can be appreciated in Fig. 1(a)–(c). In particular, at the right side of each figure, corresponding to $\cos\theta_0\to1$ or $\theta_0\to0$, the tendency toward an infinite degeneracy of the energy levels of the "one-dimensional" hydrogen atoms at the ionization threshold is clearly illustrated,

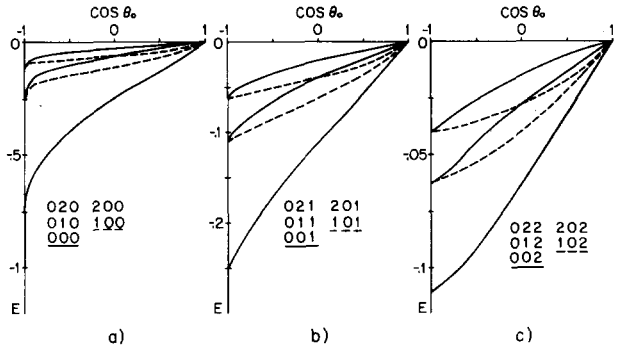

Fig. 1. Energy levels of hydrogen atom in different states (n_r, n_θ, $|m|$) for different positions of conical boundary. (a) $m=0$, (b) $m=\pm1$, and (c) $m=\pm2$. Energy unit $Z^2e^2/2a_0$.

because there are an infinite number of additional states with almost the same energy for the successively larger values of n_r, n_θ, and $|m|$. The limit of the one-dimensional hydrogen atom $\theta_0=0$ is expected to be valid only for the $m=0$ states, since according to Eq. (12) the probability amplitude for the other m states vanishes.

The discussion of the previous paragraph has been restricted to the low-lying states of the hydrogen atom, i.e., finite values of its quantum numbers. Going back to the paragraph of Eq. (14) we can consider some complementary and alternative situations in which the atom can be ionized for finite positions of the conical boundary. First, $\nu\to\infty$ can be obtained for finite values of λ and $n_r\to\infty$. Second, within the original assumption of $\lambda\to\infty$ and finite n_r, the energy threshold is reached by taking the states with high polar excitation n_θ equal to the least integer that is greater than or equal to $\lambda-|m|-1$, $\lambda-|m|-2$, ..., for which the conical boundaries are far from $\theta_0=0$. In any case, the general conclusion is that the presence of the conical boundary cannot by itself ionize the hydrogen atom in low-lying states; it can produce ionization of states that are highly excited radially or polarly.

We close this discussion by pointing out that the model studied in this paper is the limiting situation of the model of the hydrogen atom in a semi-infinite space limited by a hyperboloidal boundary[9] when the focal distance of the latter tends to vanish. Both models share the dynamical and geometrical properties studied in Sec. II and discussed in this section. The model with the conical boundary is obviously much simpler and its study may open a door for the interested reader to some of the physics of surface effects.[1-9]

[1] J. D. Levine, "Nodal hydrogenic wave functions of donors on semiconductor surface," Phys. Rev. A **140**, 586–589 (1965).
[2] Z. Liu and D. L. Lin, "Hydrogenic atom in semi-infinite space," Phys. Rev. B **28**, 4413–4418 (1983).
[3] S. Satpathy, "Eigenstates of Wannier excitons near a semiconductor surface," Phys. Rev. B **28**, 4585–4592 (1983).
[4] Y Shan, T. F. Jiang, and Y. C. Lee, "Generalized spheroidal wave equations from an image-potential method for surface effects on impurity states," Phys. Rev. B **31**, 5487–5489 (1985).
[5] Y. Shan, "Generalized spheroidal wave equations for a hydrogenic system in half space: I. General properties," J. Phys. B: At. Mol. Phys. **20**, 4275–4284 (1987).
[6] Y. Shan, P. C. Lu, and H. C. Tseng, "Generalized spheroidal wave equations for a hydrogenic system in half space: II. Exact solutions," J. Phys. B: At. Mol. Phys. **20**, 4285–4298 (1989).
[7] J. H. You, Z. G. Ye, and M. L. Du, "Properties of a substitutional and/or interstitial surface hydrogen atom," Phys. Rev. B **41**, 8180–8183 (1990).
[8] E. Ley-Koo and R. M. G. García-Castelán, "The hydrogen atom in a semi-infinite space limited by a paraboloidal boundary," J. Phys. A: Math. Gen. **24**, 1481–1493 (1991).
[9] E. Ley-Koo and S. Mateos-Cortés, "The hydrogen atom in a semi-infinite space limited space limited by a hyperboloidal boundary," to be published.
[10] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1961), pp. 186–199.
[11] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).
[12] J. D Jackson, *Classical Electrodynamics* (Wiley, New York, 1975), 2nd ed., pp. 94–98, Sec. 3.4, "Behavior of Fields in a Conical Hole."

Aspects of Debye shielding

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The Debye shielding is derived in a simple way without assuming Boltzmann's equilibrium. The conditions under which it applies and some of its consequences are discussed at the elementary level.

I. INTRODUCTION

One of the most basic ideas of plasma physics is Debye shielding, first recognized[1] when the plasma did not even have a name.[2] Yet, elementary textbooks discuss it rather briefly and in virtually the same way, and one is accustomed to take it for granted. Thinking more deeply about it, however, raises some questions and reveals a few surprises.

At first sight, the concept seems rather trivial. Since electric charges attract oppositely charged particles and repel the others, ionized matter tends to maintain electrical neutrality; but the thermal agitation counteracts this tendency. Loosely speaking, the Coulomb attraction keeps opposite charges together, whereas the particle agitation tends to separate them; the balance allows the existence of nonneutral regions whose scale—the so-called Debye length, increases with the thermal agitation—i.e., the temperature, and is an inverse function of the density (since increasing the density of charge carriers favors the shielding). Neutrality is not perfect at the Debye scale but is effective farther out, so that any charge has a dress of size the Debye length which makes it "invisible" from larger distances.

This loose argument, however, as the classical Debye–Hückel derivation that can be found in virtually any textbook, is based on thermal equilibrium. But many plasmas, and in particular most space plasmas, are collision-free,