One- and two-dimensional hydrogen atoms

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Certain one- and two-dimensional reductions of the three-dimensional Schrödinger equation of the hydrogen atom are considered. These reductions are carried out from the point of view of the two common sets of space coordinates: Cartesian and spherical. The resulting systems have features that relate more readily to the old quantum theory models of Bohr and Sommerfeld than the general three-dimensional hydrogen atom. Furthermore, the considerations yield interesting insights into the quantum mechanics of the hydrogen atom and may serve as helpful intermediary preparation, in an introductory presentation of the subject, for the unreduced three-dimensional case.

I. INTRODUCTION

It is convenient for our purposes to begin with the time-independent Schrödinger equation of a particle in a potential. This equation, when expressed in standard notation, reads as follows:

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z). \quad (1)$$

One usually illustrates this equation, in an introductory presentation of the subject, in terms of Cartesian one-dimensional systems. These systems have simple potentials, e.g., the square well and the rectangular potential barrier. The important case of the hydrogen atom, however, is dealt with from the outset in three dimensions. Yet, certain one- and two-dimensional reductions of the hydrogen atom system can be studied towards further illustration of Schrödinger's Eq. (1), and towards building up to the three-dimensional case.[1] Additionally, the study of the resulting reduced systems leads to a better appreciation of the relation between the old quantum theory and Schrödinger's theory.

II. ONE-DIMENSIONAL HYDROGEN ATOMS

The dimensional reduction of Schrödinger's equation depends on the set of coordinates in which it is expressed. Attention will be confined to the hydrogen atom in the two common sets: Cartesian and spherical coordinates, cf., Fig. 1. The potential V in Eq. (1) is then the electrostatic Coulomb potential of the electron in the field of the proton. For the one-dimensional reduction from the point of view of Cartesian coordinates, there is only one distinct reduction. This corresponds to any one of x, y, and z being variable while the remaining two are held constant. Let the chosen variable be denoted by x. The resulting reduced equation from Eq. (1) is

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} - \frac{e^2}{4\pi\epsilon_0|x|}\psi(x) = E\psi(x). \quad (2)$$

Standard notation and the mks system are used.[2] Equation (2) has already been studied by Loudon at length.[3] Its mathematical and physical properties are too specialized and technical for an introductory illustration of Eq. (1) to interest us here.

From the point of view of spherical coordinates, however, there are two distinct one-dimensional reductions. The first is where both angles θ and ϕ (Fig. 1) are constant while r is a variable. This is equivalent to the one-dimensional Cartesian reduction obtained above, confined to the positive x axis. It does not interest us here either. The second reduction is where r and one of the angles are constant while the other angle is variable. Let the variable angle be ϕ and the plane of motion be the x–y plane (Fig. 1). This is clearly the analog of the Bohr atom. It therefore could be of considerable interest. Equation (1) then reduces to

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d^2\psi(\phi)}{d\phi^2} - \frac{e^2}{4\pi\epsilon_0 r}\psi(\phi) = E\psi(\phi), \quad (3)$$

which is more conveniently written as

$$\frac{d^2\psi(\phi)}{d\phi^2} + \frac{2\mu r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\epsilon_0 r}\right)\psi(\phi) = 0. \quad (4)$$

Note that

$$E + e^2/4\pi\epsilon_0 r \equiv E - V = p^2/2\mu,$$

and

$$\frac{2\mu r^2}{\hbar^2}\frac{p^2}{2\mu}$$

is a constant; E, V, and r being constants. Thus the normalized wave-function solution of Eq. (4) is

$$\psi(\phi) = \frac{1}{\sqrt{2\pi}}\exp\left(\pm\frac{ipr}{\hbar}\phi\right). \quad (5)$$

Requiring that the wave function be single valued, i.e., $\psi(\phi) = \psi(\phi + 2\pi)$, leads to the condition

$$pr = n\hbar, \quad (6)$$

where $n = 1,2,3,\dots$. The $n = 0$ has been excluded because as seen below it implies the unphysical case of an orbit of zero radius where the electron is infinitely bound to the proton. We see that the condition of Eq. (6) is Bohr's quantization condition. Bohr's quantization condition, quite *ad hoc* in Bohr's model, is now understood as a result of the requirement that the wave-function solution of Eq. (3) be single valued. Furthermore, the picturesque and equivalent way of describing Bohr's condition as fitting for a given orbital motion an integral number of de Broglie wavelengths around the orbit, $2\pi r = n\lambda$, follows as well. This perhaps makes more evident the sense in which de Broglie's wave
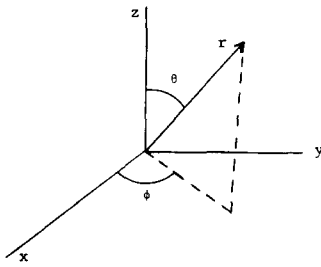
Fig. 1. Three-dimensional space characterization by the Cartesian set of coordinates x, y, and z and the spherical set of coordinates r, θ, and ϕ.

concept relates to Schrödinger's wave equation.

Let us note further that since for this system[4] $E = (1/2)V = -e^2/8\pi\epsilon_0 r$, Eq. (4) can then be expressed as follows:

$$\frac{d^2\psi(\phi)}{d\phi^2} + \left(\frac{e^2\mu r}{4\pi\epsilon_0\hbar^2}\right)\psi(\phi) = 0. \tag{7}$$

The requirement that $\psi(\phi)$ be single valued, which led above to Bohr's quantization condition Eq. (6), now leads to

$$\sqrt{\frac{e^2\mu r}{4\pi\epsilon_0\hbar^2}} = n, \tag{8a}$$

or

$$r_n = \frac{4\pi\epsilon_0\hbar^2 n^2}{\mu e^2}, \tag{8b}$$

where as before $n = 1,2,3,\ldots$. This is the orbit's quantization of the Bohr model. Substituting Eq. (8b) in the expression $-e^2/8\pi\epsilon_0 r$ for the energy, one gets

$$E_n = -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2 n^2}, \tag{9}$$

the well-known Bohr model energy levels formula.[5]

Thus it is seen that the angular momentum quantization of Eq. (6) is built into the Schrödinger analog of the Bohr model, and that otherwise the Schrödinger analog yields the same physical features as the Bohr model.

III. TWO-DIMENSIONAL HYDROGEN ATOMS

As in the one-dimensional case, the reduction of the hydrogen atom Schrödinger equation to two dimensions will be carried out from the point of view of the two common sets of coordinates: Cartesian and spherical. From the point of view of the Cartesian set of coordinates x, y, and z, there is only one distinct reduction. This corresponds to any pair of the three coordinates being variable while the third is held constant. Choosing x and y to be the pair, Eq. (1) becomes

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y)$$

$$-\frac{e^2}{4\pi\epsilon_0\sqrt{x^2+y^2}}\psi(x,y) = E\psi(x,y). \tag{10a}$$

Equation (10a), when expressed in terms of the transformed coordinates r and ϕ, has the form

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2\psi(r,\phi)}{\partial r^2} + \frac{1}{r}\frac{\partial\psi(r,\phi)}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi(r,\phi)}{\partial\phi^2}\right)$$

$$-\frac{e^2}{4\pi\epsilon_0 r}\psi(r,\phi) = E\psi(r,\phi). \tag{10b}$$

This two-dimensional hydrogen atom of Eqs. (10a) and (10b) has already been studied by Zaslow and Zandler[6] and

again by Huang and Kozycki.[1] Using the method of separation of variables (r and ϕ), the wave-function solutions of Eqs. (10a) and (10b) have been obtained along with quantization conditions on the angular momentum and energy of the system. This two-dimensional system is the Schrödinger analog of the Sommerfeld generalization of the Bohr model (Sommerfeld model) allowing elliptical orbits.[7] It is therefore of interest to compare the main results of the solutions of Eqs. (10a) and (10b) with those of the Sommerfeld model.

For the system described by Eqs. (10a) and (10b), the values of the magnitude of the angular momentum turn out to be $|l|\hbar$, where $l = 0,\pm1,\pm2,\ldots$; while those of the energy turn out to be given by the formula[6,1]

$$E_n = -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2(n - \frac{1}{2})^2}, \tag{11}$$

where n is an integer $1,2,3,\ldots$ such that $n > |l|$. The quantization of the angular momentum in the Sommerfeld case is the same as this Schrödinger analog except that in Sommerfeld's case the $l = 0$ value is not assumed while the $l = n$ value is. It is to be noted, however, that the energy formula of Eq. (11) is different from Sommerfeld's model energy formula in that the principal quantum number n in the latter is replaced by $(n - \frac{1}{2})$ here. The Sommerfeld energy formula, as is well known, is the same as that of the Bohr model, Eq. (9), and the three-dimensional Schrödinger hydrogen atom. Thus the principal quantum number n relates differently to the energy in the two cases. In view of the results of Sec. II, the modified energy formula, Eq. (11), may seem surprising, albeit instructive. The ground-state energy ($n = 1$) from Eq. (11) is four times larger than that obtained from Eq. (9). As n takes on larger values, the discrepancy becomes accordingly smaller; an illustration of Bohr's correspondence principle. As to the quantized elliptical orbits of Sommerfeld's model, they give way in the Schrödinger analog to a more general description in terms of the radial part of the wavefunction solutions of Eqs. (10a) and (10b).

Let us now turn our attention to the two-dimensional reduction of Schrödinger's Eq. (1) for the hydrogen atom from the spherical coordinates point of view. Here there are two distinct reductions from among the r, θ, and ϕ coordinates. The first is where r and one of the angles (say r and ϕ) are chosen to be variables. This choice, however, leads back to the just discussed Eq. (10b). The second distinct and last choice is where θ and ϕ are variables and r is held constant. The correspondingly reduced Schrödinger equation is

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi(\theta,\phi)}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi(\theta,\phi)}{\partial\phi^2}\right]$$

$$-\frac{e^2}{4\pi\epsilon_0 r}\psi(\theta,\phi) = E\psi(\theta,\phi). \tag{12}$$

Note that r in Eq. (12) is constant. The classical counterpart of the system described by Eq. (12) is that of an electron moving about the proton over a spherical surface of radius r in the constant Coulomb field $-e^2/4\pi\epsilon_0 r$. Classically the orbit of the electron will have to be in a fixed plane, being in a central force field. Thus the classical orbit will still be a circle. The classical counterpart of this system is therefore equivalent to the classical counterpart of both Bohr's model and its one-dimensional Schrödinger analog of Sec. II. Any differences appearing in the solutions of Eq. (12) from those

of Eq. (3) will have to be therefore of nonclassical, quantum-mechanical origin. Equation (12) can be solved by the method of separation of variables, namely, let

$$\psi(\theta,\phi) = \Theta(\theta) \, \Phi(\phi). \tag{13}$$

Substituting Eq. (13) into Eq. (12) and separating the ϕ-dependent terms from the θ-dependent terms, one gets

$$\frac{1}{\Theta(\theta)} \sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta(\theta)}{d\theta}\right) + \frac{2\mu r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\epsilon_0 r}\right)\sin^2\theta$$
$$= \frac{-1}{\Phi(\phi)} \frac{d^2\Phi(\phi)}{d\phi^2}. \tag{14}$$

Setting each side equal to a separation constant m^2, one then has

$$\frac{d^2\Phi(\phi)}{d\phi^2} + m^2\Phi(\phi) = 0 \tag{15}$$

and

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right)$$
$$+ \left[\frac{2\mu r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\epsilon_0 r}\right) - \frac{m^2}{\sin^2\theta}\right]\Theta(\theta) = 0. \tag{16}$$

Equations (15) and (16) have the same form as those of the angular equations of the three-dimensional hydrogen atom case.[9] The solution therefore may be expressed in terms of the spherical harmonics $Y_l^m(\theta,\phi)$ with $l = 1,2,3,\ldots$ and $m = 0,\pm 1,\pm 2,\ldots\pm l$. The $l = 0$ is excluded since it leads, as seen below, to the unphysical case of the electron having an orbit of zero radius and being infinitely bound to the proton. The quantity

$$\frac{2\mu r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\epsilon_0 r}\right)$$

is related to l by the condition

$$\frac{2\mu r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\epsilon_0 r}\right) = l(l + 1). \tag{17}$$

Noting that

$$E + \frac{e^2}{4\pi\epsilon_0 r} \equiv E - V = \frac{p^2}{2\mu}, \tag{18}$$

Eq. (17) may be written as

$$\frac{p^2 r^2}{\hbar^2} = l(l + 1). \tag{19}$$

Equation (19) is the angular momentum quantization condition. It results from the usual requirement of proper solutions of Eq. (16). It does not have to be separately hypothesized. It is the same quantization resulting from the three-dimensional case except for the exclusion of $l = 0$. It modifies the form of the quantization of angular momentum in both Bohr and Sommerfeld models as well as their respective Schrödinger analogs; the modification being the replacement of n (or l) there by $\sqrt{l(l + 1)}$ here. This is a quantum-mechanical, nonclassical, expression of the electron being able to move on the surface of a sphere rather than confined to a plane. The meaning of the quantum number m is exactly the same as that of the three-dimensional case. As such, $m\hbar$ is the quantized z component of the angular momentum in the state $Y_l^m(\theta,\phi)$. For a given value l, there are $(2l + 1)$ possible values of m.

Setting in Eq. (17) $E = -e^2/8\pi\epsilon_0 r$, which holds as in the one-dimensional case of Sec. II,[4] one gets a quantization condition on the orbits:

$$r_l = \frac{4\pi\epsilon_0\hbar^2 l(l + 1)}{\mu e^2}; \tag{20}$$

and the energy:

$$E_l = -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2 l(l + 1)}. \tag{21}$$

The results of Eqs. (20) and (21) differ from the corresponding ones of the one-dimensional system of Sec. II in the replacing of n^2 there by $l(l + 1)$ here; an additional quantum-mechanical manifestation of the electron being no longer confined to a circle in a plane but can move over a surface of a sphere. The ground-state angular momentum, orbit, and energy from Eqs. (19), (20), and (21) are, respectively, $\sqrt{2}$, 2, and $\frac{1}{2}$ times those of Bohr's model and its Schrödinger analog given in Sec. II by Eqs. (6), (8b), and (9). For large quantum numbers n or l as the case may be, the discrepancy becomes, however, accordingly smaller; another illustration of Bohr's correspondence principle.

IV. CONCLUDING REMARKS

It may be desirable to indicate at this point how the uncertainty principle relates to the reduced one- and two-dimensional systems discussed above. The reduced systems are bona fide quantum systems from a formal standpoint. They include uncertainty principles limited to their respective domains of applicability. Specifically, for example, the analog of the Bohr model of Sec. II is defined by a Hamiltonian

$$H = \frac{L_z^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}. \tag{22}$$

L_z is the dynamical variable of angular momentum having the operator representation $(\hbar/i)(\partial/\partial\phi)$. The other dynamical variable of the system is the angle ϕ. Note that r here is not a dynamical variable but a parameter of the system. In this reduced system, the linear momentum along r, p_r, simply does not arise; neither does the space coordinate z or its corresponding linear momentum p_z. L_z and ϕ are noncommuting and therefore are not simultaneously determinable. While L_z is completely determined in any given state ψ_n, being $n\hbar$, the angular position ϕ of the electron is completely undetermined. Thus the uncertainty principle applies within the context of the variables of the system. It would be meaningless to search for an uncertainty condition on r and p_r (or z and p_z) in the context of this reduced system. This simply lies outside the scope of the system as defined. These remarks may be extended to the two-dimensional systems as well. From a physical standpoint, on the other hand, the following question can still be raised: What physical constraints might one have which, when applied to the hydrogen atom (or otherwise) would lead to a physical situation that might be approximated by any one of the above reduced systems? This is an open question and no claim is made that such physical situations do in fact exist.[9] The primary motivations for the considerations of these systems have already been indicated in Sec. I.

Let us now turn to the case of the electron constrained to the surface of a sphere and note that the angular momentum variable $L(L_x,L_y,L_z)$ has the same properties that L has in the normal three-dimensional case. In particular

L_x, L_y, and L_z are noncommuting and not simultaneously determinable. That $(L)^2$ takes on the values $l(l + 1)\hbar^2$, Eq. (19), and not $l^2\hbar^2$, as in the cases of the Schrödinger analogs of Bohr and Sommerfeld models, is due to this nonclassical feature of noncommutativity of L_x, L_y, and L_z, and is a manifestation of the uncertainty principle at work within the context of the system as defined.

Finally, let us observe that in all the instances encountered above where the zero value of angular momentum is excluded, the electron has definite orbits. The zero angular momentum is not excluded when the radial position of the electron is described in terms of nonsingular probability distribution functions (Schrödinger's analog of Sommerfeld's model and the normal three-dimensional Schrödinger hydrogen atom). For the cases of definite orbits, the zero angular momentum leads to an unphysical consequence where either the electron has to go through the proton (Sommerfeld's model) or that the electron is infinitely bound to the proton (Bohr's model, its Schrödinger analog and Schrödinger's description of the electron confined to the surface of a sphere). From the uncertainty principle standpoint, one may see the exclusion of the zero angular momentum state as related to the absence of an operative uncertainty condition on the electron's coordinate r and its corresponding momentum p_r.

ACKNOWLEDGMENT

[1] Similar point has also been made recently by J. W. Huang and A. Kozycki, Am. J. Phys. **47**, 1005 (1979).

[2] The nuclear motion is disposed of in the usual manner by separating out the motion of the center of mass and treating only the relative motion; μ thus denotes the reduced mass.

[3] R. Loudon, Am. J. Phys. **27**, 649 (1959).

[4] This is the standard classical expression of the energy E for the electron circulating about the proton. It is nevertheless a special manifestation of the virial theorem applied to this system, yielding

$$p^2/2\mu = -(1/2)V \quad \text{and} \quad E = (1/2)V.$$

[5] Once the angular momentum quantization and the relation

$$E = -e^2/8\pi\epsilon_0 r$$

are at hand, the quantized expressions for the orbits and the energy may be obtained from the usual Bohr model analysis. The above alternate derivation, however, shows another feature of this Schrödinger system.

[6] B. Zaslow and M. E. Zandler, Am. J. Phys. **35**, 1118 (1967).

[7] For example: H. Semat, *Introduction to Atomic and Nuclear Physics* (Holt, Rinehart and Winston, New York, 1962), Chap. 8, pp. 241–246 and Appendix IX, pp. 607–610.

[8] It is to be noted that in an introductory presentation of the subject, one cannot assume the methods of the three-dimensional case to be known, and that one will have to introduce the methods of solution of Eqs. (15) and (16) without such reference. This will in turn facilitate the discussion of the three-dimensional case.

[9] See also the introduction of Ref. 6