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On the Isotropic Oscillator and the Hydrogenic Atom in Classical and Quantum Mechanics

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It is shown how one may simply associate the problem of the isotropic oscillator to that of the hydrogenic atom in classical dynamics, particularly in its action-angle variable formulation, so that the solution of the one problem implies that of the other. This relationship persists in the two-dimensional quantum mechanics and provides the key to the construction of a wave packet solution for the isotropic oscillator in the region of large principal quantum number in three dimensions.

It is customary in expositions of the later developments of classical dynamics (such as action-angle variables[1,2]) and in discussions of the early quantum theory,[3] first to work out the solution of the one-dimensional harmonic oscillator and then that of a more complex problem, typically the Kepler problem in three dimensions. The elaborate theoretical apparatus required to discuss, say, the hydrogen atom, serves to discourage the analogous treatment of other dynamical systems in more than one dimension, and one soon discovers that there are not many of these of equal pedagogical value. Thus, it may be of some interest to show that the hydrogenic atom and the isotropic oscillator are simply related in classical dynamics and that *both* these fundamental three-dimensional problems may be solved simultaneously there with little additional effort. (In the process, we confirm the basic geometric intuition that since the classical orbits of the bound Kepler problem and the harmonic oscillator are ellipses, there should exist a transformation between these two problems.[4]) Surprisingly, one finds that this relationship persists in the two-dimensional quantum mechanics as well. In three dimensions, the now approximate connection still provides the key to a wave-packet solution for the isotropic oscillator in the region of large principal quantum number. Such a wave-packet follows the classical circular orbit as in the analogous construction recently given by Brown[5] for the hydrogen atom.

We remind the reader that the solution to the problem of the hydrogenic atom in three dimensions requires the introduction of the action variables J_i $(i=r, \theta, \phi)$:

$$J_\phi = \oint p_\phi d\phi, \tag{1a}$$

$$J_\theta = \oint p_\theta d\theta = \oint (p^2 - p_\phi^2/\sin^2\theta)^{1/2} d\theta, \tag{1b}$$

$$J_r = \oint (-2m\,|\,E\,|\, + 2mZe^2/r - p^2/r^2)^{1/2} dr; \tag{1c}$$

where p is the magnitude of the total angular momentum of the planar bound orbital motion. [That motion is alternatively treated by dealing with the Hamiltonian in plane polar coordinates,[6]

$$\mathcal{H}(\rho, p_\rho; \phi, p) = (1/2m)(p_\rho^2 + p^2/\rho^2) - Ze^2/\rho, \tag{2}$$

introducing the appropriate action variables, J_ρ, $J_\phi = 2\pi p$.] From Eq. (1b) one deduces that J_θ is a homogeneous function of p, p_ϕ of first degree, i.e.,

$$p\partial J_\theta/\partial p + p_\phi \partial J_\theta/\partial p_\phi = J_\theta;$$

indeed, one has

$$p = (J_\theta + J_\phi)/2\pi, \tag{3}$$

by explicit integration.[7] The integral involved in Eq. (1c) is evaluated by elementary means or by application of the residue theorem,[8] so that we have

$$\mathcal{H} \equiv E = -2\pi^2 m Z^2 e^4/(J_r + J_\theta + J_\phi)^2. \qquad (4)$$

To simplify matters, we restrict our discussion now to the motion in the orbital plane (ρ, ϕ), where $(J_r \to J_\rho)$,

$$E = -2\pi^2 m Z^2 e^4/[J_\rho + p/2\pi]^2. \qquad (5)$$

Under the coordinate transformation given by

$$\rho = u^2, \qquad (6a)$$

$$\phi = 2\psi, \qquad (6b)$$

an ellipse of the bound motion of the planetary electron with semimajor [semiminor] axis $a[b]$, given by

$$\frac{1}{\rho} = \frac{a - (a^2 - b^2)^{1/2} \cos\phi}{b^2}, \qquad (7)$$

goes into the ellipse,[9]

$$\frac{X^2}{a + (a^2 - b^2)^{1/2}} + \frac{Y^2}{a - (a^2 - b^2)^{1/2}} = 1, \qquad (8)$$

where

$$X = u \cos\psi, \qquad (9a)$$

$$Y = u \sin\psi. \qquad (9b)$$

At the same time, via the generating function of the "third type," [1]

$$-F_3(\mathbf{p}, u) = p_x u^2 \cos 2\psi + p_y{}^2 u^2 \sin 2\psi, \qquad (10)$$

with its associated equations of transformation,

$$x = -\partial F_3/\partial p_x = u^2 \cos 2\psi, \qquad (11a)$$

$$y = -\partial F_3/\partial p_y = u^2 \sin 2\psi, \qquad (11b)$$

$$p_u = -\partial F_3/\partial u = 2u(p_x \cos 2\psi + p_y \sin 2\psi)$$
$$= 2u p_\rho, \qquad (12a)$$

$$p_\psi = -\partial F_3/\partial \psi = 2u^2(p_y \cos 2\psi - p_x \sin 2\psi)$$
$$= 2p, \qquad (12b)$$

one obtains for the new Hamiltonian $\mathcal{H}$,

$$\mathcal{H}(u, p_u; \psi, p_\psi)$$
$$= (1/2m)(p_u{}^2/4u^2 + p_\psi{}^2/4u^4) - Ze^2/u^2$$
$$= -|E|. \qquad (13)$$

In the transformed theory,[10]

$$J_\psi = \oint p_\psi d\psi = 2\pi p_\psi = 2J_\phi, \qquad (14a)$$

$$J_u = \oint p_u du$$
$$= \oint (8mZe^2 - 8m|E|u^2 - p_\psi{}^2/u^2)^{1/2} du = 2J_\rho. \qquad (14b)$$

Thus we are dealing there with the action variables for an isotropic harmonic oscillator with (positive) energy $\epsilon = 4Ze^2$, spring constant $k = 8|E|$, and angular momentum p_ψ. Since, in the case of the isotropic oscillator,

$$\epsilon = 4Ze^2 = (J_u + J_\psi)\nu, \qquad (15)$$

where

$$\nu = \pi^{-1}(2|E|/m)^{1/2}, \qquad (16)$$

one finds,

$$|E| = \frac{2\pi^2 m Z^2 e^4}{(J_\rho + p/2\pi)^2}. \qquad (17)$$

In the two-dimensional quantum mechanics, the bound state eigenvalue problem of the hydrogenic atom,

$$[-(\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2) - Ze^2/\rho]\psi = -|E|\psi, \qquad (18)$$

may be solved through the introduction of parabolic coordinates in the plane,

$$\xi = 2X^2 = \rho + x, \qquad (19a)$$

$$\eta = 2Y^2 = \rho - x, \qquad (19b)$$

with

$$\psi_{n_1 n_2}(\xi, \eta) = f_{n_1}[(|E|)^{1/2}\xi] f_{n_2}[(|E|)^{1/2}\eta]$$
$$\times \exp[-\tfrac{1}{2}(\xi + \eta)(|E|)^{1/2}],$$
$$(n_1, n_2 = 0, 1, \cdots) \qquad (20)$$

where the functions $f_n(x)$ can be identified[11] with Hermite polynomials of even order,

$$f_n(x) = \mathcal{H}_{2n}(x^{1/2}), \qquad (21)$$

and

$$|E| = mZ^2e^4/\hbar^2 2(n_1+n_2+\tfrac{1}{2})^2. \qquad (22)$$

This solution [Eqs. (19)–(22)] suggests a direct transformation of the Schrödinger equation (18) into one for an equivalent two-dimensional oscillator. This is given by

$$x = X^2 - Y^2, \qquad (23a)$$

$$y = 2XY \qquad (23b)$$

using (6a, b) and (9a, b) with $(x, y) = (\rho\cos\phi, \rho\sin\phi)$. The transformed eigenvalue problem is

$$[-(\hbar^2/2m)(\partial^2/\partial X^2+\partial^2/\partial Y^2) + 4|E|(X^2+Y^2)]\psi = 4Ze^2\psi; \qquad (24)$$

or, in a more conventional guise (after the scale transformation),

$$(|E|)^{1/2}(X\hat{\imath}+Y\hat{\jmath}) = (X'\hat{\imath}+Y'\hat{\jmath}),$$

$$[-(\hbar^2/2m)(\partial^2/\partial X'^2+\partial^2/\partial Y'^2) + 4(X'^2+Y'^2)]\psi' = [4Ze^2/(|E|)^{1/2}]\psi', \qquad (25)$$

with eigenvalues,

$$\epsilon = 4Ze^2/(|E|)^{1/2} = (2n_1+2n_2+1)\hbar(8/m)^{1/2}, \qquad (26)$$

so that the result of Eq. (22) again emerges.

Recently a wave-packet solution for a system of a hydrogenlike character which follows the corresponding classical circular orbit was constructed by Brown.[5] In that construction, one was motivated to try a radial function of the form

$$u_{nl}(r) = (\text{const.})\, r^n \exp(-\kappa_{nl}r), \qquad (27)$$

in the radial equation

$$\{-(d^2/dr^2) + [l(l+1)/r^2] - (2m/\hbar^2)(Ze^2/r) + \kappa_{nl}^2\}u_{nl}(r) = 0. \qquad (28)$$

Although our earlier connection between hydrogenic atom and isotropic oscillator breaks down in three dimensions,[11] there is the possibility that the analogous construction in the case of the isotropic oscillator may follow from the introduction of a trial radial function

$$v_{nl}(r) = (\text{const.})\,(r^2)^{n/2} \exp[-(1/2\hbar)(mk)^{1/2}r^2], \qquad (29)$$

in the corresponding oscillator radial equation

$$\{-(d^2/dr^2) + [l(l+1)/r^2] + (2m/\hbar^2)(kr^2/2) - \beta_{nl}^2\}v_{nl}(r) = 0. \qquad (30)$$

Our motivation stems from the fact that in the limit of large n, l ($n \simeq l$), the radial equation *and* radial function u_{nl} for the hydrogenic atom go over into the oscillator radial equation *and* radial function v_{nl} under the substitutions,

$$r \to r^2,$$

$$l \to l/2,$$

$$n \to n/2,$$

$$(8m/\hbar^2)Ze^2 \to \beta_{nl}^2,$$

$$\kappa_{nl}^2 \to mk/4\hbar^2.$$

Indeed, $v_{nl}(r)$ is a solution of Eq. (30) provided $n = l+1$, and $\beta_{nl}^2 = (2/\hbar)(l+3/2)(mk)^{1/2}$. Thus $E_l = \hbar\omega(l+3/2)$, with (proceeding as in Ref. 5),

$$\psi_{ll\,l+1}^{\text{osc}}(\mathbf{r}) = \text{const.}\exp\{-[l^{1/2}-(r/a)]^2\} \times \exp(il\phi)\exp[-\tfrac{1}{2}(\theta-\tfrac{1}{2}\pi)^2], \qquad (31)$$

where $a = (\hbar/m\omega)^{1/2}$ is the characteristic length for the harmonic oscillator. As in the case of the hydrogenic atom, one finds the wavefunction peaked along the circle $r = r_p = l^{1/2}a$ and with a width $\Delta r \sim l^{-1/2}r_p$. On the other hand, since we have

$$\partial^2E_l/\partial l^2|_N = 0, \qquad (32)$$

there is no spreading in this case.

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[1] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, MA, 1950), pp. 287, 299–307.

[2] H. C. Corben and P. Stehle, *Classical Mechanics* (Wiley, New York, 1950), pp. 251–257.

[3] D. Bohm, *Quantum Theory* (Prentice-Hall, New York, 1951), pp. 42–47.

[4] The connection between the Kepler problem and the harmonic oscillator has been a source of great interest for some time now though principally from the standpoint of the Runge–Lenz tensor {a vector in the former case and a symmetric tensor in the latter case [see, for example, D. M. Fradkin, Am. J. Phys. **33**, 207 (1965)]} and its properties. The works of Fradkin and of Bacry *et al.* [Commun. Math. Phys. **3**, 323 (1966)] are most pertinent to this view.

[5] L. S. Brown, Am. J. Phys. **41**, 525 (1973). It is amusing to find the scenario for this construction given on pp. 344–345 of Ref. 3.

[6] In the orbital plane, $\rho=(x^2+y^2)^{1/2}$.

[7] There is also the simple procedure suggested by J. H. Van Vleck (Ref. 1).

[8] This is due to A. Sommerfeld (Ref. 1).

[9] More concisely, in terms of the complex variable z, one finds under the transformation,

$$z=\rho\exp(i\phi)\rightarrow\zeta^2=[u\exp(i\psi)]^2,$$

that the ellipse of Eq. (7),

$$|z|+|z-2(a^2-b^2)^{1/2}|=2a$$

goes into the trajectory,

$$|\zeta^2|+|\zeta^2-2(a^2-b^2)^{1/2}|=2a,$$

which is another version of the "standard" ellipse,

$$|\zeta-\gamma|+|\zeta+\gamma|=2\alpha,$$

rewritten in the form,

$$|\zeta|^2+|\zeta^2-\gamma^2|=2\alpha^2-\gamma^2,$$

with the square of the focal separation,

$$(2\gamma)^2=8(a^2-b^2)^{1/2},$$

and the square of the semimajor axis,

$$\alpha^2=a+(a^2-b^2)^{1/2}.$$

[10] From Eq. (12b) we deduce that two cycles of motion in the (ρ,ϕ) plane correspond to one cycle of motion in the (u,ψ) plane.

[11] In the present context, in two dimensions, the radial equation for the hydrogenic bound states,

$$\left(-\frac{\hbar^2}{2m}\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}+\frac{\hbar^2l^2}{2m\rho^2}+|E|-\frac{Ze^2}{\rho}\right)P_l(\rho)=0,$$

goes over into the radial oscillator equation,

$$\left(-\frac{\hbar^2}{2m}\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}+\frac{\hbar^2l^2}{2m\rho^2}-4Ze^2+4|E|\rho^2\right)P_{l/2}(\rho^2)=0,$$

under the transformation $\rho\rightarrow\rho^2$, $l\rightarrow l/2$, with $\epsilon=4Ze^2$ and $\nu=(2|E|/m)^{1/2}\pi^{-1}$ as we obtained earlier classically. However, no such relationship follows from the analogous substitution $r\rightarrow r^2$, $l\rightarrow l/2$, in the three-dimensional radial hydrogenic equation,

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{\hbar^2l(l+1)}{2mr^2}+|E|-\frac{Ze^2}{r}\right)R_l(r)=0.$$