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Classical limit of the two-dimensional and the three-dimensional hydrogen atom

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Abstract. Using the harmonic oscillator representation of the hydrogen atom and constructing the appropriate coherent state corresponding to the minimum uncertainty product, the classical limits of the two-dimensional and the three-dimensional hydrogen atom are examined. The method adopted in this paper is similar to that used recently by Bhaumik, Dutta Roy and Ghosh. We deduce the classical limit by requiring that the expectation value $\langle r \rangle$ of the radial variable is large for the two-dimensional hydrogen atom. The resulting trajectory is an ellipse satisfying the conditions of the Kepler orbit in classical mechanics. In order to obtain the classical limit of the three-dimensional hydrogen atom, besides the condition of large $\langle r \rangle$, we make the uncertainty $\Delta r = (\langle r^2 \rangle - \langle r \rangle^2)^{1/2}$ a minimum with respect to certain parameters of the coherent state. Imposition of only the first condition leads to an elliptical orbit, which is not a Kepler orbit in general. Imposition of both conditions leads to an orbit identical with that of the two-dimensional hydrogen atom. However, the time evolution of the expectation values of position variables are consistent with the corresponding results of the Kepler problem only for small values of eccentricity, but not in general.

1. Introduction

Since its formulation in 1926, quantum mechanics has established itself as the most successful physical theory for the description of the microworld. On the other hand, the laws of classical dynamics explain many common phenomena involving larger objects moving with small velocities. The transition from quantum physics to classical physics seems to be an area which is still not thoroughly explored and fully understood. The transition has been described in general terms by Bohr's correspondence principle: quantum theory must approach classical theory asymptotically in the limit of large quantum numbers. Further, the Poisson bracket formulation of classical mechanics and commutator bracket formulation of quantum mechanics indicate a formal structural similarity between classical and quantum mechanics. The analysis of the phase of the wavefunction in the Schrödinger equation and its relation to the Hamilton principal function of the Hamilton-Jacobi theory of classical mechanics is another way of relating quantum and classical mechanics.

It is generally believed that an appropriate superposition of the relevant states resulting in a spacetime-dependent coherent state will exhibit the associated classical behaviour. This has been successfully done in the case of the one-dimensional (1D) harmonic oscillator (Schrödinger 1926, Sudarshan 1963, Glauber 1963). Schrödinger suggested that construction of such states for the hydrogen atom (H atom) should lead to a proper classical limit, namely the Kepler orbit. Recently, several attempts have been made at constructing a suitable coherent state for generalised potentials (Nieto

and Simmons 1979, Nieto 1980) as well as for the Coulomb potential in particular (Brown 1973, Snieder 1983).

The connection between the three-dimensional (3D) H atom and the four-dimensional (4D) or two two-dimensional (2D) harmonic oscillators has been established by various approaches (Kibler *et al* 1986, Chen 1987). This has provided a way of studying the classical limit of the H atom on the harmonic oscillator basis (Gerry 1986, Bhaumik *et al* 1986). Bhaumik, Dutta Roy and Ghosh (1986, hereafter referred to as BDG), have constructed a very long-lived wavepacket which traverses an elliptical orbit consistent with the corresponding results of classical mechanics. They have achieved this by imposing the constraint $\langle z \rangle = 0$ for the expectation value of position variable z and confining the analysis primarily to the motion of the wavepacket in the xy plane. In this paper, we investigate the classical limit of the 2D H atom using a procedure similar to the one adopted by BDG. Apart from making available the details of the calculation of the classical limit of the 2D H atom, our work is motivated by the following important considerations.

It is well known that the central field problem in classical mechanics conserves the angular momentum *vector* L and the motion is in a plane perpendicular to it. From this point of view, one may ask whether the corresponding formulation in quantum mechanics is the 2D Schrödinger equation having a circularly symmetric potential, because then the angular momentum conservation is retained both in quantum and in classical mechanics. In order to examine this in detail, we obtain the classical limit of the 2D H atom. We further study the equivalence of this approach to that of BDG. It is also noted that even in the case of a central potential quantum mechanics does not conserve the angular momentum *vector* but only L^2 and, say, L_z . Hence, one cannot preclude the existence of a 3D orbit for the classical limit of the 3D H atom. This aspect is investigated in the present paper starting from the 3D H atom and without imposing the condition $\langle z \rangle = 0$. The condition that the uncertainty $\Delta r = (\langle r^2 \rangle - \langle r \rangle^2)^{1/2}$ is a minimum is imposed by requiring that the wavepacket should have maximum localisation in the classical limit. We further examine whether the classical limit obtained from the 2D and the 3D H atom in the present approach is completely equivalent to the classical limit in all details, like the exact time dependence of the orbit variables.

In § 2 we study the 2D H atom in terms of the harmonic oscillator basis. Section 3 deals with the construction of coherent states and deduction of the orbit in the classical limit of the 2D H atom. In § 4 we study the 3D H atom wavepacket by suitable parametrisation which does not make $\langle z \rangle = 0$ in general and deduce the orbit in the classical limit. Section 5 deals with the discussion and conclusions.

2. Spectrum of the two-dimensional hydrogen atom using the harmonic oscillator basis

Let us consider the Schrödinger equation for the 2D H atom:

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 - \frac{k}{r} \right] \psi = E\psi \quad E < 0 \quad (1)$$

where $V(r) = -k/r$, $k > 0$, is the Coulomb potential and

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \quad (2)$$

with $x = r \cos \phi$ and $y = r \sin \phi$.

Introducing the parameters $\lambda = 8m_0k/\hbar^2 = 8/a_0$, $\eta^4 = -8m_0E/\hbar^2$ and $a_0 = \hbar^2/m_0k$ (the Bohr radius), equation (1) reduces to the form

$$[4r\nabla^2 + \lambda - \eta^4 r]\psi = 0. \tag{3}$$

It is well known that the 2D H atom problem can be solved on the harmonic oscillator basis using the coordinate system (u, v) given by (Englefield 1971)

$$x = \frac{1}{2}(u^2 - v^2) \quad y = uv. \tag{4}$$

This is equivalent to the complex coordinate system (ξ, ξ^*) given by

$$x + iy = \frac{1}{2}(u + iv)^2 = 2\xi^2 \quad x - iy = \frac{1}{2}(u - iv)^2 = 2(\xi^*)^2. \tag{5}$$

In terms of the polar coordinate system (r, ϕ)

$$\xi = \sqrt{\frac{r}{2}} \exp(\frac{1}{2}i\phi) \quad \xi^* = \sqrt{\frac{r}{2}} \exp(-\frac{1}{2}i\phi) \tag{6}$$

such that

$$r = 2\xi^*\xi \quad \phi = \tan^{-1}(y/x) = (\text{phase of } \xi - \text{phase of } \xi^*).$$

In terms of the complex coordinates ξ, ξ^* the Schrödinger equation (3) becomes

$$-\frac{1}{\eta^2} \frac{\partial^2 \psi}{\partial \xi^* \partial \xi} + \eta^2 \xi^* \xi \psi = \frac{\lambda}{2\eta^2} \psi. \tag{7}$$

Let us introduce annihilation and creation operators

$$\begin{aligned} a_+ &= \frac{1}{\sqrt{2}\eta} \left(\frac{\partial}{\partial \xi} + \eta^2 \xi^* \right) & a_- &= \frac{1}{\sqrt{2}\eta} \left(\frac{\partial}{\partial \xi^*} + \eta^2 \xi \right) \\ a_+^\dagger &= \frac{1}{\sqrt{2}\eta} \left(-\frac{\partial}{\partial \xi^*} + \eta^2 \xi \right) & a_-^\dagger &= \frac{1}{\sqrt{2}\eta} \left(-\frac{\partial}{\partial \xi} + \eta^2 \xi^* \right) \end{aligned} \tag{8}$$

satisfying the usual canonical commutation rules

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \quad [a_i, a_j^\dagger] = \delta_{ij} \quad i, j = +, -. \tag{9}$$

In terms of these operators equation (7) becomes

$$[a_+^\dagger a_+ + a_-^\dagger a_- + 1]\psi = (\lambda/2\eta^2)\psi. \tag{10}$$

This equation is formally identical to the Schrödinger equation for a 2D harmonic oscillator. $a_+^\dagger a_+$ and $a_-^\dagger a_-$ represent the number operators having eigenvalues n_+, n_- , respectively and $n_\pm = 0, 1, 2, 3, \dots$. Hence,

$$n_+ + n_- + 1 = \lambda/2\eta^2. \tag{11}$$

It can be readily seen using expressions given by (8) and (6) that

$$-\frac{\hbar}{2} (a_+^\dagger a_+ - a_-^\dagger a_-)\psi = -\frac{\hbar}{2} \left(\xi \frac{\partial}{\partial \xi} - \xi^* \frac{\partial}{\partial \xi^*} \right) \psi = -i\hbar \frac{\partial \psi}{\partial \phi}. \tag{12}$$

Since the 2D wavefunction is separable, the eigenfunction can be formally written as

$$\psi_{nm}(r, \phi) = R_{nm}(r)\Phi_m(\phi).$$

$\Phi_m(\phi)$ is an eigenfunction of $-i\hbar \partial/\partial\phi$ with eigenvalues $m\hbar$, $m=0, \pm 1, \pm 2, \dots$. Therefore, it follows that

$$-n_+ + n_- = 2m. \quad (13)$$

Hence, from (11) we get

$$E = -(2m_0k^2/\hbar^2)(n_+ + n_- + 1)^{-2}. \quad (14)$$

Therefore

$$E_n = -(m_0k^2/2\hbar^2)(n - \frac{1}{2})^{-2} \quad (15)$$

where $n = n_+ + m + 1 = 1, 2, 3, \dots$. One readily identifies E_n with the energy eigenvalue of the 2D H atom (Zaslow and Zandler 1967) obtained using other standard methods. It is noticed that the energy eigenvalues of the 2D and the 3D H atom nearly coincide for large quantum numbers.

3. Classical limit of the two-dimensional hydrogen atom

It is well-known that the classical limit of the 1D harmonic oscillator can be deduced by constructing the coherent state by superposing the harmonic oscillator eigenfunctions $|n\rangle$ (Schrödinger 1926, Sudarshan 1963, Glauber 1963). Such a coherent state is characterised by the minimum uncertainty product of position and momentum. The works of Gerry (1986) and BDG on the classical limit of the 3D H atom also adopt a procedure similar to this, using the superposition of two 2D or 4D harmonic oscillator eigenstates.

The coherent state $|\alpha\rangle$ corresponding to the 1D harmonic oscillator (Sudarshan 1963, Glauber 1963, Gerry 1986, BDG) is

$$|\alpha\rangle = \exp(-\frac{1}{2}|\alpha|^2) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (16)$$

where α is a complex number such that

$$a|\alpha\rangle = \alpha|\alpha\rangle \quad (17)$$

with a being an annihilation operator.

If H_0 denotes the Hamiltonian of a harmonic oscillator of angular frequency ω , then

$$H_0|n\rangle = (n + \frac{1}{2})\hbar\omega|n\rangle. \quad (18)$$

The time dependence of the coherent state is given by

$$|\alpha, t\rangle = \exp(-iH_0t/\hbar)|\alpha\rangle = \sum_{n=0}^{\infty} \exp(-\frac{1}{2}|\alpha|^2) \frac{\alpha^n}{\sqrt{n!}} \exp[-i(n + \frac{1}{2})\omega t]|n\rangle. \quad (19)$$

Hence, the expectation value of the position variable x is

$$\langle x \rangle = \left(\frac{2\hbar}{m_0\omega} |\alpha|^2 \right)^{1/2} \cos(\omega t - \delta_0) \quad (20)$$

where δ_0 is the argument of the complex number α . This expectation value $\langle x \rangle$ satisfies the classical equation of motion for the harmonic oscillator

$$\langle \ddot{x} \rangle + \omega^2 \langle x \rangle = 0 \quad (21)$$

where $\langle \ddot{x} \rangle = (d^2/dt^2)\langle x \rangle$.

From this basis we now proceed to study the coherent states having the minimum uncertainty, leading to the classical limit of a quantal problem in the case of the Coulomb potential $V(r) = -k/r$, $k > 0$.

In the case of the 2D H atom treated as a 2D harmonic oscillator in the new variables ξ and ξ^* , the coherent state $|\alpha_+, \alpha_-\rangle$ in terms of eigenfunctions $|n_+, n_-\rangle$ of the number operators $a_+^\dagger a_+$ and $a_-^\dagger a_-$ is:

$$|\alpha_+, \alpha_-\rangle = \sum_{\{n_\pm\}=0}^{\infty} \exp[-\frac{1}{2}(|\alpha_+|^2 + |\alpha_-|^2)] \frac{\alpha_+^{n_+} \alpha_-^{n_-}}{\sqrt{n_+! n_-!}} |n_+, n_-\rangle \quad (22)$$

where $|\alpha_+, \alpha_-\rangle$ is an eigenstate of a_+ and a_- with eigenvalues α_+ , α_- respectively. Following the method of BDG, we write

$$\alpha_\pm = |\alpha_\pm| \exp(\mp i\Delta) \quad (23)$$

along with the parametrisation

$$|\alpha_+| = \gamma \cos \chi \quad |\alpha_-| = \gamma \sin \chi \quad (24)$$

such that $|\alpha_+|^2 + |\alpha_-|^2 = \gamma^2$, which is applicable to the 2D H atom problem. It will be shown that γ^2 is proportional to $\langle r \rangle$ and hence should be assumed to be large in the classical limit.

Let us now introduce the time evolution of the state. We note that the coefficients of this coherent state are peaked around the maximum of $\alpha_+^{n_+} \alpha_-^{n_-} (n_+! n_-!)^{-1/2}$. Using Stirling's formula we see that the following values of n_+ , n_- , respectively, maximise the coefficients:

$$N_+ = \gamma^2 \cos^2 \chi \quad N_- = \gamma^2 \sin^2 \chi. \quad (25)$$

Expanding the energy E as a power series around these values, we can write from (14)

$$E = -(2m_0 k^2 / \hbar^2)(n_+ + n_- + 1)^{-2} \\ = E_{\text{peak}} + \hbar\omega_c(\delta_+ + \delta_-) - (3\hbar\omega_c/2\gamma^2)(\delta_+ + \delta_-)^2 + \dots \quad (26)$$

where

$$E_{\text{peak}} \approx -2m_0 k^2 / \hbar^2 \gamma^4 \quad (27)$$

$$\omega_c \approx 4m_0 k^2 / \hbar^3 \gamma^6 \quad \delta_\pm = n_\pm - N_\pm. \quad (28)$$

The energy dependence of the state, entering through the factor $\exp(-iEt/\hbar)$, induces, to the leading order in $1/\gamma^2$, a simple time dependence of $\exp(-i\omega_c t)$ on each of α_+ and α_- . Thus, the time dependence of the state over and above the phase factor $\exp(-iE_{\text{peak}}t/\hbar)$ is given by

$$|\alpha_+, \alpha_-\rangle = |\gamma^2, \chi, \Delta; t\rangle = |\gamma \cos \chi \exp[-i(\Delta + \omega_c t)], \gamma \sin \chi \exp[i(\Delta - \omega_c t)]\rangle. \quad (29)$$

Using this, the expectation values of the dynamical variables x , y , r and angular momentum L can be found after expressing them in terms of annihilation and creation operators. The results are

$$\langle x \rangle = (\gamma^2 / \eta^2) [\cos 2\Delta (\cos 2\omega_c t + \sin 2\chi) - \cos 2\chi \sin 2\Delta \sin 2\omega_c t] \quad (30a)$$

$$\langle y \rangle = (\gamma^2 / \eta^2) [\sin 2\Delta (\cos 2\omega_c t + \sin 2\chi) + \cos 2\chi \cos 2\Delta \sin 2\omega_c t] \quad (30b)$$

$$\langle r \rangle = (\gamma^2 / \eta^2) (1 + \sin 2\chi \cos 2\omega_c t) \quad (30c)$$

$$\langle L \rangle = \frac{1}{2} \hbar \gamma^2 \cos 2\chi \quad (30d)$$

where $L = xp_y - yp_x$.

If the coordinate system is rotated by an angle -2Δ , the resulting values of $\langle x \rangle$ and $\langle y \rangle$ satisfy the equation of an ellipse with its symmetry axes coinciding with the new coordinate axes:

$$\frac{[\langle x \rangle - (\gamma^2/\eta^2) \sin 2\chi]^2}{(\gamma^2/\eta^2)^2} + \frac{(\langle y \rangle)^2}{[(\gamma^2/\eta^2) \cos 2\chi]^2} = 1. \quad (31)$$

The angle -2Δ is the angle between the major axis of the ellipse and the original x axis. In the case of this ellipse, the variables $\langle x \rangle$ and $\langle y \rangle$ are defined in a coordinate system in which one of the foci is at the origin. The parameters of the ellipse are

$$\text{semimajor axis: } a = \gamma^2/\eta^2 \quad (32a)$$

$$\text{semiminor axis: } b = (\gamma^2/\eta^2) \cos 2\chi \quad (32b)$$

$$\text{eccentricity: } \varepsilon = \sin 2\chi. \quad (32c)$$

The expectation value of the energy is

$$\langle E \rangle = -2m_0k^2/\hbar^2\gamma^4. \quad (33)$$

Since $\langle x \rangle$ and $\langle y \rangle$ are periodic with frequency $2\omega_c$, the time period of revolution is

$$T = 2\pi/2\omega_c = \pi/\omega_c \quad (34a)$$

and hence

$$T^2 = (4\pi^2m_0/k)a^3. \quad (34b)$$

This is identical with Kepler's third law.

Equations (30d), (32a)-(32c) and (33) lead to the following relations among the semimajor axis, semiminor axis, eccentricity, energy and angular momentum:

$$a = |k/2\langle E \rangle| \quad (35a)$$

$$b = |k/2\langle E \rangle|(1 - \varepsilon^2)^{1/2} \quad (35b)$$

$$\varepsilon = [1 + (2\langle E \rangle \langle L \rangle^2/m_0k^2)]^{1/2}. \quad (35c)$$

The ellipse obtained by BDG in the xy plane also satisfies the above relations. These are the same as the standard results of elliptical orbits of the Kepler problem in classical mechanics (see, for example, Goldstein 1978).

Following the procedure of BDG, let us now estimate the lifetime of a wavepacket as it dissipates with time. Let us consider the simple case of a special state of the wavepacket moving in a circular trajectory ($\varepsilon = 0$ and hence $\chi = 0$). Then, $\alpha_+ = \gamma \exp(-i\omega_c t)$ and $\alpha_- = 0$. The appropriate wavepacket in this case is obtained from (22) by setting $n_- = 0$. Writing the symbol n for n_+ for convenience, we get

$$|\alpha_+, \alpha_- \rangle = \exp(-\frac{1}{2}\gamma^2) \sum_{n=0}^{\infty} \frac{\alpha_+^n}{\sqrt{n!}} |n, 0 \rangle. \quad (36)$$

The coefficient of expansion in (36) is a maximum for $n = N_+ = \gamma^2$. Let $\nu = n - N_+ = n - \gamma^2$. Expanding the coefficients around the maximum value and using Stirling's formula and noting that $\gamma^2 \gg 1$, we get

$$\frac{|\alpha_+|^n}{\sqrt{n!}} \approx (2\pi\gamma^2)^{-1/4} \exp\left[\frac{1}{2}\left(\gamma^2 - \frac{\nu^2}{2\gamma^2}\right)\right].$$

Hence

$$|\alpha_+, \alpha_- \rangle = \sum_{\nu=-\infty}^{\infty} (2\pi\gamma^2)^{-1/4} \exp\left(-\frac{\nu^2}{4\gamma^2}\right) |\gamma^2 + \nu, 0 \rangle. \quad (37)$$

Introducing the time dependence over and above the phase factor $\exp(-iE_{\text{peak}}t/\hbar)$ and considering up to the third term in the energy expansion of equation (26) and replacing the summation by integration over ν , we get the state for $\chi = 0$, $n_- = 0$ as

$$|\gamma^2, t\rangle = (2\pi\gamma^2)^{-1/4} \int_{-\infty}^{\infty} d\nu \exp\left(-\frac{\nu^2}{4\gamma^2} - i\omega_c t\nu + \frac{3}{2}i\omega_c t\frac{\nu^2}{\gamma^2}\right) |\gamma^2 + \nu, 0\rangle. \quad (38)$$

The value of $\langle r \rangle$ obtained using equation (38) is independent of time:

$$\langle r \rangle = \gamma^2 / \eta^2.$$

The expectation values $\langle x \rangle$ and $\langle y \rangle$ are determined similarly for the special state given by equation (38) (Gradshteyn and Ryzhik 1965):

$$\langle x \rangle = \frac{1}{\eta^2} \exp\left(-\frac{18\omega_c^2 t^2}{\gamma^2} - \frac{1}{2\gamma^2}\right) (\gamma^2 \cos 2\omega_c t + 6\omega_c t \sin 2\omega_c t) \quad (39a)$$

$$\langle y \rangle = \frac{1}{\eta^2} \exp\left(-\frac{18\omega_c^2 t^2}{\gamma^2} - \frac{1}{2\gamma^2}\right) (\gamma^2 \sin 2\omega_c t - 6\omega_c t \cos 2\omega_c t). \quad (39b)$$

As $t \rightarrow \infty$, both the expectation values $\langle x \rangle$ and $\langle y \rangle$ tend to zero, keeping $\langle r \rangle$ constant. This means that the wavepacket ultimately gets smeared over a circular ring of large radius. From the equations (39a) and (39b) we see that

$$T_s = \frac{\gamma}{\sqrt{18}\omega_c} = \sqrt{\frac{2m_0 \langle r \rangle}{\hbar\omega_c}} \quad (40)$$

is the time in which the wavepacket gets smeared over a circular orbit. For a large planet like the Earth moving around the Sun, the decay time is of the order of 10^{36} yr which is very large compared to the present age of the Earth. Just for curiosity, if one evaluates T_s in the case of the Bohr H atom for a coherent state around energy E_n , $n \gg 1$, one gets

$$T_s \approx \frac{2^{3/4}}{3} \frac{m_0^{3/4} a_0^{3/2}}{(E_0 \hbar^2)^{1/4}} n^{7/2} \approx 1.6 \times 10^{-17} n^{7/2} \text{ s}$$

where E_0 is the ground-state energy of the 3D H atom. For $n = 10^4$, T_s is of the order of 10^{-3} s. This time is significantly larger than the decay times of the highly excited H atom states and hence unlikely to have any observable consequence. We see that the nature of the Kepler orbit, the time period of revolution of the wavepacket and the mean life T_s of the wavepacket moving in a circular orbit are found to be the same as those calculated by BDG starting from the 3D H atom and imposing the condition $\langle z \rangle = 0$. Thus the present analysis shows that the classical limit is achieved in the following respects: (i) Kepler's first law is obtained; (ii) Kepler's third law is obtained; (iii) Kepler's second law, which describes the conservation of angular momentum is automatically guaranteed while it has been imposed in the BDG treatment of the 3D H atom.

4. Classical limit of the three-dimensional hydrogen atom

The analysis of the 3D H atom has been done by BDG using 2D harmonic oscillators in terms of the four variables ξ_A , ξ_A^* , ξ_B and ξ_B^* which are related to the four variables r , θ , ϕ , σ , the first three being the usual spherical polar coordinates. The hydrogenic

spectrum was obtained by applying the constraint that the wavefunction is independent of σ . In order to obtain a wavepacket moving in a plane as required by classical mechanics, BDG set the expectation value $\langle z \rangle = 0$. This condition, together with the associated results that $\langle L_x \rangle = \langle L_y \rangle = 0$, enabled them to obtain a wavepacket such that the time variations of expectation values $\langle x \rangle$ and $\langle y \rangle$ follow an elliptical orbit:

$$\frac{[\langle x \rangle - (2\mu\rho/\eta^2) \sin 2\chi]^2}{(2\mu\rho/\eta^2)^2} + \frac{(\langle y \rangle)^2}{[(2\mu\rho/\eta^2) \cos 2\chi]^2} = 1 \quad (41)$$

where the parameters μ , ρ and χ are as defined by BDG. This is consistent with Kepler's first law. The condition $\langle L_x \rangle = \langle L_y \rangle = 0$ guarantees Kepler's second law. BDG also established Kepler's third law and the decay time of the coherent wavepacket.

We now make the following observations. (i) Imposition of the condition $\langle z \rangle = 0$ does not necessarily confine the wavepacket to a plane. Such may be the case if $\langle z^2 \rangle$ is equal to or close to zero. This aspect is made clear by noting that in the case of the 1D harmonic oscillator of mass m_0 , angular frequency ω and energy E , the time average $\langle \overline{x(t)} \rangle$ is zero whereas the time average $\langle \overline{x^2(t)} \rangle$ is $E/m_0\omega^2$, which is positive and can be large. Similarly, for a coherent state which depends upon all three position variables x , y and z (or r , θ , ϕ), $\langle z^2 \rangle$ is positive and non-zero even if $\langle z \rangle = 0$. Hence one might ask whether the Kepler orbit obtained by BDG starting from the 3D H atom is only a kind of projection of the evolution of the coherent state onto the xy plane. (ii) It is well known that unlike the case in classical mechanics, the 3D quantum mechanical central field problem does not conserve all the three components L_x , L_y and L_z of the angular momentum simultaneously. Hence, *a priori* one cannot rule out the possibility that a coherent state constructed starting from a superposition of two 2D harmonic oscillator wavefunctions corresponding to a 3D H atom may have motion in 3D space, in a non-trivial sense. Therefore, it is of interest to investigate the nature of the orbit if the condition $\langle z \rangle = 0$ is not imposed.

In order to do this, we consider the parametrisation such that $\langle z \rangle \neq 0$ in general in the case of the 3D H atom. A suitable parametrisation which can be analysed analytically is

$$\begin{aligned} |\alpha_+\rangle &= \gamma \cos \chi \cos \delta & |\alpha_-\rangle &= \gamma \sin \chi \cos \delta \\ |\beta_+\rangle &= \gamma \sin \chi \sin \delta & |\beta_-\rangle &= \gamma \cos \chi \sin \delta. \end{aligned} \quad (42)$$

This parametrisation retains $|\alpha_+|^2 + |\alpha_-|^2 + |\beta_+|^2 + |\beta_-|^2 = \gamma^2$. As before, for classical orbits $\gamma^2 \gg 1$. Following the procedure of BDG, with appropriate orientation of the x , y and z axes, (i.e. $\Delta = 0$) we get

$$\langle x \rangle = (\gamma^2/\eta^2) \sin 2\delta [\cos 2\omega_c t + \frac{1}{2} \sin 2\chi (\cos^2 \chi \cos^2 \delta + \sin^2 \chi \sin^2 \delta)^{-1/2} \\ \times (\cos^2 \chi \sin^2 \delta + \sin^2 \chi \cos^2 \delta)^{-1/2}] \quad (43a)$$

$$\langle y \rangle = (\gamma^2/\eta^2) \sin 2\delta \cos 2\chi \sin 2\omega_c t \quad (43b)$$

$$\langle z \rangle = (\gamma^2/\eta^2) \cos 2\delta \sin 2\chi [\cos 2\omega_c t + \frac{1}{2} \sin 2\chi (\cos^2 \chi \cos^2 \delta + \sin^2 \chi \sin^2 \delta)^{-1/2} \\ \times (\cos^2 \chi \sin^2 \delta + \sin^2 \chi \cos^2 \delta)^{-1/2}] \quad (43c)$$

$$\langle r \rangle = (\gamma^2/\eta^2) [2(\cos^2 \chi \cos^2 \delta + \sin^2 \chi \sin^2 \delta)^{1/2} \\ \times (\cos^2 \chi \sin^2 \delta + \sin^2 \chi \cos^2 \delta)^{1/2} + \sin 2\chi \cos 2\omega_c t] \quad (43d)$$

$$\langle L_z \rangle = \gamma^2 \hbar \cos 2\chi \quad (43e)$$

$$\langle E \rangle = -2m_0 k^2 / \hbar^2 \gamma^4 \quad (43f)$$

where $\omega_c = 4m_0 k^2 / \hbar^3 \gamma^6$.

Now, let us examine the general case given by equations (43). Equations (43a) and (43c) show that

$$\langle z \rangle = (\sin 2\chi / \tan 2\delta) \langle x \rangle. \quad (44)$$

This implies that the projection of the actual orbit for our particular choice of coordinate axes is a straight line in the zx plane, making an angle $\theta_0 = \tan^{-1}(\sin 2\chi / \tan 2\delta)$ with the x axis. This implies that in the present case the actual orbit in the classical limit lies in a plane which is perpendicular to the zx plane and makes an angle θ_0 with the xy plane. Now, we rotate the zx plane around the y axis through angle θ_0 so that the new $x'y'$ plane coincides with the plane of the orbit. Then, we get the expectation values $\langle x' \rangle$, $\langle y' \rangle$ and $\langle z' \rangle$ in the new coordinate system (x', y', z') as

$$\begin{aligned} \langle x' \rangle &= (\gamma^2 / \eta^2) \sin 2\delta (1 + \sin^2 2\chi / \tan^2 2\delta)^{1/2} [\cos 2\omega_c t \\ &\quad + \frac{1}{2} \sin 2\chi (\cos^2 \chi \cos^2 \delta + \sin^2 \chi \sin^2 \delta)^{-1/2} \\ &\quad \times (\cos^2 \chi \sin^2 \delta + \sin^2 \chi \cos^2 \delta)^{-1/2}] \end{aligned} \quad (45a)$$

$$\langle y' \rangle = (\gamma^2 / \eta^2) \sin 2\delta \cos 2\chi \sin 2\omega_c t \quad (45b)$$

$$\langle z' \rangle = 0. \quad (45c)$$

This leads to the following equation for the trajectory as an ellipse in the $x'y'$ plane:

$$\frac{(\langle x' \rangle - g)^2}{[(\gamma^2 / \eta^2) \sin 2\delta (1 + \sin^2 2\chi / \tan^2 2\delta)^{1/2}]^2} + \frac{(\langle y' \rangle)^2}{[(\gamma^2 / \eta^2) \sin 2\delta \cos 2\chi]^2} = 1 \quad (46)$$

where

$$\begin{aligned} g &= \frac{1}{2} (\gamma^2 / \eta^2) \sin 2\delta \sin 2\chi (1 + \sin^2 2\chi / \tan^2 2\delta)^{1/2} \\ &\quad \times (\cos^2 \chi \cos^2 \delta + \sin^2 \chi \sin^2 \delta)^{-1/2} (\cos^2 \chi \sin^2 \delta + \sin^2 \chi \cos^2 \delta)^{-1/2}. \end{aligned}$$

Thus, we find that a coherent state constructed starting from the harmonic oscillator basis of the 3D H atom leads to an elliptical orbit in a plane in the limit of large quantum numbers. However, this ellipse given by (46) is not identical with the Kepler ellipse. We further impose the physically meaningful condition for the correct classical limit that the wavepacket should have maximum localisation. That is, $\Delta r = (\langle r^2 \rangle - \langle r \rangle^2)^{1/2}$ is a minimum. The expression for Δr in terms of the parametrisation given by equation (42) shows that for $\delta = \frac{1}{4}\pi$, Δr has its minimum value. It may be mentioned that in the particular case of circular orbits $(\Delta r)_{\min} = [-3\gamma^2 \hbar^2 / 4m \langle E \rangle]^{1/2}$. On putting $\delta = \frac{1}{4}\pi$, we find that $\theta_0 = 0$, i.e. the plane of the elliptical orbit coincides with the original xy plane and this also leads to the result $\langle z \rangle = 0$. Also, the condition $\delta = \frac{1}{4}\pi$ shows that the ellipse given by (46) is identical with the ellipse given by (31) in the 2D H atom case. Hence, Kepler's third law and the relations given by (35) are satisfied by the parameters of the elliptical orbit in the 3D H atom case in the classical limit.

5. Discussion and conclusion

Based on the present work and that of BDG, we make the following observations.

(i) The Kepler orbit obtained by starting from the 2D H atom is identical to the Kepler orbit obtained by BDG starting from the 3D H atom and imposing the condition $\langle z \rangle = 0$.

(ii) If one starts with the 3D H atom and uses a parametrisation which does not necessarily imply $\langle z \rangle = 0$, the coherent wavepacket still leads to an elliptical orbit in the large quantum number limit. However, this is not identical to the Kepler orbit and not confined to the xy plane. But if one further demands that the parametrisation should be such that the uncertainty Δr is a minimum, one automatically gets the orbit in the xy plane, which is identical to Kepler's ellipse. We offer the following plausible explanation to understand the situation.

Using the spherical polar coordinates (r, θ, ϕ) the 3D hydrogenic time-independent wavepacket can be formally written as

$$\psi_{3D}(r, \theta, \phi) = \sum_{n,l,m} c_{nlm} R_{nl}(r) y_{lm}(\theta, \phi). \quad (47)$$

If the wavepacket is restricted to the xy plane by putting $\theta = \frac{1}{2}\pi$, then the angular part of the wavefunction is $y_{lm}(\theta = \frac{1}{2}\pi, \phi) = \text{constant} \times \exp(im\phi)$. The corresponding 2D hydrogenic wavepacket can be written with (r, ϕ) variables as

$$\psi_{2D}(r, \phi) = \sum_{n,m} c'_{nm} U_{nm}(r) \exp(im\phi). \quad (48)$$

The symbol r denotes $(x^2 + y^2 + z^2)^{1/2}$ in 3D and $(x^2 + y^2)^{1/2}$ in 2D space. The expressions for $R_{nl}(r)$ and $U_{nm}(r)$ are

$$R_{nl}(r) = - \left[\left(\frac{2m_0 k}{n\hbar^2} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right]^{1/2} \exp(-\frac{1}{2}\beta r) (\beta r)^l L_{n+l}^{2l+1}(\beta r) \quad (49a)$$

$$U_{nm}(r) = - \frac{2m_0 k}{n\hbar^2} \left(\frac{(n-|m|-1)!}{(2n-1)[(n+|m|-1)!]^3} \right)^{1/2} \exp(-\frac{1}{2}\beta r) (\beta r)^{|m|} L_{n+|m|-1}^{2|m|}(\beta r) \quad (49b)$$

where $\beta = 2m_0 k / n\hbar^2$.

Obviously the radial parts of ψ_{3D} and ψ_{2D} coincide asymptotically for $|m| = l = n - 1$, $n \rightarrow \infty$. It may also be mentioned here that in case of large $l = |m|$, we have (Abramowitz and Stegun 1964):

$$P_l^l(\cos \theta) = 2^l \pi^{-1/2} \Gamma(l + \frac{1}{2}) \xrightarrow{l \rightarrow \infty} (2/e)^{1/2} [(2l+1)/e]^l \xrightarrow{l \rightarrow \infty} \infty \quad \theta = \frac{1}{2}\pi$$

$$P_l^l(\cos \theta) = \frac{\Gamma(2l+1)}{\Gamma(l+\frac{3}{2})} (\frac{1}{2}\pi \sin \theta)^{-1/2}$$

$$\times \cos[(l+\frac{1}{2})\theta - \frac{1}{4}\pi + \frac{1}{2}l\pi] + O(l^{-1}) \quad \varepsilon < \theta < \pi - \varepsilon \quad \varepsilon > 0 \quad (50)$$

$$P_l^l(\cos \theta) = 0 \quad \theta = 0, \pi \quad l = 1, 2, \dots$$

These observations indicate that enforcing the condition $\langle z \rangle = 0$ (as in BDG) amounts to the large cancellation of the coherent states for angles $\theta \neq \frac{1}{2}\pi$ due to rapid oscillation of $P_l^l(\cos \theta)$ and the accumulation of large amplitudes at $\theta = \frac{1}{2}\pi$, i.e. the xy plane. Similarly our procedure for obtaining the Kepler orbit starting from the 3D H atom by imposing the condition that Δr is to be a minimum with respect to the parametrisation used, seems to be equivalent to constructing a wavepacket of the type given by (47)

with $|m| = l = n - 1$, $n \rightarrow \infty$, because our procedure also automatically leads to the Kepler orbit in the xy plane and the condition $\langle z \rangle = 0$. Hence, we believe that our results and that of BDG are in agreement with the correspondence principle. It should be mentioned that our 3D H atom results are achieved by assuming the particular convenient parametrisation given by (42). Hence, it may still be incorrect to conclude that any arbitrarily constructed coherent wavepacket starting from the 3D H atom always leads to a planar orbit in general.

From the discussion so far one may naively conclude that coherent state wavepackets lead to the correct classical limit in the 2D as well as the 3D case and a connection between classical and quantum mechanics has been achieved for this problem. Unfortunately, this is not entirely true. A correct description of the central field problem for the inverse-square force in classical mechanics requires in addition to the description of the orbits, the correct time dependence of the position variables $x(t)$ and $y(t)$ or, equivalently $r(t)$ and $\phi(t)$. It is well known that in the case of $V(r) = -(k/r)$, $x(t)$, $y(t)$ and $r(t)$ are not simple harmonic in general, but are much more complicated functions of time. The harmonic time dependence of $x(t)$ and $y(t)$ are reasonably correct only when the energy of the particle is equal to or close to the minima $r = r_0$ of the effective potential $V_{\text{eff}}(r) = -(k/r) + (L^2/2mr^2)$. Hence, the classical limit of the H atom obtained by BDG or in this paper are correct descriptions only when the eccentricity of the Kepler orbit is close to or equal to zero. For highly eccentric Kepler orbits the time dependence given by (30) or (43) is not the correct approximation, notwithstanding the fact that the resulting orbit is a Kepler ellipse. In other words, deduction of the Kepler orbit is not a guarantee of a completely justified correct classical limit of the quantal problem for the potential $V(r) = -k/r$.

The origin of the harmonic time dependence of the expectation values $\langle x \rangle$ and $\langle y \rangle$ in this treatment can be elaborated as follows: One expects that the appropriate superposition needed to obtain a coherent state is of the form

$$|\alpha, t\rangle = \sum_n d_n \exp(-iE_n t/\hbar) |n\rangle \quad (51)$$

where

$$d_n = \exp(-|\alpha|^2/2) \alpha^n / \sqrt{n!}.$$

In the present and earlier treatments, the time evolution is closely approximated by expanding the energy in equation (26) only about the value for which d_n is a maximum. Hence, all the other contributing wavepackets are made to have the same time dependence through the factor $\exp[-i(E_{\text{peak}}/\hbar + \omega_c)t]$. This is made clear by noting that E_{peak} corresponds to the classical energy for the minima $r = r_0$ of V_{eff} corresponding to which the trajectory is circular. The present and earlier approaches therefore amount to the consideration of wavepackets corresponding to elliptical orbits of low eccentricity, which have harmonic time dependence to a reasonable degree of accuracy.

Before concluding, we make an additional observation. The classical limit of the H atom in terms of the Kepler orbit is a problem which is of interest in general aspects of quantum mechanics and its classical limit. As a physical problem, however, it has additional complications when the classical limit is reached. This is due to the fact that interaction in the H atom is electrodynamic in nature and hence in the classical limit the actual H atom will have to satisfy the laws of classical electrodynamics, such as radiation by accelerating charge, etc. Hence the results of the present paper should be understood purely as a bound-state problem under the central potential $V(r) = -k/r$

in quantum mechanics and its classical limit. It would be erroneous to deduce the properties of the physical H atom in the classical limit without incorporating additional features arising due to electrodynamical considerations.

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