

Coherent states for general potentials. IV. Three-dimensional systems

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The minimum-uncertainty coherent-states formalism is extended to higher-dimensional systems. Specifically, for spherically symmetric three-dimensional potentials the formalism looks for coherent states which are products of an angular wave function times a radial wave function. After reviewing the many studies on angular coherent states, I concentrate on the physically distinguishing radial coherent states. The radial formalism is explained in detail and contrasted with the effective one-dimensional formalism. The natural classical variables in the radial formalism are those which vary sinusoidally as $g(E,L)\theta(t)$, where $\theta(t)$ is the real azimuthal angular variable and $g(E,L)$ is the number of oscillations between apsidal distances per classical orbit. When changed to natural quantum operators, these operators can be given as the Hermitian sums and differences of the "l" raising and lowering operators. The formalism is applied to the three-dimensional harmonic-oscillator and Coulomb problems.

I. INTRODUCTION

Having discussed¹⁻³ the minimum-uncertainty coherent-states (MUCS) formalism for one-dimensional systems in great detail with Simmons, Jr., I now proceed to higher-dimensional systems. For explicitness, in this section I limit myself to spherically symmetric potentials in three dimensions. The generalization to N dimensions will be obvious.

Given a specific physical problem, one hopes to find a separable set of coordinates in which one can work. One can then attempt to find the coherent states as product wave functions in these coordinates. Of course, for spherically symmetric potentials a separable set of coordinates is (r, θ, ϕ) , so one can look for coherent states in the forms $\psi(r)\psi(\theta, \phi)$ or $\psi(r)\psi(\theta)\psi(\phi)$. Many discussions have appeared concerning coherent states for angular coordinates. These discussions are reviewed in Appendix A. Since the angular part of the entire coherent states will be the same for all spherically symmetric potentials, I refer the reader to Appendix A and the references listed there. In this paper I will concentrate on the physically distinguishing part of the problem, the radial part.

The radial part can be attacked in more than one fashion. The first method is to consider the potential plus angular momentum barrier $L^2/(2mr^2)$ as an effective one-dimensional potential. This was done for the harmonic oscillator with centripetal barrier (HOCB) potential in paper II.² There, we took the effective potential as

$$V(x) = U_0 \left(ax - \frac{1}{ax} \right)^2, \quad U_0 = \epsilon_0 \nu^2. \quad (1.1)$$

The natural classical variable X_c is

$$X_c = (ax)^2 - \left(1 + \frac{E}{2U_0} \right). \quad (1.2)$$

and it varies as the sine of the classical angular velocity multiplied by time:

$$X_c = \left[\frac{E}{U_0} \left(1 + \frac{E}{4U_0} \right) \right]^{1/2} \sin \omega_c t. \quad (1.3)$$

The quantum version of X_c is the natural quantum operator

$$X = (ax)^2 - \left(1 + \frac{H}{2U_0} \right), \quad (1.4)$$

where H is the effective one-dimensional Schrödinger Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x). \quad (1.5)$$

X is related to the "n" raising and lowering operators as

$$X_n = X(H - E_n) = \frac{1}{\nu} (A_n^- + A_n^+). \quad (1.6)$$

Note that these A_n^\pm operators raise and lower the ψ_n which correspond to the $\chi_{n_l} = R_{n_l}/r$ of the radial problem.

The above description represents the chain which we discussed in paper I: (a) the classical problem, (b) the natural classical variables, (c) the natural quantum operators, and (d) the "n" raising and lowering operators for the quantum eigenvalue problem. On this last point, recall our emphasis in paper III that the raising and lowering operators we use are for the n quantum number, not other raising and lowering operators which one could obtain from certain Infeld-Hull factorizations.⁴ (These might, for example, change both the shape of the potential and the quantum number n . See the Introduction

of paper III.³) As will be discussed in paper VI,⁵ a physical justification can be given in terms of WKB arguments⁶ for choosing the n raising and lowering operators. [This justification amounts to completing the bridge between (c) and (d) of the above chain.] But independent of this, the procedure has worked every time in our one-dimensional examples.^{2,3} Our program clearly relates to many of the connections between classical and quantum motion.^{6,7}

However, if one tries to apply the above chain to the hydrogen atom, the problem turns out to be analytically intractable. This can be immediately realized by observing that the n raising and lowering operators for the hydrogen atom *cannot* be put in analytic closed form. This is because the wave functions $R_{n,l}$ or $\chi_{n,l} = R_{n,l}/r$ are functions of the quantity

$$\rho_n = r/r_0^n. \quad (1.7)$$

Thus, even given the raising and lowering operators which change $R_{n,l}$ (or $\chi_{n,l}$) to $R_{n\pm 1,l}$, they *do not* also change ρ_n to $\rho_{n\pm 1}$. The new quantities $R_{n\pm 1,l}(\rho_n)$ are *not* the $(n\pm 1, l)$ eigenfunctions. To make then the new eigenfunctions ρ_n must be raised or lowered to $\rho_{n\pm 1}$ by hand. At root, this is the reason it was not possible to use the Perelomov technique⁸ to obtain *exact* hydrogen-atom coherent states in terms of the exponential of the group generators of the hydrogen atom.⁹

The futility of this approach for the hydrogen atom can also be seen by solving the classical problem for the natural classical variable X_c . As is shown in Appendix B, the answer is

$$X_c = \pm \cos \left\{ -\frac{2E}{e^2} \left(\frac{L^2}{2mE} - \frac{e^2 r}{E} - r^2 \right)^{1/2} + \sin^{-1} \left[\frac{e^2 + 2Er}{(e^4 + 2EL^2/m)^{1/2}} \right] \right\}, \quad (1.8)$$

where the plus sign is for $2n\pi \leq \omega_c t \leq (2n+1)\pi$. The natural quantum operator X would be Eq. (1.8) *symmetrized* in $E \rightarrow H$ and r . To obtain the analytic MUCS from this operator and the associated quantum operator P would be heroic. However, the complicated, nonanalytic raising and lowering operators at one end of the chain make the complicated X_c at the other end of the chain mutually believable.

Is there, though, another MUCS procedure that can be used? The answer is "yes." For spherically symmetric three-dimensional problems, it is not just the cyclic variable ($\omega_c t$) which can be used to obtain natural classical¹⁰ variables. There is also the real angular variable $\theta(t)$, where classically

$$\dot{\theta} = L/mr^2. \quad (1.9)$$

(The azimuthal angle is often labeled θ in classical mechanics instead of by the ϕ of quantum physics.) For spherically symmetric potentials,¹⁰ the classical orbit varies between the interior perigee and exterior apogee apsidal distances r_1 and r_2 . The orbit is closed for all E and L only for the harmonic-oscillator and Kepler-Coulomb potentials.¹¹ However, since for all spherical potentials the orbit is symmetric about any apsidal vector,¹⁰ the orbit will start at an apsidal position, vary to the other, and come back again, in some fraction $1/g(E, L)$ of 2π . [The case $g(E, L) = 0$ corresponds to just unbound motion, and so is excluded.] Thus, a natural classical variable can be chosen as that variable which varies as the sine and cosine of $\theta(t)g(E, L)$. $g(E, L)$ is "2" and "1" for the harmonic oscillator and the hydrogen atom, respectively.

Now, in terms of this angular variable, the MUCS procedure works thusly:

- (a) Solve the classical problem.
- (b) Find the "natural classical variables" which vary as $\sin[\theta(t)g(E, L)]$ and $\cos[\theta(t)g(E, L)]$.
- (c) Turn these natural classical variables into "natural quantum operators" and find the minimum-uncertainty states of the associated uncertainty relation, subject to restriction that the ground state is one of them. (The ground state is taken to be minimum n for a given l . This is circular motion, so the particle is at the bottom of the radial potential plus angular momentum barrier.)
- (d) These natural quantum operators will be able to be written in terms of Hermitian sums and differences of the " l " raising and lowering operators.

Given the classical problem, properties (a) and (b) can be satisfied as a matter of principle. Properties (c) and (d) are satisfied explicitly for the two examples given in Sec. III. The generality of these last two properties will be discussed in the concluding paper of our series.⁵

In Sec. II, I describe this MUCS procedure in detail, emphasizing the differences between this procedure and that for real one-dimensional problems. In Secs. III and IV, I implement this procedure for the radial parts of the harmonic oscillator and the hydrogen atom. The results are compared to those which can be obtained from other procedures in Sec. V. As I emphasize, the different methods for obtaining MUCS for a particular system do not yield identical MUCS. However, they all follow the classical motion. The wave packets have slightly different shapes be-

cause they are MUCS for different uncertainty relations.

II. CLASSICAL RADIAL PROBLEM

Starting from the classical Hamiltonian equation for a conservative system with constant energy

$$H = E = \frac{p_{cr}^2}{2m} + V(r) + \frac{L^2}{2mr^2} \quad (2.1a)$$

$$= \frac{m}{2} \dot{r}^2 + V(r) + \frac{L^2}{2mr^2}, \quad (2.1b)$$

one has

$$\dot{r} = \left(\frac{2}{m}\right)^{1/2} \left[E - V(r) - \frac{L^2}{2mr^2} \right]^{1/2}. \quad (2.2)$$

Our natural classical variable

$$X_c = X_c(r, E, L) \quad (2.3)$$

varies with time as

$$X_c = A_c(E, L) \sin[g(E, L)\theta(t)]. \quad (2.4)$$

With a prime denoting the derivative with respect to r , taking the time derivative of X_c yields

$$\dot{X}_c = X_c' \dot{r} = g \dot{\theta} A \cos(g\theta) \quad (2.5)$$

$$= \frac{gLA}{mr^2} \cos(g\theta), \quad (2.6)$$

where we have used

$$\dot{\theta} = \frac{L}{mr^2}. \quad (2.7)$$

Combining Eq. (2.6) with Eq. (2.2), X_c is the solution of the equation

$$X_c' = \left(\frac{g}{r^2} \frac{L}{m}\right) \left(\frac{m}{2}\right)^{1/2} \left[\frac{A^2 - X_c^2}{E - V(r) - L^2/2mr^2} \right]^{1/2}. \quad (2.8)$$

The main difference between this and the one-dimensional formula¹ (I3.4) is the factor (g/r^2) . Here (L/m) takes the place of ω_c in the one-dimensional case. The other natural variable P_c is given by

$$P_c = -m\dot{X}_c r^2 / g \quad (2.9a)$$

$$= -p_{cr} X_c' r^2 / g \quad (2.9b)$$

$$= -LA \cos(g\theta). \quad (2.9c)$$

The factor $(-g^{-1})$ in (2.9a) is a convenient normalization, but the factor r^2 is absolutely necessary. Otherwise, the time variation of (2.9c) would not be $\cos[g\theta(t)]$ since r also varies with t .

The reader should here recall that the variation of θ with r will also be found by integrating Eq. (2.7), using (2.2) to change variables, leading to

$$\begin{aligned} \theta - \theta_0 &= \int_0^t \frac{dt L}{mr^2} \\ &= \int_{r_0}^r \frac{dr}{[(2m/L^2)(E - V) - 1/r^2]^{1/2} r^2} \\ &= - \int_{u_0}^u \frac{du}{[(2m/L^2)(E - V) - u^2]^{1/2}}, \end{aligned} \quad (2.10)$$

$$u \equiv 1/r. \quad (2.11)$$

Putting Eqs. (2.8) and (2.9b) into Eq. (2.1a), one can rewrite the Hamiltonian equation in the form

$$\frac{A^2 L^2}{2m} = \frac{P_c^2}{2m} + \frac{1}{2} m \left(\frac{L}{m}\right)^2 X_c^2. \quad (2.12)$$

This means that once again, when one uses the natural classical variables X_c and P_c , the Hamiltonian equation is in the form of that for a harmonic oscillator. The classical equations of motion are

$$\dot{X}_c = -\frac{g}{mr^2} P_c, \quad (2.13)$$

$$\dot{P}_c = \frac{gL^2}{mr^2} X_c. \quad (2.14)$$

III. HARMONIC OSCILLATOR

A. Natural classical variables and quantum operators

For

$$V(r) = \frac{1}{2} m \omega^2 r^2 \quad (3.1)$$

the natural classical variables are

$$X_c = \left(\frac{1}{r^2} - \frac{mE}{L^2}\right) = A(E, L) \sin 2\theta, \quad (3.2)$$

$$P_c = \frac{p_{cr}}{r} = -AL \cos 2\theta. \quad (3.3)$$

This is the correct angular variation,

$$g(E, L) = 2, \quad (3.4)$$

since the orbit of the harmonic oscillator undergoes two oscillations between apsidal distances for every angular rotation of 2π . The reader can verify that the above results satisfy the equations of Sec. II, specifically, Eqs. (2.8), (2.10) with the appropriate phase, and (2.11)–(2.14).

The natural quantum operators should thus have forms like

$$X \sim \left(\frac{1}{r^2} - \frac{mH}{\hbar^2(l + \frac{1}{2})^2}\right), \quad (3.5)$$

$$P \sim \frac{1}{2} \left\{ \frac{1}{r}, p_r \right\} = \frac{\hbar}{i} \left(\frac{1}{2r^2} + \frac{2}{r} \frac{d}{dr} \right), \quad (3.6)$$

where the use of $(l + \frac{1}{2})^2$ vs $l(l+1)$ in (3.5) will be understood shortly. p_r is the quantum radial momentum operator

$$p_r = \frac{\hbar}{i} \left(\frac{1}{r} + \frac{d}{dr} \right) \quad (3.7)$$

and H is the radial quantum Hamiltonian

$$H = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} + \frac{1}{2} m\omega^2 r^2. \quad (3.8a)$$

The quantum analogs to the classical equations of motion (2.13) and (2.14) are

$$\dot{X} = \frac{1}{i\hbar} [X, H] = -\frac{1}{m} \left\{ \frac{1}{r^2}, P \right\}, \quad (3.8b)$$

$$\dot{P} = \frac{1}{i\hbar} [P, H] = \frac{\hbar^2}{m} \left\{ \frac{1}{r^2}, (l + \frac{1}{2})^2 X - \frac{1}{r^2} \right\}. \quad (3.8c)$$

The above natural quantum operators are in agreement with those obtained from the l raising and lowering operators. For the harmonic oscillator,

$$E_n = \hbar\omega(n + \frac{3}{2}), \quad (3.9)$$

$$R_{n1} = N_{n1} \phi_{n1}, \quad (3.10)$$

$$N_{n1} = \left[\frac{2\alpha^2 \Gamma(\frac{1}{2}n - \frac{1}{2}l + 1)}{\Gamma(\frac{1}{2}n + \frac{1}{2}l + \frac{3}{2})} \right]^{1/2}, \quad (3.11)$$

$$\phi_{n1} = \exp(-\frac{1}{2}\rho^2) \rho^l L_n^{(l+1/2)}(\rho^2), \quad (3.12)$$

$$\rho \equiv ar \equiv \left(\frac{m\omega}{\hbar} \right)^{1/2} r, \quad (3.13)$$

$$A_{\pm}^{\dagger} = \left[\frac{(l - \frac{1}{2} \pm \frac{1}{2})(l + \frac{5}{2} \pm \frac{1}{2})}{\rho^2} - \frac{(l + \frac{1}{2} \pm 1)}{\rho} \frac{d}{d\rho} - (n + \frac{3}{2}) \right], \quad (3.14)$$

$$A_{\pm}^{\dagger} R_{n1} = [(n + l + 2 \pm 1)(n - l + 1 \mp 1)]^{1/2} R_{n, l \pm 2}. \quad (3.15)$$

Observe that, as is necessary, l is changed by two units to go to the next allowed eigenstate. In terms of these operators the natural quantum operators are

$$X_n = \frac{1}{(2l+1)^2} \{ [A_{\pm}^{\dagger} + (A_{\pm}^{\dagger})^{\dagger}] + [A_{\pm}^{\dagger} + (A_{\pm}^{\dagger})^{\dagger}] \} \\ = \left[\frac{1}{\rho^2} - \frac{(n + \frac{3}{2})}{(l + \frac{1}{2})^2} \right], \quad (3.16)$$

or

$$X = \left[\frac{1}{\rho^2} - \frac{H}{\hbar\omega(l + \frac{1}{2})^2} \right] \quad (3.17)$$

and

$$P = \frac{1}{2(2l+1)^2} \{ [A_{\pm}^{\dagger} + (A_{\pm}^{\dagger})^{\dagger}] - [A_{\pm}^{\dagger} + (A_{\pm}^{\dagger})^{\dagger}] \} \\ = \frac{1}{i} \left(\frac{1}{2\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} \right) = \frac{1}{2} \left\{ \frac{1}{\rho}, p_{\rho} \right\}. \quad (3.18)$$

Equations (3.17) and (3.18) are the dimensionless forms of (3.5) and (3.6), with the zero-point contribution explicitly giving the change of $l(l+1)$ to $(l + \frac{1}{2})^2$ in (3.5) and (3.17).

B. Minimum-uncertainty coherent states

The commutator of X and P is

$$[X, P] = iG, \quad (3.19)$$

$$G = -\frac{1}{\rho^4} - \frac{i}{(l + \frac{1}{2})^2} \left(\frac{3}{4\rho^4} - \frac{1}{\rho^2} \frac{d^2}{d\rho^2} + 1 \right), \quad (3.20)$$

defining the uncertainty relation

$$(\Delta X)^2 (\Delta P)^2 \geq \frac{1}{4} \langle G \rangle^2. \quad (3.21)$$

The equality in the uncertainty relation is obtained when

$$(X + iBP)\psi = C\psi, \quad (3.22)$$

$$B = \frac{1}{2} \langle G \rangle / (\Delta P)^2, \quad (3.23)$$

$$C = \langle X \rangle + iB \langle P \rangle. \quad (3.24)$$

The "ground state" R_{11} satisfies (3.22) since

$$\langle X \rangle_{11} = -\frac{1}{(l + \frac{1}{2})^2}, \quad (3.25)$$

$$\langle X^2 \rangle_{11} = \frac{1}{(l + \frac{1}{2})(l - \frac{1}{2})} - \frac{2(l + \frac{3}{2})}{(l + \frac{1}{2})^2} + \frac{(l + \frac{3}{2})^2}{(l + \frac{1}{2})^4}, \quad (3.26)$$

$$(\Delta X)_{11}^2 = \frac{1}{(l + \frac{1}{2})^2 (l - \frac{1}{2})}, \quad (3.27)$$

$$\langle P \rangle_{11} = 0, \quad (3.28)$$

$$\langle P^2 \rangle_{11} = (\Delta P)^2 = \frac{1}{(l - \frac{1}{2})}, \quad (3.29)$$

$$\langle G \rangle_{11} = \frac{-2}{(l + \frac{1}{2})(l - \frac{1}{2})}. \quad (3.30)$$

This corresponds to a B of

$$B = -\frac{1}{(l + \frac{1}{2})}. \quad (3.31)$$

We take (3.31) to hold, leaving the two-parameter complex constant C to label the coherent states.

Putting all our results into Eq. (3.22) and changing variables to

$$y = \rho^2, \quad (3.32)$$

the defining equation for the MUCS is

$$0 = \left[2y \frac{d^2}{dy^2} - 2(l-1) \frac{d}{dy} - \frac{1}{2}y + \frac{l^2}{2y} - (l + \frac{1}{2})^2 C \right] \psi. \quad (3.33)$$

The large- y behavior is determined by the first and second terms of (3.33), and yields $\exp(\pm \frac{1}{2}y)$. Since the ground state goes as $y^{l/2} \exp(-\frac{1}{2}y)$, one would think that this would be a good trial function. However, the techniques used below which yield the final MUCS show that this trial function leads to unnormalizable solutions of (3.33), except for values of C of $[-(2k+1)/(l+1/2)^2]$, $k=0, 1, 2, \dots$. The normalizable solutions of (3.33) are found by the trial wave function

$$\psi = Ny^{l/2} \exp(+\frac{1}{2}y)g. \quad (3.34)$$

Inserting this in (3.33) yields

$$0 = yg'' + (1+y)g' + \frac{1}{2}[1 - (l + \frac{1}{2})^2 C]g. \quad (3.35)$$

The large- y behavior of (3.35) is $\exp(-y)$, meaning (3.34) will be normalizable. Using a power-series solution of the form

$$g = \sum_{j=0}^{\infty} a_j y^j \quad (3.36)$$

in (3.35) gives

$$\frac{a_{j+1}}{a_j} = -\frac{j + \frac{1}{2}[1 - (l + \frac{1}{2})^2 C]}{(j+1)^2}, \quad (3.37)$$

so that

$$g = {}_1F_1\left(\frac{1}{2}[1 - (l + \frac{1}{2})^2 C]; 1; -y\right) \quad (3.38a)$$

$$= \sum_{j=0}^{\infty} \frac{(\frac{1}{2}[1 - (l + \frac{1}{2})^2 C])_j}{(1)_j} \frac{(-y)^j}{j!}. \quad (3.38b)$$

For large y , g does vary as $\exp(-y)$, so ψ is normalizable. From (3.24), (3.25), and (3.27), C is $-1/(l + \frac{1}{2})^2$ for the ground state. Then g is exactly $\exp(-y)$, meaning ψ does indeed check out to be the ground state. Also, observe that the special values

$$C = \frac{2k+1}{(l + \frac{1}{2})^2}, \quad k=0, 1, 2, \dots \quad (3.39)$$

are excluded. For these C the power series in g terminates after $(k+1)$ terms so ψ cannot be normalized. However, all other complex values of C are allowed.

C. Other calculations

By taking

$$\alpha_{i,m}^{\pm} = A_i^{\pm} (n + l + 2 \pm 1)^{-1/2} \quad (3.40)$$

and making the transformation

$$n \rightarrow (H/h\omega - \frac{3}{2}) \equiv h - \frac{3}{2}, \quad (3.41)$$

one can define the n -independent l raising and lowering operators

$$\alpha_i^{\pm} = \left[\frac{(l - \frac{1}{4} \pm \frac{1}{4})(l + \frac{5}{4} \pm \frac{1}{4})}{\rho^2} - \frac{(l + \frac{1}{2} \pm 1)}{\rho} \frac{d}{d\rho} - h \right] [h + (l + \frac{1}{2}) \pm 1]^{-1/2} \quad (3.42)$$

with the properties

$$\alpha_i^{\pm} R_{nl} = (n - l + 1 \mp 1)^{1/2} R_{n, l \pm 2}. \quad (3.43)$$

In terms of these one has

$$\mathcal{H} R_{nl} = (n + \frac{3}{2}) R_{nl}, \quad (3.44)$$

$$\mathcal{H} = \frac{1}{2}(\alpha_i^{\dagger} \alpha_i + \alpha_i \alpha_i^{\dagger}) + (l + \frac{1}{2}). \quad (3.45)$$

These α_i could serve as the basis for a discussion of annihilation-operator or displacement-operator coherent states.

It is also possible to define simpler "approximate" minimum-uncertainty coherent states by substituting $\langle H \rangle = \bar{E}$ for H in the quantum operator X . Then one could drop the second term in X to have

$$\bar{X} = \frac{1}{\rho^2}, \quad (3.46)$$

$$\bar{P} = \frac{1}{2i} \left\{ \frac{1}{\rho}, \frac{d}{d\rho} + \frac{1}{\rho} \right\} = \frac{1}{i} \left(\frac{1}{2\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} \right), \quad (3.47)$$

$$[\bar{X}, \bar{P}] = i\bar{G} = -i \frac{2}{\rho^4}. \quad (3.48)$$

These relations lead to the approximate minimum-uncertainty coherent states

$$\psi = \left[\frac{2(u)^{l+3/2} a^3}{\Gamma(l + \frac{3}{2})} \right]^{1/2} \rho^l \exp(-\frac{1}{2}\bar{C}\rho^2), \quad (3.49)$$

$$\bar{C} \equiv u + iv = (l + \frac{1}{2}) \langle \bar{X} \rangle - i \langle \bar{P} \rangle. \quad (3.50)$$

For these states, $0 < u < \infty$. From Eq. (3.49), $u=1$ corresponds to the ground state R_{1l} . This agrees with (3.50), since

$$\langle \bar{X} \rangle_{1l} = \frac{1}{(l + \frac{1}{2})}. \quad (3.51)$$

Finally, one calculates \bar{E} as

$$\bar{E} = \langle H \rangle = \frac{1}{2} \hbar \omega (l + \frac{3}{2}) \left(u + \frac{1}{u} + \frac{v^2}{u} \right). \quad (3.52)$$

IV. HYDROGEN ATOM

A. Natural classical variables and quantum operators

For

$$V(r) = -\frac{e^2}{r}, \quad (4.1)$$

the natural classical variables are

$$X_c = \left(\frac{1}{r} - \frac{me^2}{L^2} \right) = \left(\frac{me^4}{L^4} + \frac{2me}{L^2} \right)^{1/2} \sin\theta, \quad (4.2)$$

$$P_c = p_{rc} = -LA \cos\theta. \quad (4.3)$$

This is the correct angular variation,

$$g(E, L) = 1, \quad (4.4)$$

since the Kepler-Coulomb particle undergoes one oscillation between apsidal distances for every angular rotation of 2π . Again the reader can verify that the above results satisfy the equations of Sec. II.

The natural quantum operators should thus be of the form

$$X = \left(\frac{1}{r} - \frac{1}{2r_0 l(l+1)} \right), \quad (4.5)$$

$$r_0 = \frac{\hbar^2}{2me^2}, \quad (4.6)$$

$$P = p_r = \frac{\hbar}{i} \left(\frac{1}{r} + \frac{d}{dr} \right). \quad (4.7)$$

Using the radial quantum Hamiltonian

$$H = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{e^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2}, \quad (4.8)$$

one can show that these operators obey the quantum analogs of the classical equations of motion (2.13) and (2.14),

$$\begin{aligned} \dot{X} &= \frac{1}{i\hbar} [X, H] \\ &= -\frac{1}{2m} \left\{ \frac{1}{r^2}, P \right\}, \end{aligned} \quad (4.9)$$

$$\begin{aligned} \dot{P} &= \frac{1}{i\hbar} [P, H] \\ &= \frac{\hbar^2 l(l+1)}{mr^2} X. \end{aligned} \quad (4.10)$$

The X and P of (4.5) and (4.6) are in agreement with those obtained from the l raising and lowering operators. For the hydrogen atom,¹²

$$\begin{aligned} E_n &= -\frac{e^2}{n^2} \equiv -\frac{e^2}{4r_0 n^2} \\ &= -\left(\frac{me^4}{2\hbar^2} \right) \frac{1}{n^2}, \quad n=1, 2, \dots \end{aligned} \quad (4.11)$$

$$R_{nl} = N_{nl} \phi_{nl}, \quad l=0, 1, \dots, n-1, \quad (4.12)$$

$$N_{nl} = \left[\frac{\Gamma(n-l)}{n^3 r_0^3 2n \Gamma(n+l+1)} \right]^{1/2}, \quad (4.13)$$

$$\phi_{nl} = \exp\left(-\frac{1}{2}\rho_n\right) \rho_n^l L_{n-l-1}^{(2l+1)}(\rho_n), \quad (4.14)$$

$$\rho_n \equiv \frac{\rho}{n} \equiv \frac{r}{r_0 n}, \quad (4.15)$$

$$A_l^\dagger = \left(\frac{l + \frac{1}{2} \mp \frac{1}{2}}{\rho_n} \mp \frac{d}{d\rho_n} - \frac{n}{2l+1 \pm 1} \right), \quad (4.16)$$

$$A_l^\dagger R_{nl} = \left\{ \frac{[n^2 - (l + \frac{1}{2} \pm \frac{1}{2})^2]^{1/2}}{2l+1 \pm 1} \right\} R_{n, l \pm 1}. \quad (4.17)$$

Thus, X and P can be given dimensionlessly as

$$X = \left[\frac{1}{\rho} - \frac{1}{2l(l+1)} \right] \quad (4.18a)$$

$$= \frac{2}{n(2l+1)} \{ [A_l^\dagger + (A_l^\dagger)^\dagger] + [A_l^\dagger + (A_l^\dagger)^\dagger] \}, \quad (4.18b)$$

$$P = \frac{1}{i} \left(\frac{1}{\rho} + \frac{d}{d\rho} \right) \equiv p_\rho \quad (4.19a)$$

$$= \frac{1}{ni} \{ [A_l^\dagger + (A_l^\dagger)^\dagger] - [A_l^\dagger + (A_l^\dagger)^\dagger] \}, \quad (4.19b)$$

where from now on we will be discussing things in terms of the dimensionless variable $\rho = r/r_0$ of (4.15).

B. Minimum-uncertainty coherent states

The commutator of X and P is

$$[X, P] = -\frac{i}{\rho^2}, \quad (4.20)$$

defining the uncertainty relation

$$\begin{aligned} (\Delta X)^2 (\Delta P)^2 &= \left[\Delta \left(\frac{1}{\rho} \right) \right]^2 (\Delta p_\rho)^2 \\ &\geq \frac{1}{4} \left\langle \frac{1}{\rho^2} \right\rangle. \end{aligned} \quad (4.21)$$

Taking, for convenience, a different convention for the minimum-uncertainty states defining equation, the equality in the uncertainty relation is obtained when

$$\left[\frac{1}{i} \left(\frac{1}{\rho} + \frac{d}{d\rho} \right) + iB \left(\frac{1}{\rho} \right) \right] \psi = \left\langle p_\rho \right\rangle + iB \left\langle \frac{1}{\rho} \right\rangle \psi, \quad (4.22)$$

$$B = \frac{\langle 1/\rho^2 \rangle}{2[\Delta(1/\rho)]^2}. \quad (4.23)$$

The "ground state" $R_{l+1, l}$ satisfies (4.22) with

$$B = (l+1). \quad (4.24)$$

Putting (4.24) into (4.22), solving the differential equation, and normalizing, one obtains

$$\psi = r_0^{3/2} (2u)^{l+3/2} [\Gamma(2l+3)]^{-1/2} \rho^l \exp(-C\rho), \quad (4.25)$$

$$C = (l+1) \langle 1/\rho \rangle - i \langle P \rangle \quad (4.26a)$$

$$\equiv u + iv. \quad (4.26b)$$

The ground state has $C = [2(l+1)]^{-1}$ or $\langle 1/\rho \rangle = [2(l+1)^2]^{-1}$. In general,

$$\left\langle \frac{1}{\rho} \right\rangle = \frac{u}{l+1}, \quad (4.27)$$

$$\left\langle \frac{1}{\rho^2} \right\rangle = \frac{u^2}{(l+1)(l+\frac{1}{2})}, \quad (4.28)$$

$$(\Delta X)^2 = \left(\Delta \frac{1}{\rho} \right)^2 = \frac{1}{2(l+1)^2} \frac{u^2}{(l+\frac{1}{2})}, \quad (4.29)$$

$$\langle P \rangle = -v, \quad (4.30)$$

$$\langle P^2 \rangle = v^2 + \frac{u^2}{2(l+\frac{1}{2})}, \quad (4.31)$$

satisfying the uncertainty relation (4.21). The energy of a coherent state is

$$\langle H \rangle = +4\mathcal{E}_0 \left(u^2 + v^2 - \frac{u}{l+1} \right), \quad (4.32)$$

which is a minimum as $v=0$ and $u=[2(l+1)]^{-1}$, i.e., the ground state $R_{l+1,1}$. We will discuss the time evolution of these states in the following paper V.

C. Other calculations

By taking

$$\alpha_{l,n}^{\pm} = A_l^{\pm} \left(\frac{2}{n} \right) \quad (4.33)$$

and making the transformation

$$n \rightarrow (-\mathcal{E}_0/H)^{1/2} \equiv (-h)^{-1/2}, \quad (4.34)$$

one can define n -independent l raising and lowering operators

$$\alpha_l^{\pm} = \left(\frac{2l+1 \mp 1}{\rho} \mp \frac{d}{d\rho} \right) (-h)^{1/2} - \left(\frac{1}{l+\frac{1}{2} \pm \frac{1}{2}} \right) \quad (4.35)$$

with the properties

$$\alpha_l^{\pm} R_{n,l} = \left[\frac{1}{(l+\frac{1}{2} \pm \frac{1}{2})^2} - \frac{1}{n^2} \right]^{1/2} R_{n,l \pm 1}. \quad (4.36)$$

In terms of these, one then has

$$\mathcal{K} R_{n,l} = -\frac{1}{n^2} R_{n,l}, \quad (4.37)$$

$$\mathcal{K} = \frac{1}{2} (\alpha_l^+ \alpha_l^+ + \alpha_l^- \alpha_l^-) - \left[\frac{1}{l^2} + \frac{1}{(l+1)^2} \right]. \quad (4.38)$$

These α_l^{\pm} could therefore serve as the basis for a discussion of generalized annihilation-operator or displacement-operator coherent states.

V. DISCUSSION

For the harmonic oscillator, the MUCS methods we have proposed allow a discussion of more than one set of coherent states. Taking the effective one-dimensional potential of Eq. (1.1), the natural variable X_c which varies as $\sin(\omega_c t)$ yields the coherent states which were obtained in Sec. II of

paper II. In Sec. II of this paper we obtained coherent states from the real radial part of the three-dimensional problem, the natural variable X_c varying as $\sin[2\theta(t)]$. A comparison of the analytic results obtained shows that for this potential the results for the effective one-dimensional HOCB formulation are simpler to handle.

Both these sets of states can be used with the angular coherent states discussed in Appendix A. Further, if one uses angular coherent states of the type where J is not a definite integer (see Appendix A), the value of " l " used in the radial problem need not be an integer, but can be considered some average $\langle J \rangle$. The radial problem only demands that $(n-l)/2$ be an integer for the harmonic oscillator [or $(n-l)$ be an integer for the hydrogen atom].

For the harmonic-oscillator problem alone one can also factorize the problem into (x, y, z) coordinates. Therefore, one can construct coherent states as product wave functions of ordinary coherent states $\psi(x)\psi(y)\psi(z)$ and then write them as sums of the ψ_{nlm} . This has been done by Mikhailov.¹³ All three of these sets of states are minimum-uncertainty coherent states, but since they are in terms of different natural classical variables, they minimize different uncertainty relations and are not identical.

The differences in the properties of the various MUCS can be easily visualized if one considers the two-dimensional case with the wave packet plotted in the z direction. An MUCS wave packet that minimizes the position-momentum uncertainty relations in the x and y directions can be thought of as the product of two Gaussian-shaped cylinders. One cylinder axis is oriented normal to the x axis and it always travels in the x direction. The other cylinder is oriented normal to the y axis and it always travels in the y direction. Each cylinder always has its original orientation and moves parallel to its original velocity. The point which is at the simultaneous maximum of the two cylinders follows the classical motion.

On the other hand, if one uses angular and radial variables, the coherent state is the product of two bell-shaped cylinders which *do* change orientation and shape in time. One always has its axis normal to the vector from the origin to the classical position (the radial wave packet), and one has its axis parallel to that vector (the angular wave packet). For this state the point which is at the simultaneous maximum of the two cylinders again follows the classical motion. However, in following the classical motion the two cylinders reorient themselves as described above.

In any event, since the harmonic oscillator is

an equally spaced level system, all the wave packets mentioned above will return to their original shapes after one classical oscillation. Therefore, the three sets of states serve as complements to each other in intuitively understanding the MUCS method.

Near Eq. (2.54) of paper II,² it was pointed out that for the equally spaced level system defined by the HOCB potential, any wave packet will return to its original shape after one classical oscillation. The arguments given there apply to any quantum system with equally spaced eigenvalues. For one-dimensional potential systems, there are systems whose classical oscillation frequencies are independent of energy. All such classical potentials can be obtained in principle.¹⁴ For further insight into this phenomenon, the reader can consult Ref. 15, where time-evolution studies of the HOCB system are given.

For the hydrogen-atom problem, on the other hand, there is a clear preference for using the three-dimensional radial formalism rather than the one-dimensional effective formalism. As noted in the Introduction, the effective one-dimensional formalism cannot be handled analytically. From the first part of our chain this is because the natural classical variables are mathematically so complicated, as evidenced by Eq. (1.8). From the other end of the chain, this is because the n raising and lowering operators cannot be handled analytically, whereas the l raising and lowering operators can. This last point also holds even if one tries to use group-theory methods. The states of Mostowski,⁹ using the Perelomov⁸ formulation, become exact only in the limit where one can ignore "one" with respect to n . In this limit one also gets the circular orbit results obtained by Brown¹⁶ on physical grounds.

In the following paper, numerical integration of the defining differential equation will be used to study the time evolution of our radial coherent states for the hydrogen atom.

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APPENDIX A: COHERENT STATES FOR ANGULAR COORDINATES

To discuss the complete coherent-states problem for angular coordinates in three dimensions, one must deal with a two-dimensional system to cover the θ - ϕ coordinates. Thus, one's states must be able to be written as combination of the Y_{Jm} for all J and m .

Among the first to do this were Atkins and Dobson.¹⁷ They combined the discussion of the harmonic-oscillator coherent states in Ref. 18 with Schwinger's two-boson formulation of the quantum theory of angular momentum.¹⁹ The formulation uses two pairs of boson creation and annihilation operators,

$$[a_u, a_v^\dagger] = \delta_{uv}, \quad (\text{A1})$$

$$[a_u, a_v] = [a_u^\dagger, a_v^\dagger] = 0, \quad (\text{A2})$$

$$(u \text{ or } v) = (+ \text{ or } -). \quad (\text{A3})$$

These operators can be identified with the angular momentum operators as

$$J_z = \frac{1}{2}(a_+^\dagger a_+ - a_-^\dagger a_-) \equiv \frac{1}{2}(n_+ - n_-), \quad (\text{A4})$$

$$J_\pm = J_x \pm iJ_y = a_\pm^\dagger a_\mp, \quad (\text{A5})$$

$$J^2 = \frac{1}{2}(n_+ + n_-)[\frac{1}{2}(n_+ + n_-) + 1]. \quad (\text{A6})$$

The $|J, m\rangle$ states are

$$|J, m\rangle = [(J+m)!(J-m)!]^{-1/2} \times (a_+^\dagger)^{J+m} (a_-^\dagger)^{J-m} |0, 0\rangle. \quad (\text{A7})$$

The simultaneous eigenstates of a_+ and a_- with eigenvalues α_+ and α_- are referred to as the *angular momentum coherent states*. They can be written in the form^{17,20}

$$|\alpha_+, \alpha_-\rangle = \exp[-\frac{1}{2}(|\alpha_+|^2 + |\alpha_-|^2)] \times \sum_{J=0}^{\infty} \sum_{m=-J}^J \frac{(\alpha_+)^{J+m} (\alpha_-)^{J-m}}{[(J+m)!(J-m)!]^{1/2}} |J, m\rangle. \quad (\text{A8})$$

Atkins and Dobson¹⁷ showed that these states are mathematically equivalent to the two-dimensional harmonic-oscillator coherent states studied in Ref. 21. Therefore, thinking of the bosons as defining (x, y) and (p_x, p_y) operators, these angular momentum coherent states can be thought of as minimum-uncertainty states for (x, p_x) and (y, p_y) operators. The above led them to the comment "... one would expect a coherent state of a three-dimensional harmonic oscillator to be equivalent to a product of an angular momentum coherent state and a coherent state connected with a radial excitation."¹⁷ Our position, that for spherically symmetric potentials one can consider coherent states to be a product of an angular part times a radial part, can be viewed as a generalization

of the earlier Atkins-Dobson comment. Finally, to within uncertainties, the angular momentum coherent states lead to a $\langle \vec{J} \rangle$ which is classical.

A similarly inspired¹⁹ set of angular momentum coherent states has been recently discussed by Bhaumik, Nag, and Dutta-Roy.²² They looked for the simultaneous eigenvectors of the operators $a_+ a_+$ and $a_- a_-$ with eigenvalues β and γ , where $a_+ a_+ |J, m\rangle \propto |J-1, m-1\rangle$ and $a_- a_- |J, m\rangle \propto |J-1, m\rangle$. This leads to the set of states

$$|\beta, \gamma\rangle = [\cosh(|\beta| + |\gamma|/|\beta|)]^{-1/2} \times \sum_{J=0}^{\infty} \sum_{m=-J}^J \frac{\beta^m \gamma^{J-m}}{[(J+m)!(J-m)!]^{1/2}} |J, m\rangle. \quad (\text{A9})$$

This set of states also leads to a $\langle \vec{J} \rangle$ which, within uncertainties, is classical. However, here the states are minimum-uncertainty states for the uncertainty relation defined by

$$[K_1, K_2] \equiv [\frac{1}{2}(a_+ a_- + a_+^\dagger a_-^\dagger), \frac{1}{2}i(a_+ a_- - a_+^\dagger a_-^\dagger)] \\ = -iK_3 \equiv -i[\frac{1}{2}(a_+^\dagger a_+ + a_-^\dagger a_- + 1)] \quad (\text{A10})$$

and nearly minimum-uncertainty states for the uncertainty relation defined by

$$[I_1, I_2] \equiv [\frac{1}{2}(a_+ a_+ + a_+^\dagger a_+^\dagger), \frac{1}{2}i(a_+ a_+ - a_+^\dagger a_+^\dagger)] \\ = -iI_3 \equiv -i(2a_+^\dagger a_+ + 1). \quad (\text{A11})$$

The above two sets of states^{17,22} are pertinent for us as they stand. They can be used to write the entire coherent states for spherically symmetric potentials in the form $\psi(r)\psi(\theta, \phi)$. Also, other states could be investigated by using some of the different ladder operators in the Schwinger two-boson formulation.^{23,24} Consult Ref. 22 for a description of these operators.

However, in addition to the above ideas, there has been even more work on sets of states with definite J . Although these are states in (θ, ϕ) , they are defined in terms of only one space of operators (J_+, J_-), which is what yields the definite J .

One line of research was started by Radcliffe's²⁵ "coherent spin states." These turned out to be Block states,²⁶ and were later independently discussed from another point of view as "atomic coherent states" by Arecchi, Courtens, Gilmore, and Thomas.^{27,28} These states can be defined as²⁵⁻³²

$$|J, \mu\rangle = N \exp(\mu J_-) |J, J\rangle \\ = \frac{1}{(1 + |\mu|^2)^J} \sum_{p=0}^{2J} \left[\frac{p!(2J-p)!}{(2J-p)!} \right]^{1/2} \frac{\mu^p}{p!} |J, J-p\rangle. \quad (\text{A12})$$

These states do have desirable classical prop-

erties and are obviously states of definite J . Further, they satisfy the uncertainty relation³²

$$\Delta(\vec{J} \cdot \vec{u}) \Delta(\vec{J} \cdot \vec{v}) \geq \frac{1}{2} |\langle \vec{J} \cdot \vec{w} \rangle|, \quad (\text{A13})$$

where $(\vec{u}, \vec{v}, \vec{w})$ form an arbitrary orthonormal basis.

A related set of states, called "intelligent spin states," were described by Aragone, Guerri, Salamó, and Tani.³³ They can be defined³³⁻³⁵ as the minimum-uncertainty states of the equally spaced level system

$$[J_x, J_y] = iJ_z, \quad (\text{A14})$$

$$(\Delta J_x)^2 (\Delta J_y)^2 \geq \frac{1}{4} \langle J_z \rangle^2. \quad (\text{A15})$$

Relationships among all the above states have been studied. For instance, it has been shown^{33,34,36,37} that some, but not all (or even most), of the coherent spin states of Radcliffe are intelligent spin states. The reverse statement is also true. Further, Takahashi and Shibata²⁰ have observed that by projecting out a particular J part of the Atkins-Dobson¹⁷ angular momentum coherent states, one obtains "atomic" or coherent spin states. The reader can verify this by comparing Eq. (A8) for a given J and no sum over J with Eq. (A10). Finally, Bhaumik, Nag, and Dutta-Roy,²² going in the opposite direction, have shown that their "angular momentum coherent states" can be given as an explicit infinite sum over all J of specific coherent spin states.

Before ending this appendix I wish to mention that all these states are related in some way to the methods proposed for generalized coherent states in Refs. 8, 38, and 39, which have often been applied to equally spaced eigenvalue systems. There are also many other pertinent articles, and I list a few in Refs. 40-43. Finally, an extensive review and discussion of these types of states from the boson representation and group theory points of view has recently appeared.⁴⁴

APPENDIX B: X_c FOR THE HACB POTENTIAL

For the hydrogen atom with centripetal barrier (HACB) potential of Fig. 1,

$$V(r) = -\frac{e^2}{r} + \frac{L^2}{2mr^2}, \quad (\text{B1})$$

the natural classical variable X_c can be found with the aid of Kepler's laws of planetary motion. The parameters in Fig. 2, defining the bound ($E = -|E|$) elliptical motion, are

$$1 = \frac{x^2}{a^2} + \frac{y^2}{b^2}, \quad (\text{B2})$$

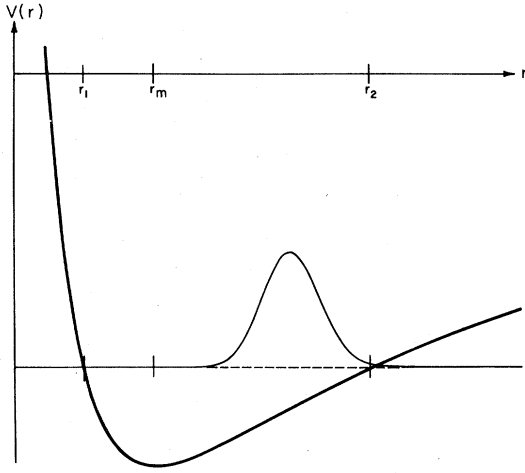


FIG. 1. The effective one-dimensional potential of Eq. (B1) for the hydrogen atom with centripetal barrier. The turning-point apsidal distances r_1 and r_2 are shown, along with $r_m = 2r_1$, the position where the potential is a minimum. As an example, a minimum-uncertainty coherent-state wave packet is also shown. It has an average energy $\frac{1}{4}$ of the distance up from $V(r_m)$ to the continuum. The given starting position is halfway in time between the turning points. Here $L^2 = \hbar^2 l(l+1)$, $l = 75$.

$$a = \frac{1}{2}(r_1 + r_2) \equiv e^2/2|E|, \quad (\text{B3})$$

$$b = (r_1 r_2)^{1/2}, \quad (\text{B4})$$

$$c = \frac{1}{2}(r_2 - r_1) \equiv a\epsilon, \quad (\text{B5})$$

$$a^2 = c^2 + b^2, \quad (\text{B6})$$

$$r_{1,2} = \frac{e^2}{2|E|} \left[1 \mp \left(1 - \frac{2|E|L^2}{me^4} \right)^{1/2} \right] \equiv a(1 \mp \epsilon). \quad (\text{B7})$$

a , b , and c are the semimajor axis, the semiminor axis, and the distance from the origin to the foci. r_1 and r_2 are the perigee and apogee turning points. ϵ is the eccentricity.

Kepler's third law states that the square of the period is proportional to the cube of the semimajor axis a . When the constants are put in, one has

$$\omega_c = \frac{2\pi}{\tau} = \left(\frac{e^2}{m} \right)^{1/2} a^{-3/2} \quad (\text{B8a})$$

$$= \left(\frac{8|E|}{me^4} \right)^{1/2}. \quad (\text{B8b})$$

By Kepler's second law, the radius vector from the "Sun," located at $(-c, 0)$, to the position (x, y) of the "planet" sweeps out equal areas in equal times. Taking the starting position at $a\vec{i}$ and going counterclockwise in Fig. 1, the area swept out is

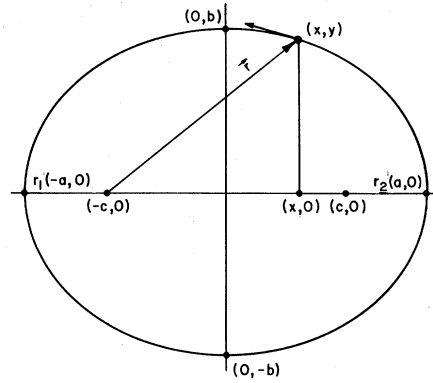


FIG. 2. The Kepler-Coulomb classical elliptical orbit, used to find the natural classical variable X_c for the effective one-dimensional HACB potential. (r_1 , r_2) are the apsidal distances. (a , b , c) are the semimajor axis, the semiminor axis, and the distance from the origin to the foci. \vec{r} shows the vector from the "Sun" at $(-c, 0)$ to the orbiting "planet" at (x, y) .

$$\begin{aligned} \alpha(t) &= \frac{1}{2}(c+x)y + \int_x^a \frac{b}{a}(a^2 - x^2)^{1/2} dx \\ &= \frac{1}{2} \frac{cb}{a} (a^2 - x^2)^{1/2} + \frac{ba\pi}{4} - \frac{ba}{2} \sin^{-1} \left(\frac{x}{a} \right). \end{aligned} \quad (\text{B9})$$

Since (πab) is the area of an entire ellipse,

$$\frac{\alpha(t)}{\pi ab} = \frac{\omega_c t}{2\pi}. \quad (\text{B10})$$

Further, using elementary trigonometry and algebra, x can be expressed in terms of r as

$$\frac{x}{a} = \frac{r-a}{c}. \quad (\text{B11})$$

Putting this into Eq. (B10), multiplying by 2π , and taking the sine of both sides, one has X_c as

$$X_c = \sin \omega_c t \quad (\text{B12})$$

$$\begin{aligned} &= \sin \left\{ \frac{\pi}{2} - \frac{2E}{e^2} \left(\frac{L^2}{2mE} - \frac{e^2 r}{E} - r^2 \right)^{1/2} \right. \\ &\quad \left. + \sin^{-1} \left[\frac{e^2 + 2Er}{(e^4 + 2EL^2/m)^{1/2}} \right] \right\} \\ &\equiv \sin\{\eta(r)\}. \end{aligned} \quad (\text{B13})$$

Using either (B12) or (B13) and (B9) for ω_c , it is straightforward to verify that X_c satisfies the defining one-dimensional equation for X_c ,

$$X_c' = \omega_c \left[\frac{m}{2} \frac{(A^2 - X_c^2)^{1/2}}{(E - V)} \right]^{1/2}. \quad (\text{B14})$$

Here a prime denotes the derivative with respect to r and $A(E) = 1$.

However, the above Eq. (B13) holds only for $2n\pi \leq \omega_c t \leq (2n+1)\pi$. Basically the reason is that the square-root function of r in (B13) is proportional to $|y|$ instead of y . But by the symmetry of the problem, one can make the formula valid for $(2n+1)\pi \leq \omega_c t \leq 2(n+1)\pi$ by writing

$$\begin{aligned} \sin \omega_c t &= \sin[2\pi - \eta(r)], \\ (2n+1)\pi &\leq \omega_c t \leq 2(n+1)\pi. \end{aligned} \quad (\text{B15})$$

Then using trigonometry one obtains

$$\begin{aligned}
 X_c &= \sin \omega_c t \\
 &= \pm \cos \left\{ -\frac{2E}{e^2} \left(\frac{L^2}{2mE} - \frac{e^2 r}{E} - r^2 \right)^{1/2} \right. \\
 &\quad \left. + \sin^{-1} \left[\frac{e^2 + 2Er}{(e^4 + 2EL^2/m)^{1/2}} \right] \right\} \\
 &= \pm \cos \left\{ \left[(\epsilon^2 - 1) + 2 \left(\frac{r}{a} \right) - \left(\frac{r}{a} \right)^2 \right]^{1/2} \right. \\
 &\quad \left. + \sin^{-1} \left(\frac{1 - r/a}{\epsilon} \right) \right\}, \quad (B16)
 \end{aligned}$$

$$\begin{pmatrix} + \text{sign} \\ - \text{sign} \end{pmatrix} \leftrightarrow \begin{cases} 2n\pi \leq \omega_c t \leq (2n+1)\pi \\ (2n+1)\pi \leq \omega_c t \leq 2(n+1)\pi \end{cases}. \quad (B17)$$

There still remains a double solution for $r(t)$, which is fixed by the initial value and demanding that the solution be a continuous function of time.

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