Quantum wave packets on Kepler elliptic orbits

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Wave-packet solutions of the Schrödinger equation for the Coulomb potential are obtained that travel along classical elliptic orbits of fixed mean eccentricity and angular momentum. These wave packets are coherent states that have minimal quantum fluctuations in the noncommuting components of the Lenz vector in the plane of the orbit. For large quantum numbers the asymptotic form of the wave packet and the classical equations of the orbit are obtained analytically.

A fundamental problem in physics is to understand the transition from quantum to classical mechanics. Since Schrödinger's pioneering work,[1] it has been known that coherent states are optimal quantum-mechanical states to describe the classical limit. While there has been widespread application of these states to many physical systems,[2] it is surprising that for the Coulomb potential the evaluation of coherent states traveling along Keplerian elliptic orbits, which was first attempted by Schrödinger, has not been successfully carried out yet. Following the work of Brown[3] on circular wave packets, Mostowski[4] gave a formal solution for elliptic coherent states by applying the general theory of coherent states developed by Barut[5] and Perelomov.[6] However, the *superposition of energy eigenstates* given by this theory[4-6] does not lead to a classical limit for the Coulomb case. Moreover, some incorrect conclusions have been reached regarding the long-time behavior[3,4,7] of superpositions of energy eigenstates, which will be discussed in this paper. Another construction, based on the mapping of the Coulomb Hamiltonian to a four-dimensional harmonic-oscillator Hamiltonian,[8] gives wave packets[7] which spread out asymptotically into a circular ring.

Recently, interest in this problem has been revived due to the experimental study of Rydberg atoms in external fields.[9,10] Such studies also provide an arena to explore the manifestations of classical chaos in quantum mechanics.[11] In particular, Gay and his collaborators[12,13] have evaluated numerically the coherent energy eigenstates first discussed by Mostowski, and proposed experimental methods to create these states in Rydberg atoms in crossed electric and magnetic field. An angularly localized wave packet in atomic sodium has been excited by a pulsed laser, and observed experimentally to exhibit classical behavior.[14]

In this paper we construct and evaluate the most general time-dependent localized wave packets which travel along a Kepler elliptical orbit *for all times*. The physical principle which leads to these coherent wave packets is the requirement that the two noncommuting components of the Lenz vector in the plane of the orbit have minimal quantum fluctuations *independent of time*. This leads directly to an analytic solution for the coefficients of the expansion of coherent energy eigenstates in terms of the conventional angular momentum eigenstates of the Coulomb Hamiltonian. For large quantum numbers we obtain a Gaussian linear superposition of these eigenstates with mean angular momentum corresponding to the classical value, and dispersion proportional to the eccentricity and to the square root of the principal quantum number of the state. For simplicity we confine our discussion to the Coulomb problem in two dimensions which contains the essential physical ideas, and then give the extension to the three-dimensional case.

In classical physics it is well known that the eccentricity and direction of the major axis of the elliptical Kepler orbit is determined by the magnitude and direction of the Lenz vector **M**. In quantum mechanics, the corresponding symmetrized Hermitian operator, which commutes with the Coulomb Hamiltonian, was introduced by Pauli[15] as $\mathbf{M}=\frac{1}{2}(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})-\mathbf{r}/r$ (in units where $e^2=m=\hbar=1$), where $\mathbf{p}$ is momentum, $\mathbf{L}$ is the angular momentum, and $\mathbf{r}$ is the coordinate of the electron. In two dimensions the commutation relations for the two components of M_x,M_y of the Lenz vector and L_z, which are the generators of the O(3) symmetry group of the Coulomb Hamiltonian H for bound states ($E<0$), are

$$[M_x,M_y]=-2iHL_z,\ \ [L_z,M_x]=iM_y,\ \ [L_z,M_y]=-iM_x\ , \tag{1}$$

where $H=p^2/2-1/r$. For $d=3$, the corresponding symmetry group of H is O(4),[15,16] but the same O(3) subgroup is the relevant group for this problem.

In order to obtain appropriate quantum states with a given mean value of the eccentricity, the direction of the major axis, and the angular momentum which corresponds asymptotically to the classical case, we will show that it is sufficient to find states which minimize the product of the quantum fluctuations ΔM_x and ΔM_y of the Lenz vector. The commutation relations, Eq. (1), lead to the uncertainty relation

$$\Delta M_x \Delta M_y \geq \frac{1}{2}\left|\langle -2HL_z\rangle\right|\ , \tag{2}$$

where $\langle\,\rangle$ indicates the mean value in a given state. The required quantum states are the solutions of H pertaining to the equality sign in Eq. (2). These states are determined by the eigenfunction equation

$$(M_x+i\delta M_y)\psi=\eta\psi\ , \tag{3}$$

where δ is a real parameter which will be related to the eccentricity e, and η is an eigenvalue of the non-Hermitian operator $M_x + i\delta M_y$. The state ψ is also an eigenstate of the Coulomb Hamiltonian H with energy E_n.

It can be readily shown for the solutions of Eq. (3) that

$$(\Delta M_x)^2 = -E_n \delta \langle L_z \rangle,\ (\Delta M_y)^2 = -\frac{E_n}{\delta} \langle L_z \rangle . \qquad (4)$$

Further properties of this eigenvalue equation can be obtained by introducing the ladder operators

$$A_{\pm} = \pm \frac{1}{(-2H)^{1/2}} (\delta M_x + i M_y) - (1-\delta^2)^{1/2} L_z , \qquad (5)$$

for $0 \leq \delta^2 \leq 1$. These operators give the additional solutions $A_{\pm}^m \psi$ of Eq. (3) with eigenvalues $\eta \pm m[-2E_n \times (1-\delta^2)]^{1/2}$, where m is an integer. We find that the eigenvalue η is real and corresponds to the mean value of the eccentricity e of the elliptic orbit

$$e = \langle M_x \rangle = m[-2E_n(1-\delta^2)]^{1/2},\ \langle M_y \rangle = 0 . \qquad (6)$$

Here $m = l_n, l_n - 1, \ldots, -l_n$, where l_n is an integer that is related to the energy eigenvalue $E_n = -1/2n^2$, and $n = l_n + \frac{1}{2}$ for $d = 2$, while $n = l_n + 1$ for $d = 3$. Of particular interest to our discussion is the eigenstate ψ_n^δ of maximal eigenvalue $m = l_n$. This eigenstate satisfies the additional condition [17]

$$A_+ \psi_n^\delta = 0 , \qquad (7)$$

and we label these solutions by the continuous parameter δ and the principal quantum number n. In this case it can be readily shown that $\langle L_z \rangle = \delta l_n$. It will be shown that this corresponds to the classical value of the angular momentum for a given eccentricity e and energy E_n. Together with Eq. (4), this result implies that the quantum fluctuations ΔM_x and ΔM_y are proportional to $1/(l_n)^{1/2}$. For large quantum numbers l_n, it follows from Eq. (6) that the eccentricity e for this coherent state depends only on δ and is independent of l_n. Hence *a general linear superposition of these states* for large quantum number also satisfies Eq. (3), and therefore has minimal quantum fluctuations in M_x and M_y. Furthermore, in this limit we obtain for this state from Eq. (6) the classical relation for the eccentricity,

$$e = (1-\delta^2)^{1/2} = (1 - 2E_n \langle L_z \rangle^2)^{1/2} . \qquad (8)$$

We can readily solve Eqs. (3) and (7) by expanding $\psi_n^\delta(\mathbf{r})$ in the conventional eigenfunctions $\psi_{n,l}(\mathbf{r})$ of the Coulomb Hamiltonian H and the angular momentum L_z for $d = 2$ (and L^2 with maximum eigenvalue of L_z for $d = 3$)

$$\psi_n^\delta(\mathbf{r}) = \sum_{l=-l_n}^{l_n} c_{n,l}^\delta \psi_{n,l}(\mathbf{r}) , \qquad (9)$$

and obtain for the coefficients $c_{n,l}^\delta$,

$$c_{n,l}^\delta = \frac{1}{2^{l_n}} \left[\frac{(2l_n)!}{(l_n+l)!(l_n-l)!} \right]^{1/2} (1-\delta^2)^{l_n/2} \left[\frac{1+\delta}{1-\delta} \right]^{l/2} . \qquad (10)$$

For large l_n, these coefficients are approximated very well

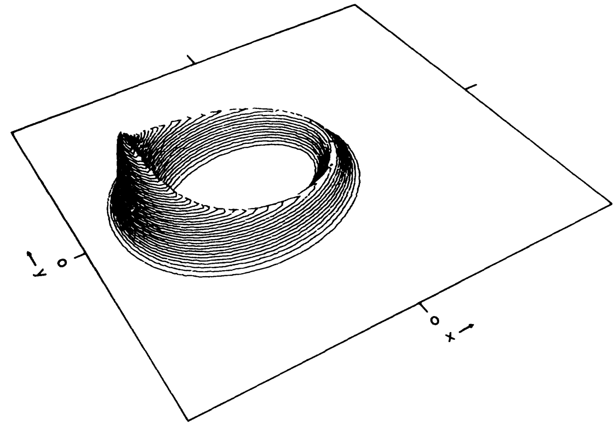

FIG. 1. The probability distribution for a coherent energy eigenstate, Eq. (9), with principal quantum number $l_n = 40$ and $\delta = 0.8$, which correspond to eccentricity $e = 0.6$ and mean angular momentum $\langle L_z \rangle = 32$.

by a Gaussian distribution in l:

$$c_{n,l}^\delta \cong \left[\frac{\pi}{2} l_n (1-\delta^2) \right]^{1/4} \exp[-(1-\delta l_n)^2 / l_n (1-\delta^2)] .$$

Similar expressions are obtained by expanding in the eigenstates of the components M_x or M_y of the Lenz vector. Asymptotically the coefficients are approximated by a Gaussian distribution in the corresponding eigenvalues, with a dispersion and mean value given by Eqs. (4) and (6), respectively. This coherent energy eigenstate[4,13,18] has a spatial probability distribution strongly peaked along the Kepler orbit with the corresponding eccentricity e and major axis; see Fig. 1.

To obtain a localized wave packet we must take a superposition of these coherent energy eigenstates,

$$\psi^\delta(\mathbf{r},t) = \sum_n a_n \psi_n^\delta(\mathbf{r}) \exp(-iE_n t) . \qquad (11)$$

The general results are reasonably independent of details of the coefficients a_n assuming that the distribution is sharply peaked about some principal quantum number. We have carried out calculations with a Gaussian superposition,

$$a_n = (2\pi\sigma^2)^{-1/4} \exp[-(l_n - l_0)^2 / 4\sigma^2] ,$$

and we have numerically evaluated the time dependence of such wave packets in two and three space dimensions, and recorded the results on video tape. In Figs. 2 and 3 we show contours of $|\psi^\delta(\mathbf{r},t)|^2$ in two dimensions at various times along an elliptic orbit with eccentricity $e = 0.6$ and angular momentum $\langle L_z \rangle = 32$ obtained by setting $\delta = 0.8$, $l_0 = 40$, and $\sigma^2 = 3.0$. Very similar results were obtained for a wave packet in three dimensions for the same parameters when observed in the plane of the classical orbit, but there is an additional time-independent Gaussian spread of the wave packet along the polar angle. The wave packet turns around the orbit with the Kepler period $\tau = 2\pi l_0^3$. It has been launched at perihelion [Fig. 2(a)] and it slows down, contracts, and becomes steeper as

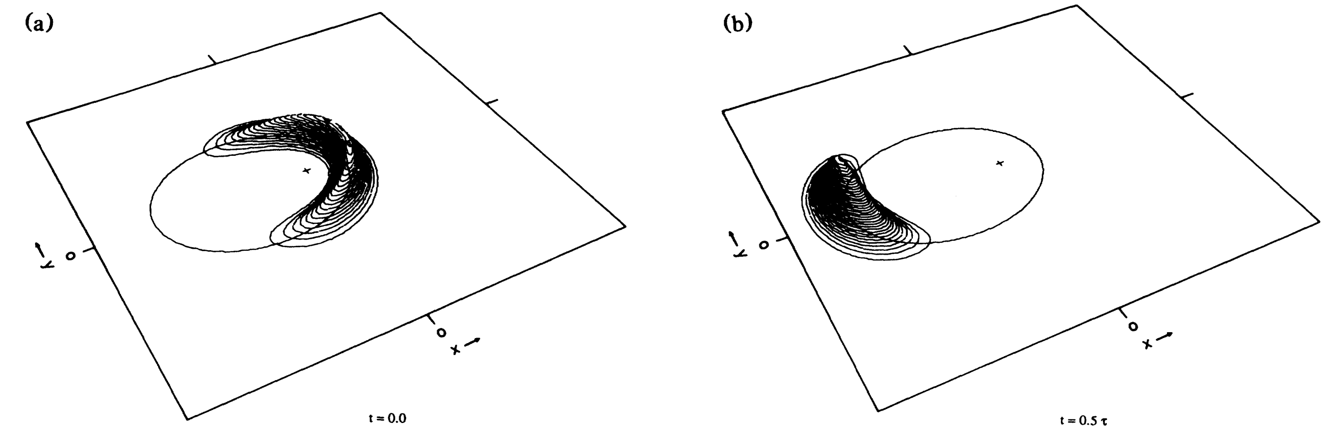

FIG. 2. (a),(b) A wave packet with eccentricity $e=0.6$ and mean angular momentum $\langle L_z\rangle = 32$ at $t=0$ and $t=0.5\tau$, where τ is the Kepler period of this orbit. For reference, the classical elliptic orbit for this eccentricity and angular momentum is drawn on the plane.

it reaches aphelion [Fig. 2(b)]. This is the expected behavior from classical mechanics. As the wave packet returns to perihelion it speeds up and spreads faster. The overall spreading of the wave packet is of classical origin, due to the initial uncertainty in position and momentum demanded by Heisenberg's principle. However, important quantum-mechanical interference effects occur when the head of the wave packet catches up with its tail. This interference leads to a nonuniform varying amplitude of the wave packet along the ellipse (Fig. 3). This phenomenon has been overlooked in the past,[3,4,8] but it is important in showing how quantum effects occur at long times in a semiclassical regime. In fact, these interference effects mark a breakdown of the semiclassical approximation at long times, and should be important in experiments in atomic physics in the semiclassical domain.

In the asymptotic regime of large principal quantum numbers $n_0 \cong l_0$, the summation over angular momentum states in Eq. (9) and energy eigenstates in Eq. (10) can be carried out analytically, using the Wentzel-Kramers-Brillouin approximation for the radial wave functions of the hydrogen atom. We obtain for $d=3$,

$$\begin{aligned}\psi^{\delta}(r,\theta,\phi,t) \cong & \left[\frac{2\omega_0}{\pi p_0(r)}\right]^{1/2} \exp[iS_0(r)] \left[\frac{\delta l_0}{\pi}\right]^{1/4} \exp\left[-\left(\theta-\frac{\pi}{2}\right)^2 \frac{\delta l_0}{2}\right] \\ & \times \sum_{\mu=-\infty}^{\infty} \exp\left[i\delta l_0(\phi+2\pi\mu) - [\phi+2\pi\mu-\phi_0(r)]^2 \frac{l_0}{2}(1-\delta^2)\right] \\ & \times \frac{1}{[2\pi\alpha_0(r,t)]^{1/2}} \exp\left[-\left(\delta(\phi+2\pi\mu-\phi_0(r)) - \frac{1}{l_0^3}[t-t_0(r)]\right)^2 \Big/ 2\alpha_0(r,t)\right], \end{aligned} \tag{12}$$

where the classical action in radial coordinates is

$$S_0(r) = \int^r p_0(r')dr' ,$$

the mean radial momentum is

$$p_0(r) = \left(2E_{n_0} - \frac{l_0^2}{r^2} + \frac{2}{r}\right)^{1/2} ,$$

the classical relation for an ellipse corresponds to

$$\phi_0(r) = -\frac{\partial S_0}{\partial l_0} , \quad \text{or} \quad r = \frac{(l_0)^2}{(l+e\cos\phi)} ,$$

and the classical time dependence along the orbit with the Kepler period $\tau = 2\pi/\omega_0 = 2\pi l_0^3$ is given by

$$t_0(r) = \frac{\partial S_0}{\partial E_n} .$$

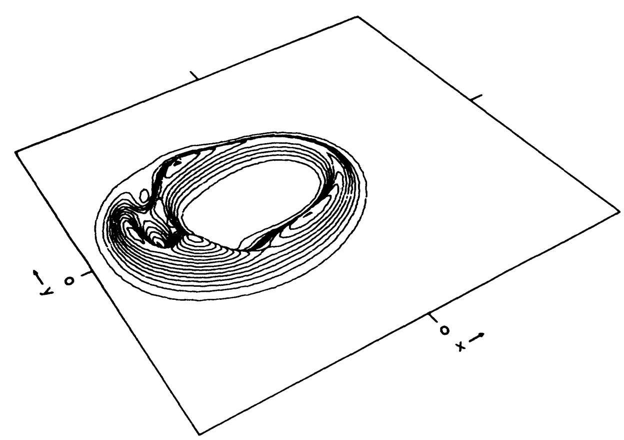

FIG. 3. The wave packet after completing two orbital periods.

The summation over integers μ in Eq. (12) comes from applying the Poisson summation formula to Eq. (9), as required by the periodicity of ψ_n^δ in the azimuthal angle ϕ. This sum accounts for the interference phenomena discussed previously when the wave packet has spread along the elliptical orbit. The rate of spreading is determined by the complex width

$$\alpha_0(r,t,\delta)=\frac{1}{2\sigma^2}-i\left[3\frac{t}{l_0^4}+2f_0(r)\right],$$

where

$$f_0(r)=\frac{\partial^2 S}{\partial E_n^2}.$$

In conclusion, it has been shown that for large quantum numbers, there exists coherent wave-packet solutions of the time-dependent Schrödinger equation which travel along Kepler elliptic orbits. Thus, it is expected that electrons in excited hydrogenlike atoms can exhibit all the classical phenomena associated with planetary motion for a limited number of revolutions. Afterwards, quantum interference phenomena set in which lead to important quantum corrections. However, the initial state will recur after a definite time. These results may also elucidate the successes as well as limitations of recent applications of classical physics to the study of manifestations of chaos in atomic physics.[11]

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