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Coherent states for the hydrogen atom

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We construct wave packets for the hydrogen atom labeled by the classical action-angle variables with the following properties. (i) The time evolution is exactly given by classical evolution of the angle variables. (The angle variable corresponding to the position on the orbit is now noncompact and we do not get exactly the same state after one period; however, the gross features do not change. In particular, the wave packet remains peaked around the labels.) (ii) The resolution of the identity using this overcomplete set involves exactly the classical phase-space measure. (iii) The semiclassical limit is related to Bohr-Sommerfeld quantization. (iv) They are almost minimum uncertainty wave packets in position and momentum. [S1050-2947(97)51111-5]

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I. INTRODUCTION

Schrödinger [1] attempted to construct wave packets for the hydrogen atom that were related to classical orbits. Such a construction was easy for the harmonic oscillator, and these are the well known coherent states [2,3]. The hydrogen atom, however, proved to be more difficult, and the question was not resolved at that time. The issue has become relevant again in connection with the Rydberg atoms [4] in microwave cavities. Various considerations have led to different proposals [5] for the coherent states of the hydrogen atom. Some used the dynamical groups SO(4) or SO(4,2). However, a state of the class did not go into a state of the same class under time evolution. Klauder [6] has constructed coherent states with the property that under time evolution these remain coherent states. Recently one of us [7] constructed a set of coherent states for the anharmonic oscillator that was unique when precise connection to the classical phase space and dynamics was demanded.

We construct wave packets for the hydrogen atom labeled by classical phase-space variables.

$$|R,\alpha,\beta,\gamma,\delta,\theta\rangle=\sum_{n=1}^{\infty}\sum_{j,m_1,m_2,l,m}\exp(-R/2\hbar)\frac{(R/\hbar)^{\frac{n-1}{2}}}{\sqrt{(n-1)!}}e^{-i\alpha m_1}e^{-i\gamma m_2}\exp\left(i\,\frac{R^3\theta}{2n^2h^3}\right)$$
$$\times\frac{(2j)!}{\sqrt{(j+m_1)!(j-m_1)!(j+m_2)!(j-m_1)!}}\left(\sin\frac{\beta}{2}\right)^{j-m_1}\left(\cos\frac{\beta}{2}\right)^{j+m_1}\left(\sin\frac{\delta}{2}\right)^{j-m_2}\left(\cos\frac{\delta}{2}\right)^{j+m_2}C^{lm}_{jm_1jm_2}|n,l,m\rangle. \quad (1)$$

The definition of these variables and their relation to the classical orbit are explained later. The angle variable θ now has the range $(-\infty,\infty)$. Note that only the bound-state spectrum has been used. Wave packets built out of scattering states with similar properties can also be constructed using our techniques, but they will not be considered here. We have the resolution of the identity in the subspace of the Hilbert space spanned by the bound states,

$$\mathbf{1}_{\rm BS}=\frac{1}{h^3}\int_0^{\infty}dR\left[\int\right]d\theta\int_{-1}^{1}d[(j+1/2)\hbar\ \cos\beta] \quad (2)$$
$$\times\int_0^{2\pi}d\alpha\int_{-1}^{1}d[(j+1/2)\hbar\ \cos\delta]$$
$$\times\int_0^{2\pi}d\gamma|R,\alpha,\beta,\gamma,\delta,\theta\rangle\langle R,\alpha,\beta,\gamma,\delta,\theta|,$$

where

$$\left[\int\right]d\theta\equiv\lim_{N\to\infty}\frac{1}{N}\int_{-N\pi}^{N\pi}d\theta. \quad (3)$$

This corresponds to an averaging over an infinite number of classical orbits. The measure is exactly the classical phase-space measure, which is invariant under canonical transformations. Under time evolution,

$$|R,\alpha,\beta,\gamma,\delta,\theta\rangle\xrightarrow{t}|R,\alpha,\beta,\gamma,\delta,\theta+\omega(R)t\rangle. \quad (4)$$

The wave packets peak around the point in the classical phase space represented by the labels. The expectation values of position and momenta do not exactly correspond to the labels, and the wave packets are not of minimal uncertainty, in contrast to the harmonic-oscillator coherent states. But these features of the latter are present in the semiclassical limit.

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II. CORRESPONDENCE TO THE KEPLER PROBLEM

The bound-state Kepler problem is conveniently described [8] by three action variables M,L,R and their corresponding angle variables $\omega_1,\omega_2,\omega_3$. (These are related to the variables in Ref [8] through $J_3=R$, $J_2=2\pi L$, $J_3=2\pi M$, $\omega_i=2\pi w_i$, $i=1,2,3$.) The Hamiltonian $\mathcal{H}$ involves only R:

$$\mathcal{H}=-\frac{2\pi^2 me^4}{R^2}. \tag{5}$$

L is the magnitude of the total angular momentum, and M is the z component of the angular momentum. The angle variables ω_1 and ω_2 are also constants of motion in this problem because their corresponding frequencies are zero. Only ω_3 changes in time as

$$\omega_3(t)=\frac{2\pi}{T(R)}t \quad \text{with} \quad \frac{1}{T(R)}=\frac{4\pi^2 me^4}{R^3}, \tag{6}$$

where $T(R)$ is the time period of the orbit.

It has been observed in [6,7] that the time evolution in Eq. (4) is possible only if the angle variable ω_3 is extended to the covering space; $\omega_3\in(-\infty,\infty)$. This is because the energy levels are incommensurate. After one period the wave packet is not reproduced, though grossly it has the same features. This uniquely fixes the dependence on ω_3:

$$|R,L,M,\omega_1,\omega_2,\omega_3\rangle=\sum_{nlm} C_{nlm}(R,L,M,\omega_1,\omega_2,)\times\exp\left(-i\frac{E_nT(R)\omega_3}{2\pi\hbar}\right)|nlm\rangle. \tag{7}$$

Under rotation we require these wave packets to go into one another as these labels do:

$$|R,L,M,\omega_1,\omega_2,\omega_3\rangle\overset{\mathcal{R}}{\to}|R,L,M(\mathcal{R}),\omega_1(\mathcal{R}),\omega_2(\mathcal{R}),\omega_3\rangle \tag{8}$$

(R,L and ω_3 do not change under rotation of axes).

ω_1 is the angle between the y axis and the line of nodes (i.e., the line of intersection between the orbital plane and the x-y plane). ω_2 is the angle between the line of nodes and the major axis (Fig. 1). Also $M/L=\cos\omega_4$, where ω_4 is the inclination of the orbit. (i.e., the angle between the normal **n** to the orbit and the z axis). Thus under rotation of the orbit around the z axis (by angle ψ_1), ω_1 increases by ψ_1, while ω_2 and ω_4 do not change. This uniquely requires the dependence on ω_1 to involve $\exp(-i\omega_1\hat{J}_z)$, where $\hat{J}_z$ is the generator of rotations about the z axis. A rotation about the line of nodes by an angle ψ_4 increases ω_4 by ψ_4 while keeping ω_1 and ω_2 unchanged. This fixes the dependence on ω_4 and ω_1 so that it involves $\exp(-i\omega_1\hat{J}_z)\exp(-i\,\omega_4\hat{J}_y)$. This is because the rotation about the line of nodes corresponds to $\exp(-i\omega_1\hat{J}_z)\exp(-i\psi_4\hat{J}_y)\exp(\omega_1\hat{J}_z)$. Finally a rotation about the normal **n** by the angle ψ_4 increases ω_2 by ψ_4 while keeping the other two angles constant. This rotation corresponds to

$$\exp(-i\omega_1\hat{J}_z)\exp(-i\omega_4\hat{J}_y)\exp\times(-i\psi_2\hat{J}_z)\exp(i\omega_4\hat{J}_y)\exp(i\omega_1\hat{J}_z).$$

Therefore the dependence on ω_4, ω_1, ω_2 is required to be

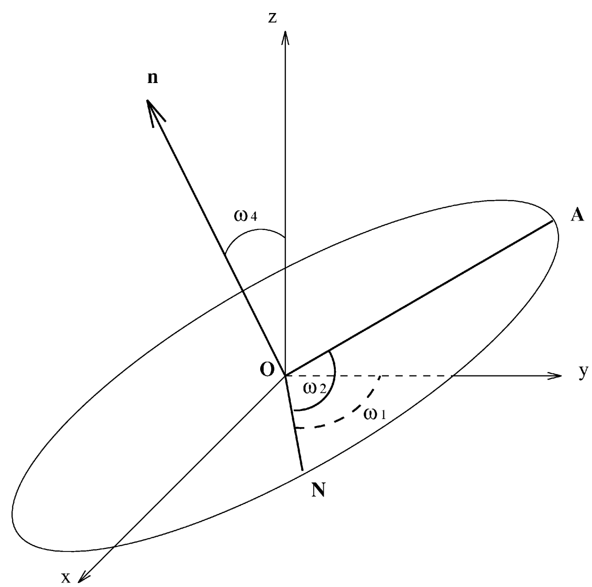

FIG. 1. The classical elliptic orbit. **ON**: line of nodes. **OA**: major axis.

$$\exp(-i\omega_1\hat{J}_z)\exp(-i\omega_4\hat{J}_y)\exp(-i\omega_2\hat{J}_z).$$

Note that this rotation precisely corresponds to taking an orbit in the x-y plane with the major axis along the x direction into the orbit labeled by $(R,L,M,\omega_1,\omega_2,\omega_3)$.

We may exploit the dynamical O(4) symmetry of the hydrogen atom to fix the dependence on L also. In addition to the conserved vector **J** related to rotational invariance, we have another conserved vector **K** along the major axis (Fig. 2) related to the Laplace-Runge-Lenz vector. We have $(\mathbf{J}+\mathbf{K})^2=(\mathbf{J}-\mathbf{K})^2=R^2$, $\mathbf{J}^2=L^2$, and the eccentricity of the orbit is $e=\sqrt{1-L^2/R^2}$. The role of the vector **K** is to deform the orbits by changing L. The O(4) symmetry corresponds to

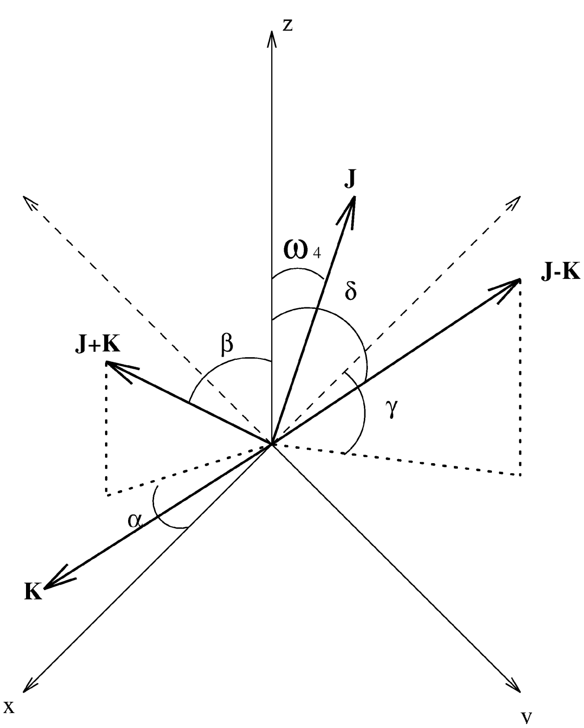

FIG. 2. The vectors **J** and **K** and the angles associated with them.

independent rotations of the vectors $(\mathbf{J}+\mathbf{K})/2$ and $(\mathbf{J}-\mathbf{K})/2$ in the three-dimensional space.

Consider a circular orbit in the x-y plane. Now $\mathbf{K}=0$ and $\mathbf{J}\pm\mathbf{K}$ are in the z direction. Imagine a rotation of $(\mathbf{J}+\mathbf{K})/2$ about the 2 axis by an angle ω_5 and an equal and opposite rotation of $(\mathbf{J}-\mathbf{K})/2$. This will give a nonzero $\mathbf{K}$ of magnitude $R\sin\omega_5$ along the x direction and $\mathbf{J}$ of magnitude $R\cos\omega_5$ along the z direction. Thus the orbit has been deformed into an elliptic orbit in the x-y plane with $L/R=\cos\omega_5$.

The above analysis shows the following. In order to have the correct transformation properties of the classical variables $R,L,M,\omega_1,\omega_2,\omega_3$ under the full O(4) symmetry, the dependence on R,L,ω_1,ω_2 has to be via

$$e^{-i\omega_1 J_z}e^{-i\omega_4\hat{J}_y}e^{-i\omega_2\hat{J}_z}e^{-i\omega_5[(\hat{J}_y+\hat{K}_y)/2]}e^{i\omega_5[(\hat{J}_y-\hat{K}_y)/2]},$$

where $\cos\omega_5=L/R$ and $\cos\omega_4=M/L$. Classically this will rotate and deform a circular orbit in the x-y plane into the orbit with the labels $(R,L,M,\omega_1,\omega_2,\omega_3)$ (without changing the size of the major axis). Quantum mechanically the former corresponds to the state $|n,n-1,n-1\rangle$. Therefore we may expect the coherent state to have the form

$$|R,L,M,\omega_1,\omega_2,\omega_3\rangle = \sum_n C_n(R)e^{-i\omega_1\hat{J}_z}e^{-i\omega_4\hat{J}_y}e^{-i\omega_2\hat{J}_z} \times e^{-i\omega_5(\hat{K}_y/2)}e^{i(\omega_3 R^3/2n^2h^3)}|n,n-1,n-1\rangle. \tag{9}$$

With a proper choice of $C_n(R)$ this will have the properties we require. However, we find that it is much more natural and convenient to use a different set of action angle variables. Note the close relation to the angular-momentum coherent states. Note also that the angle variables ω_1,ω_2 are involved in rotation about the third axis, whereas the angles ω_4 and ω_5 related to the action variables are involved in rotation about the 1 and 2 axes. This is a general feature, as seen below.

III. COHERENT STATES FOR A PRECESSING SPIN

Consider a spinning object with spin quantum number j and gyromagnetic ratio μ in an external magnetic field B in the z direction. The Hamiltonian is $\hat{\mathcal{H}}=\mu B\hat{J}_z$. Classically the spin will precess about the z axis with frequency μB. The action variable is J_z, which measures the inclination to the z axis and the angle variable $\theta\in(0,2\pi)$ is the azimuthal angle of the precessing spin. We now show that, by requiring the classical time evolution, semi-classical limit, and correct rotation property for the states $|J_z,\theta\rangle$ labeled by the classical phase space of this system, we obtain uniquely the angular-momentum coherent states [9] . We have

$$|J_z,\theta\rangle=\sum_m C_m(J_z)\exp\left(\frac{-i}{\hbar}\mu Bm\hbar\frac{\theta}{\mu B}\right)|j,m\rangle \tag{10}$$

to reproduce the classical evolution, $|J_z,\theta\rangle\overset{t}{\rightarrow}|J_z,\theta+\mu Bt\rangle$. Under rotation by the angle ψ about the x axis, ω goes to $\omega+\psi$, where $\cos\omega=J_z/J$ and J is the classical spin to be associated with the spin quantum number j. In order that $|J_z,\theta\rangle$ have this property, we have to choose

$$|J_z,\theta\rangle=e^{-i\theta\hat{J}_z}e^{-i\omega\hat{J}_y}|jj\rangle. \tag{11}$$

This is precisely the rotation that takes the z axis to the instantaneous axis of the classical spin. The correct semiclassical limit requires the choice $|jj\rangle$ as seen below. Note that we have precisely got the angular-momentum coherent state labeled by ω and θ. We now show that this has the right semiclassical limit and resolution of identity

$$|J_z,\theta\rangle=\sum_m d^j_{jm}(\omega)e^{-im\theta}|jm\rangle, \tag{12}$$

where

$$d^j_{jm}(\omega)=\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\left(\sin\frac{\omega}{2}\right)^{j-m}\left(\cos\frac{\omega}{2}\right)^{j+m}. \tag{13}$$

For large j, $d^j_{jm}(\omega)$ peaks at $\cos\omega=m/j$ i.e., the dominant contributions come from the states $m\hbar\approx J_z$.

As J_z and θ are action angle variables, the phase-space measure is $dJ_z d\theta$. Now

$$\frac{1}{h}\int_{-J}^{J}dJ_z\int_0^{2\pi}d\theta|J_z,\theta\rangle\langle J_z,\theta|$$

$$=\sum_m\frac{J}{\hbar}\int_{-1}^{1}d(\cos\omega)d^j_{jm}(\omega)d^j_{jm}(\omega)|jm\rangle\langle jm| \tag{14}$$

$$=\frac{J}{\hbar}\frac{2}{2j+1}|jm\rangle\langle jm| \tag{15}$$

$$=\mathbf{1}, \tag{16}$$

with the identification $J=(j+1/2)\hbar$. [This means that we must associate the classical $J=(j+1/2)\hbar$ to the spin quantum number j.] Thus the angles ω and θ appearing in the angular-momentum-coherent-state Eq. (12) can be interpreted as classical phase-space variables for a precessing spin with θ as the angle variable and $(j+1/2)\cos\omega$ as the corresponding action variable.

IV. COHERENT STATES FOR THE HYDROGEN ATOM

In place of the conserved variables L,M,ω_1,ω_2 we will use other variables suggested by the O(4) symmetry. We will use the two O(3) subgroups in O(4) generated by $(\hat{\mathbf{J}}\pm\hat{\mathbf{K}}/2)$. We define

$$|R,\alpha,\beta,\gamma,\delta,\theta\rangle=\sum_j C_j(R)\exp\left[-i\alpha\left(\frac{\hat{J}+\hat{K}}{2}\right)\right]\times\exp\left[-i\beta\left(\frac{\hat{J}+\hat{K}}{2}\right)\right]\exp\left[-i\gamma\left(\frac{\hat{J}-\hat{K}}{2}\right)\right]\times\exp\left[-i\delta\left(\frac{\hat{J}-\hat{K}}{2}\right)\right]\exp\left(\frac{-iR^3\theta}{2n^2h^3}\right)|jj\rangle|jj\rangle. \tag{17}$$

In place of quantum states $|n,l,m\rangle$ we are now using $|jm_1\rangle|jm_2\rangle$ of $(\hat{\mathbf{J}}+\hat{\mathbf{K}})/2$ and $(\hat{\mathbf{J}}-\mathbf{K})/2$, respectively. [The j quantum number is the same because $(\hat{\mathbf{J}}+\hat{\mathbf{K}})^2=(\hat{\mathbf{J}}-\hat{\mathbf{K}})^2$]. j takes half integer values $0,\frac{1}{2},1,\frac{3}{2},\ldots$. We get the states $|nlm\rangle$ by going to the coupled basis

$$|jm_1\rangle|jm_2\rangle=\sum_{lm}C^{lm}_{jm_1jm_2}|2j+1,l,m\rangle. \tag{18}$$

The new angles are related to the earlier angles as follows (see Fig. 2). The $(\hat{\mathbf{J}}+\hat{\mathbf{K}})/2$ rotation rotates the classical vector $\mathbf{J}+\mathbf{K}$ from the z axis to $(R\sin\beta\cos\alpha,\ R\sin\beta\sin\alpha,\ R\cos\beta)$ without affecting $(\hat{\mathbf{J}}-\hat{\mathbf{K}})/2$. Similarly the $(\hat{\mathbf{J}}-\hat{\mathbf{K}})/2$ rotation rotates the classical vector $\mathbf{J}-\mathbf{K}$ from z axis to $(R\sin\delta\cos\gamma,\ R\sin\delta\sin\gamma,\ R\cos\delta)$. Therefore the projection of $\mathbf{J}$ on the z axis gives $\cos\psi_4=R(\cos\beta+\cos\delta)/|\mathbf{J}|$ where $|\mathbf{J}|=R\sqrt{2+2\sin\beta\sin\delta\cos(\alpha-\gamma)+2\cos\beta\cos\delta}$. The line of nodes is along $\hat{z}\times\hat{J}$ and therefore has the direction cosines $(\sin\delta\sin\gamma+\sin\beta\sin\alpha,-\sin\beta\cos\alpha-\sin\delta\cos\gamma)$. Therefore $\cos\omega=(\sin\delta\sin\gamma+\sin\beta\sin\gamma)/|\mathbf{ON}|$ with $|\mathbf{ON}|=R\sqrt{\sin^2\beta+\sin^2\gamma+2\sin\beta\sin\gamma\cos(\alpha-\delta)}$. Ω is obtained by taking the component of $\mathbf{K}$ along the line of nodes, and therefore $\cos\Omega=|\mathbf{K}|(\sin^2\beta\cos 2\alpha-\sin^2\gamma\cos 2\delta)/|\mathbf{ON}|$ and $|\mathbf{K}|=R\sqrt{2-2\sin\beta\sin\delta\cos(\alpha-\gamma)-2\cos\beta\cos\delta}$. The orbit is simply obtained from the vectors $\mathbf{J}+\mathbf{K}$ and $\mathbf{J}-\mathbf{K}$ because it is perpendicular to $\mathbf{J}$ and has the major axis along the direction $\mathbf{K}$ with magnitude $(R/2\pi h)^2 a$, where a is the Bohr radius. Also the eccentricity is given by $e=\sqrt{1-\mathbf{J}^2/(\mathbf{J}\pm\mathbf{K})^2}$.

The classical phase-space measure in the new variables is $dR\, d\theta\, d((j+1/2)\hbar\cos\beta)\, d\alpha\, d((j+1/2)\hbar\cos\delta)\, d\gamma$. For large J, the state $|R,\alpha,\beta,\gamma,\delta,\theta\rangle$ gets its dominant contribution from $m_1=(j+1/2)\cos\beta$ and $m_2=(j+1/2)\cos\delta$. This is exactly what is wanted by Bohr quantization of the action angle pairs because $\cos\beta=(J+K)_z/R$ and $\cos\delta=(J-K)_z/R$. Therefore we only have to fix $C_j(R)$ by requiring the correct semiclassical limit and resolution of identity. We want $C_j(R)$ to peak at $R=(2j+1)\hbar$, as Bohr quantization gives $R=n\hbar$. Also to get a resolution of identity we require

$$\frac{1}{\hbar}\int_0^\infty dR\ |C_j(R)|^2=1 \tag{19}$$

for all j. For normalization we require $\Sigma_j|C_j(R)|^2=1$, where $j=0,\frac{1}{2},1,\frac{3}{2},\ldots$. All these requirements are met by

$$C_j(R)=\exp(-R/2\hbar)\frac{(R/\hbar)^j}{\sqrt{(2j)!}}. \tag{20}$$

Thus we get the coherent state, as in Eq. (1).

V. WAVE-PACKET PROPERTIES

In case of the harmonic-oscillator coherent states $|z\rangle$ the expectation values of the position and momentum operators are directly given by the real and imaginary parts of the label z. Also they are minimal uncertainty states. For our coherent states, these properties are not valid exactly, but are valid asymptotically in the semiclassical region [7]. This is a consequence of the semiclassical limit of our coherent states, where the correspondence principle may be applied. Consider the expectation value of an operator $\hat{O}(\hat{p},q)$ in a coherent state. For large values of R, L, and M (in units of $\hbar$), the coherent state is dominated by the states $|nlm\rangle$ with $n\approx R/\hbar$, $l\approx L/\hbar$, and $m\approx M/\hbar$. Now, the correspondence principle relates the expectation value of $\hat{O}$ to the value of the corresponding classical variable $O(p,q)$ for the corresponding classical orbit. Thus, asymptotically, our coherent states are wave packets peaked around position, momenta etc. corresponding to the action angle variables labeling them. Also, asymptotically they would be minimum uncertainty states. A more detailed consideration of these properties for small values of the action variables will be considered elsewhere.

VI. CONCLUSION

We have constructed wave packets for the hydrogen atom, labeled by points of the classical phase space which follow classical orbits very closely. They have the correct semiclassical limit corresponding to Bohr quantization. In addition, they have the desirable property that the resolution of identity involves exactly the classical phase-space measure. As a consequence of incommensurate energy levels, our wave packets do not return to the original state after one period, but the overall features do not change. One may interpret this as follows: the wave packet has (an infinite number of) internal degrees of freedom, which may not return to the original state after a period.

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