Brief Reports

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Atomic quantum states with maximum localization on classical elliptical orbits

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We show how to build atomic states that mimic the classical Bohr-Sommerfeld elliptic orbits with minimum quantum fluctuations. These elliptic states are *uniquely* defined from symmetry considerations. They are the coherent states of the SO(4) symmetry group of the Coulomb interaction in three dimensions and are superpositions of the usual spherical states with well-defined weights and phases. They can be experimentally produced from laser excitation of Rydberg atoms in crossed electric and magnetic fields. We finally indicate how to build Coulomb wave packets localized both in space and time.

In spite of early interest,[1] a still elusive question in quantum mechanics is the one of building quantum wave packets that mimic the familiar classical behavior of the electron on Bohr-Sommerfeld ellipses.[2] We give here part of the answer, namely the general solution leading to a perfect geometrical localization of the quantum electronic motion along a classical ellipse.[3] This solution, which builds a set of stationary states of the Coulomb Hamiltonian, is perfect in the sense that the states are coherent states of some rotation group in four dimensions, thus leading to minimum quantum fluctuations, independent of time. We then briefly indicate how to generalize this analysis in order to create time-dependent Bohr-Sommerfeld atomic wave packets. We finally describe a practical way of building these elliptic states[4] using a crossed electric and magnetic fields arrangement. This has already been experimentally demonstrated.[5,6]

Recent studies on Rydberg atoms in external fields have revealed the importance of symmetry considerations for understanding their dynamics.[7,8] In a given n shell, the SO(4) symmetry group is such a key notion which also applies quite successfully to the problem of quantum elliptic states. Let us recall that a classical Kepler ellipse can be defined through the set of constants of the motion, the angular momentum $\mathbf{l}$, and the Runge-Lenz vector $\mathbf{a}$,

$$\mathbf{a}=(-2E)^{-1/2}[\tfrac{1}{2}(\mathbf{p}\times\mathbf{l}-\mathbf{l}\times\mathbf{p})-\mathbf{r}/r] , \qquad (1)$$

which fulfill the conditions $\mathbf{l}\cdot\mathbf{a}=0$ and $\mathbf{l}^2+\mathbf{a}^2=-1/2E$ where E is the energy. $\mathbf{l}$ is perpendicular to the plane of the ellipse and $\mathbf{a}$ is directed along the major axis and measures the eccentricity e.

In the quantum picture, $\mathbf{l}$ and $\mathbf{a}$ build the six components of an angular momentum $\mathcal{L}$ in a fictitious four-dimensional space.[7–9] That is $\mathcal{L}$ ($\mathcal{L}_{ij}=\epsilon_{ijk}\cdot l_k$; $i,j,k=1,2,3$ and $\mathcal{L}_{i4}=-\mathcal{L}_{4i}=a_i$; $i=1,2,3$) satisfies the following commutation relations ($\hbar=1$):

$$[\mathcal{L}_{ij},\mathcal{L}_{ik}]=i\mathcal{L}_{jk} , \qquad (2)$$

otherwise 0 (if the four indices are different). The classical relations extend as

$$\mathcal{L}^2=\mathbf{l}^2+\mathbf{a}^2=-1/2E-1=n^2-1, \quad \mathbf{l}\cdot\mathbf{a}=0 \qquad (3)$$

$\mathcal{L}$ is the generator of four-dimensional rotations that leave the n Coulomb shell invariant. These rotations do not have a simple geometrical interpretation. They allow us to transform a Kepler trajectory into another one with the same energy but different eccentricity as demonstrated hereafter.

The solutions to the Coulomb problem having semiclassical behaviors and minimizing quantum fluctuations are readily deduced from this SO(4) symmetry. They are the states for which the fluctuations of $\mathcal{L}$ are the minimum ones compatible with the commutation relations (2) and constraints (3), hence the coherent states of SO(4). They can be built from the coherent states of SO(3),[10,11] those of the angular momentum in three dimensions, as SO(4)=SO(3)⊗SO(3). The two operators

$$\mathbf{j}_{1,2}=\tfrac{1}{2}(\mathbf{l}\mp\mathbf{a}) \qquad (4)$$

fulfill the standard commutation relations of two commuting three-dimensional (3D) angular momenta,[12] with, from Eq. (3), $j_1=j_2=(n-1)/2$.

The coherent state $|j\mathbf{u}\rangle$ of a 3D angular momentum $\mathbf{j}$ is the eigenstate of $\mathbf{j}\cdot\mathbf{u}$ with maximum eigenvalue j. It verifies $\langle \mathbf{j} \rangle = j\mathbf{u}$, where $\langle \mathbf{j} \rangle$ denotes the average value $\langle j\mathbf{u}|\mathbf{j}|j\mathbf{u}\rangle$. The fluctuation $\Delta j = (\langle \mathbf{j}^2\rangle - \langle \mathbf{j}\rangle^2)^{1/2}$ is the minimum one $\Delta j = \sqrt{j}$ compatible with quantum mechanics. Classically, this means that $\mathbf{j}$ points in the $\mathbf{u}$ direction. The coherent states are deduced from the one $|j\mathbf{z}\rangle = |j\, j_z = j\rangle$ (quantized along the $\mathbf{z}$ axis) through a rotation $R = e^{-i\mathbf{j}\cdot\mathbf{\Omega}}$ with axis $\mathbf{z}\times\mathbf{u}$ and the angle $\alpha = \angle(\mathbf{z},\mathbf{u})$. For SO(3), the Heisenberg uncertainty relation expresses as

$$\Delta j_i \cdot \Delta j_j \geq \tfrac{1}{2}\epsilon_{ijk}|\langle j_k\rangle| \, . \tag{5}$$

For the $|j\mathbf{u}\rangle$ state, the fluctuations of the transverse components of $\mathbf{j}$ fulfill $\Delta j_v = \Delta j_w = \sqrt{j/2}$ (where j_v and j_w are the rotated components of $\mathbf{j}$: $j_{v,w} = R j_{x,y} R^+$). The Heisenberg relation holds with the equality sign. Fluctuations are minimum for these states which are thus "semiclassical."

From $SO(4) = [SO(3)]_{j_1} \otimes [SO(3)]_{j_2}$, the coherent states of SO(4) are generated through the direct product $|j_1\mathbf{u}_1\rangle \otimes |j_2\mathbf{u}_2\rangle$ of coherent states for each SO(3) subgroup. For these states, $\mathcal{L}$ takes its maximum average value ($|\langle \mathcal{L}\rangle| = n-1$) with minimum fluctuations,

$$\Delta\mathcal{L}^2 = \Delta l^2 + \Delta \mathbf{a}^2 = 2(\Delta \mathbf{j}_1^2 + \Delta \mathbf{j}_2^2) = 2(n-1) \, . \tag{6}$$

Choosing, without loss of generality, the $\mathbf{z}$ axis as the first bisector of $(\mathbf{u}_1, \mathbf{u}_2)$ and $\mathbf{x}$ along the second bisector, one obtains

$$|n\alpha\rangle = |j_1\mathbf{u}_1\rangle \otimes |j_2\mathbf{u}_2\rangle = e^{i\alpha(j_{1y} - j_{2y})}|j_1\mathbf{z}\rangle \otimes |j_2\mathbf{z}\rangle \, . \tag{7}$$

The angle α is half the angle between $\mathbf{u}_1$ and $\mathbf{u}_2$. The generator of the rotation thus coincides with $a_y = j_{2y} - j_{1y}$. The state $|j_1\mathbf{z}\rangle \otimes |j_2\mathbf{z}\rangle$ for which $l_z = j_{1z} + j_{2z} = n-1$ and $a_z = j_{2z} - j_{1z} = 0$ is the so-called circular state.[13] It is well known to be a minimum uncertainty state for which the spatial representation of the wave function is localized on a thin torus. Transformed through the nongeometrical $e^{-i\alpha a_y}$ rotation, it is still a state localized with minimum fluctuations but the localization is on some elliptic trajectory. We will name this $|n\alpha\rangle$ state "elliptic."

The operator a_y is one of the components of the 3D angular momentum $\boldsymbol{\lambda}(a_x, a_y, l_z)$.[4,5,8] Hence the operator $e^{-i\alpha a_y}$ is a rotation operator for this angular momentum $\boldsymbol{\lambda}$. The circular state is an eigenvector of $(\boldsymbol{\lambda}^2, \lambda_z = l_z)$ with respective eigenvalues $\lambda(\lambda+1)$ and $\lambda_z = \lambda = n-1$. Hence the elliptic state [Eq. (7)] is a coherent state of the angular momentum $\boldsymbol{\lambda}$, i.e., an eigenstate of $\boldsymbol{\lambda}^2$ and $\boldsymbol{\lambda}\cdot\mathbf{u}_2$ with maximum eigenvalue $\lambda = n-1$,

$$|n\alpha\rangle = |\lambda\mathbf{u}_2\rangle = e^{-i\alpha\lambda_y}|\lambda\lambda_z = \lambda\rangle \, . \tag{8}$$

We show now that the elliptic state presents the best possible localization, within quantum-mechanical constraints, on the classical Kepler trajectory. The average values of $\mathbf{l}$ and $\mathbf{a}$ on such a state can be evaluated from conventional 3D angular momentum algebra. This yields

$$\langle a_x\rangle = (n-1)\sin\alpha \, ,$$
$$\langle l_z\rangle = (n-1)\cos\alpha \, , \tag{9}$$
$$\langle a_y\rangle = \langle a_z\rangle = \langle l_x\rangle = \langle l_y\rangle = 0 \, .$$

The associated classical trajectory is thus an ellipse in the (x,y) plane, with major axis along $\mathbf{x}$ and eccentricity

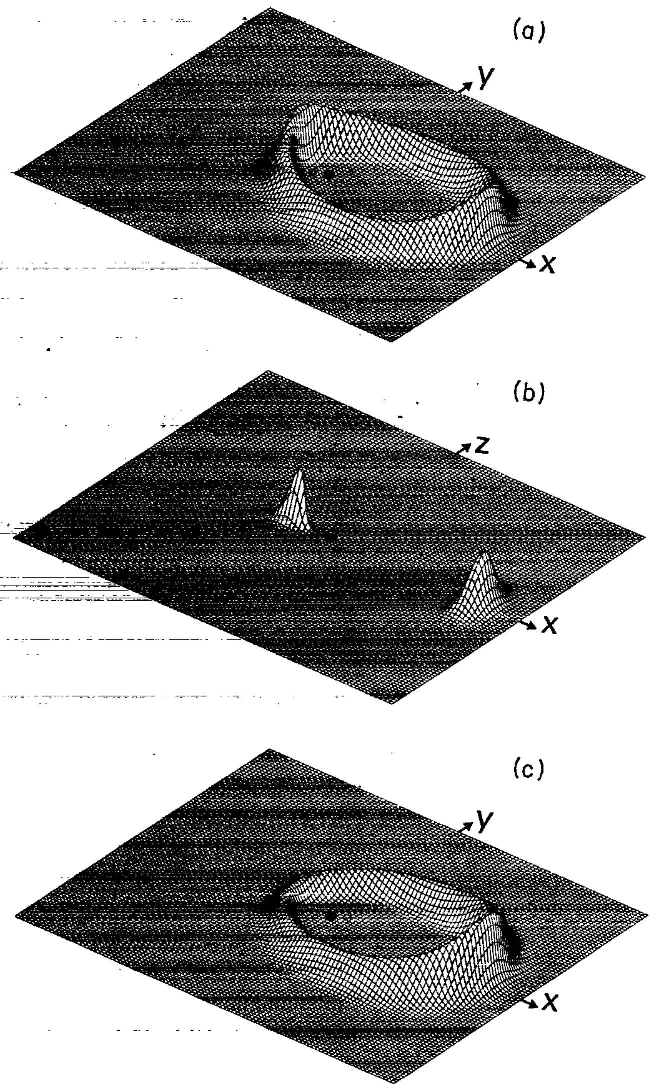

FIG. 1. Electronic density plots for the stationary elliptic state $|n\alpha\rangle$ defined through Eqs. (7) and (8) ($n=50$; eccentricity $e=0.6$; coordinates range $\mp 2n^2a_0$). (a) Distribution in the $z=0$ plane showing the elliptic localization; (b) distribution in the $y=0$ plane showing the localization near the $z=0$ plane and the focusing role of the nucleus at perihelion; (c) distribution averaged over z. The maximum at perihelion has been smoothed out. The one at aphelion is expected from semiclassical arguments. The quantum state is thus fairly localized on a Kepler orbit with eccentricity $e=\sin\alpha$ and angular momentum $l=(n-1)\cos\alpha$. The quantum fluctuations from the construction of the elliptic state are minimum and scale as $n^{3/2}$. The size of the elliptic orbit scales as n^2.

$\sin\alpha$. The fluctuations are

$$\Delta l_x = \Delta a_x = [(n-1)/2]^{1/2}\cos\alpha \ ,$$
$$\Delta l_y = \Delta a_y = [(n-1)/2]^{1/2} \ , \qquad (10)$$
$$\Delta l_z = \Delta a_z = [(n-1)/2]^{1/2}\sin\alpha \ .$$

They fulfill the minimum fluctuations criteria of Eq. (6).

The electronic density plots of the elliptic state are displayed in Fig. 1 for $e=0.6$ ($\alpha=0.6435$) and $n=50$. Figure 1(a) is a plot of the electronic density in the (x,y) plane showing localization on the Bohr-Sommerfeld ellipse. Figure 1(b) is a cut in the (z,x) plane showing that the elliptic state is strongly localized near the $z=0$ plane. Figure 1(c) represents the electronic density in the (x,y) plane after averaging over z motion. It is still localized on the ellipse and the distribution is peaked at aphelion (minimum velocity) as expected from semiclassical arguments. The peaking at the perihelion (maximum velocity) which Fig. 1(a) exhibits is smoothed out. This manifests the focusing effect of the nucleus leading to smaller z dispersion at the perihelion [see Fig. 1(b)]. Finally, geometrical fluctuations are on the order of $n^{3/2}a_0$ while the dimensions scale as n^2a_0.

For various applications, the expansion of the elliptic state $|n\alpha\rangle$ in terms of the usual spherical states $|nlm\rangle$ is needed. We first expand it on the $|\lambda\lambda_z\rangle$ basis (quantized along z axis) using the Wigner formula and Eq. (8). This yields

$$|n\alpha\rangle = \sum_m \left[\frac{2\lambda!}{(\lambda-m)!(\lambda+m)!}\right]^{1/2}\left[\sin\frac{\alpha}{2}\right]^{\lambda-m}\left[\cos\frac{\alpha}{2}\right]^{\lambda+m}|\lambda\,\lambda_z=m\rangle \ , \qquad (11)$$

with $\lambda=n-1$.

The coefficients depend on the angle α and are simply related to the eccentricity $e=\sin\alpha$ of the ellipse. Similar expansion on the (j_{1z},j_{2z}) basis can be obtained from Eq. (7). The second step is to expand the $|\lambda\lambda_z\rangle$ states onto the $|nlm\rangle$ spherical states (quantized along z). Using[5] $\lambda=e^{-i\pi j_{1z}}l e^{i\pi j_{1z}}$ this yields

$$|n\alpha\rangle = \sum_{l,m}(-1)^{(l+m)/2}\frac{2^{n-l-1}(n-1)!}{[(l-m)/2]![(l+m)/2]!}\left[\frac{(l+m)!(l-m)!(2l+1)}{(n-l-1)!(n+l)!}\right]^{1/2}$$
$$\times\left[\sin\frac{\alpha}{2}\right]^{n-m-1}\left[\cos\frac{\alpha}{2}\right]^{n+m-1}|n\,l\,l_z=m\rangle \ . \qquad (12)$$

This summation involves $n(n+1)/2$ terms, and every l and m values such that $l+m$ is even (the elliptic state has well-defined even z parity). This strongly contrasts with the expansion on the λ basis which involves only $(2n-1)$ values of λ_z.[14] In the limit of high n, the distribution of l and m values are peaked at the classical values $l_0=m_0=(n-1)$. $\cos\alpha$ with a Gaussian dispersion on the order of $\sqrt{n}$.

These results find a simple interpretation in momentum space. An explicit realization of the SO(4) symmetry group is built by adding a fourth dimension to 3D momentum space. Considering the hypersphere with radius $p_0=1/n$ (the so-called Fock hypersphere) centered at the origin, the stereographic projection of p space onto the sphere, transforms the atomic wave functions of the n Coulomb shell into the 4D spherical harmonics.[9] This establishes the 4D rotational invariance. Classically, the Kepler trajectory transforms into a "great" circle of the Fock hypersphere. The operator $e^{-i\alpha a_y}$ is just a geometrical rotation on the hypersphere and transforms any great circle into another one which is still associated with a solution to the Coulomb problem in the n shell.

Hence in 3D momentum space, the elliptic state is deduced from the circular state by the product of the three transformations: stereographic projection, rotation on the hypersphere, and inverse stereographic projection. This yields simply the analytical expression of the wave function of the elliptic state in momentum representation

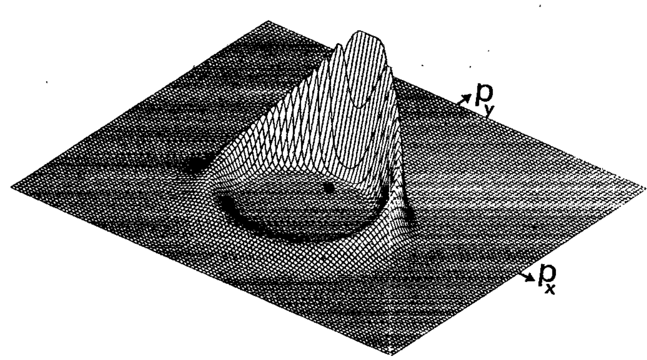

FIG. 2. Electronic density of the elliptic state in momentum space [conditions as in Fig. 1; coordinates range $\mp 3/n$ a.u.]. The density is peaked on a circle, followed with minimum fluctuations scaling as $n^{-3/2}$. The radius of the circle scales as $1/n$. The distance between the center and the origin measures the eccentricity.

$$\langle \mathbf{p}|n\alpha\rangle = \frac{2\sqrt{2}}{\pi}\frac{n^2}{(1+n^2p^2)^2}\left[\frac{2n[p_x+i(\cos\alpha)p_y]+i(\sin\alpha)(n^2p^2-1)}{1+n^2p^2}\right]^{n-1},$$

which actually presents a localization on a circle (the classical trajectory in **p** space is a circle) followed with minimum fluctuations scaling as $n^{-3/2}$ (see Fig. 2).

Previous sets of elliptic states $\{|n\alpha\rangle; 0\le\alpha\le\pi\}$ are stationary states of the Coulomb Hamiltonian which are localized on the classical Kepler trajectory, with minimum fluctuations independent on time. In order to further localize the electron on such an orbit, it is necessary to build a wave packet by mixing several n values. Getting the best localization with minimum spreading in time along the orbit requires that the n mixing respects defined rules. They can be obtained from our previous analysis combined with the Coulomb dynamical group concept.[7,9]

Finally, the stationary elliptic states should have applications to spectroscopy. They can be simply produced by the means of laser excitation of Rydberg atoms in a crossed-fields arrangement. They key point lies in that two-limiting cases of the elliptic state [Eqs. (7) and (8)] are, respectively, the circular state ($\alpha=0$) and the Stark state (quantization along the **x** axis) with extremum parabolic quantum numbers ($\alpha=\pi/2$; $l_x=0$; $a_x=n-1$; the ellipse is a straight line). Optical excitation of the latter is thus possible in the Stark limit. Subsequent adiabatic switching off of the electric field to some nonzero value produces an elliptic state $|n\alpha\rangle$ with an eccentricity $\sin\alpha$, tunable through the fields strengths.[3,4] This method has been recently demonstrated to be efficient for the building of circular states.[6] Early spectroscopic investigations of the crossed-field spectrum of rubidium also gave evidence for these elliptic states (see the plot in Fig. 11 of reference;[5] the points for $k=-33$ refer to elliptic states).

Among various applications, especially to fundamental questions (chaos, wave packets, relativistic effects, etc.), the quantum elliptic states may lead us to overcome some of the limitations of conventional optical spectroscopy. They are, from Eq. (12), coherent superpositions of all l and m values, the weights of which can be conveniently tuned through the eccentricity e. Combined with stepwise excitation, this is likely to open new fields for the studies of autoionization at high l and doubly excited systems.

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