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Wave Functions of Atomic Elliptic States.

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Abstract. – The elliptic eigenstates of the hydrogen atom are the quantum analogs of the classical trajectories of the electron around the nucleus in the sense that they have the best transverse localization compatible with the uncertainty relations. The equivalence of the hydrogen atom with a harmonic oscillator provides us with a realization of the symmetry group and allows for the analytical study of the elliptic states. In particular we derive the 2D and 3D wave functions in a simple closed form.

These last years have seen a renewed interest in building experimentally and theoretically [1-4] atomic wave packets localized along Kepler orbits. In an attempt at clarifying the theoretical background, a recent work [4, 5] has shown in an algebraic way the existence of stationary «elliptic» states. They are a class of eigenstates of the Coulomb Hamiltonian with the best transverse localization on the Bohr-Sommerfeld orbits, compatible with the uncertainty relations. However, from their stationary character, they do not have the longitudinal localization and time dependence of the classical motion.

The classical elliptic trajectories are characterized by the two constants of motion: the angular momentum $\boldsymbol{L}$ and the Runge-Lenz vector $\boldsymbol{A} = (-2E)^{-1/2}((1/2)(\boldsymbol{p} \times \boldsymbol{L} - \boldsymbol{L} \times \boldsymbol{p}) - \boldsymbol{r}/|\boldsymbol{r}|)$ (in atomic units; E is the energy) which is along the major axis (pointing towards the perihelion) and is proportional to the eccentricity of the trajectory.

The elliptic state localized on an ellipse in the (x, y)-plane with major axis along x and eccentricity $e = \sin\theta$ is deduced from the circular state $|\mathrm{Circ}(n)\rangle = |n, l = l_z = n-1\rangle$ (with maximum angular momentum $l = l_z$) through [5]

$$|\mathrm{Ell}(n, \theta)\rangle = \exp[-i\theta A_y]|\mathrm{Circ}(n)\rangle = T_\theta|\mathrm{Circ}(n)\rangle, \tag{1}$$

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where T_θ is a rotation of the $SO(4)$ symmetry group of which $\boldsymbol{L}$ and $\boldsymbol{A}$ are the generators. The elliptic state fulfills the general form for coherent states of the $SO(4)$ rotation group [6]. This leads to $\langle L_z \rangle = (n-1)\cos\theta$ and $\langle A_x \rangle = (n-1)\sin\theta$.

Equation (1) may not be appropriate for getting analytical representations as wave functions (A_y being a complicated operator in $\boldsymbol{r}$, $\boldsymbol{p}$). In the following, we exemplify one way of overcoming this difficulty and for simplicity, we first consider the two-dimensional case for which eq. (1) extends straightforwardly.

The energy spectrum of the two-dimensional hydrogen atom is $E_n = -1/[2(n+1/2)^2]$, where the principal quantum number n is a nonnegative integer. The degeneracy of each energy level is $2n+1$. The symmetry group is generated by A_x, A_y and L_z which are the classical constants of motion in the two-dimensional case; their commutation relations are those of the generators of an $SO(3)$ group. The circular state is the one for which the angular-momentum quantum number is maximum: $|\mathrm{Circ}^{(2D)}(n)\rangle = |n, l_z = n\rangle$. The elliptic states are deduced as in eq. (1) where T_θ is now a rotation of the $SO(3)$ symmetry group which is not a rotation in space (whose generator would be L_z).

The mapping of the 2D hydrogen atom onto the 2D isotropic oscillator dynamics provides us with a realization of $SO(3)$ giving more insight into the structure of the elliptic states. This can be established using the 2D parabolic coordinates (u, v) [7]:

$$x = \frac{u^2 - v^2}{2}, \qquad y = uv \tag{2}$$

in which the Schrödinger equation of the hydrogen atom for the energy E_n is cast into the one for a harmonic oscillator of frequency $\omega_n = \sqrt{-2E_n}$ and energy equal to 2:

$$\left(\frac{1}{2}\Delta_{u,v} = E_n(u^2+v^2) + 2\right)\psi_n(u, v) = 0\,. \tag{3}$$

There is an additional constraint arising from the mapping $(x, y) \leftrightarrow (\pm u, \pm v)$ being double-valued. Only the even-parity eigenfunctions of the oscillator are physically relevant for the 2D hydrogen atom.

We introduce the creation-annihilation operators in the (u, v) coordinates in the standard way with, *e.g.*, $a_u = (u\sqrt{\omega_n} + ip_u/\sqrt{\omega_n})/\sqrt{2}$. The generators of the symmetry group $SU(2)$ of the 2D oscillator are readily deduced; they are quadratic in the Fock operators and commute with the Hamiltonian. They can be identified with the $SO(3)$ symmetry group generators of the hydrogen atom for the energy level n. This yields [8]

$$\begin{cases} A_x = -\dfrac{1}{2}(a_u^\dagger a_u - a_v^\dagger a_v)\,, \\ A_y = -\dfrac{1}{2}(a_u^\dagger a_v + a_v^\dagger a_u)\,, \\ L_z = -\dfrac{i}{2}(a_u^\dagger a_v - a_v^\dagger a_u)\,, \\ H' = \omega_n(a_u^\dagger a_u + a_v^\dagger a_v + 1)\,, \end{cases} \tag{4}$$

where H' is the Hamiltonian of the oscillator; introducing the excitation numbers n_u and n_v, one gets $n_u + n_v = 2n$. (A_x, A_y, L_z) builds a 3D angular momentum with modulus $j = n$. The action of the rotation $T_\theta = \exp[-i\theta A_y]$ on the Fock operators (a_u, a_v) yields, respectively,

$a_u \cos(\theta/2) - ia_v \sin(\theta/2)$ and $a_v \cos(\theta/2) - ia_u \sin(\theta/2)$ from which we easily deduce the transformation of the coherent states $|\alpha_u \alpha_v\rangle$ (eigenstates of a_u and a_v) under T_θ. Those states are Gaussian wave packets whose wave functions have a simple expression (1). In addition, the «coherent-state representation» of the circular state, *i.e.* its projection onto the coherent-state basis, is very simple (2):

$$\langle \alpha_u, \alpha_v | \mathrm{Circ}^{(2D)}(n)\rangle = \frac{1}{\sqrt{(2n)!}}\left(\frac{\alpha_u^* + i\alpha_v^*}{\sqrt{2}}\right)^{2n} \exp\left[-\frac{1}{2}|\alpha_u|^2 - \frac{1}{2}|\alpha_v|^2\right] \tag{5}$$

from which the coherent-state representation of the elliptic state follows:

$$\langle \alpha_u, \alpha_v | \mathrm{Ell}^{(2D)}(n,\theta)\rangle = \frac{1}{\sqrt{(2n)!}}\left(\alpha_u^* \frac{\cos(\theta/2) - \sin(\theta/2)}{\sqrt{2}} + i\alpha_v^* \frac{\cos(\theta/2) - \sin(\theta/2)}{\sqrt{2}}\right)^{2n} \exp\left[-\frac{1}{2}|\alpha_u|^2 - \frac{1}{2}|\alpha_v|^2\right]. \tag{6}$$

By using the closure relation on the coherent states

$$\iint |\alpha_u \alpha_v\rangle\langle \alpha_u \alpha_v| \frac{d^2\alpha_u\, d^2\alpha_v}{\pi^2} = 1 \tag{7}$$

and the expression of their wave function $\langle uv|\alpha_u \alpha_v\rangle$ [9], this yields through a straightforward but tedious integration,

$$[\mathrm{Ell}^{(2D)}(n,\theta)](x,y) = \frac{1}{(n+1/2)\sqrt{2\pi(2n+1)!}}\left(-\frac{\sin\theta}{2}\right)^n \cdot \exp\left[\frac{-r}{n+1/2}\right] H_{2n}\left(\sqrt{\frac{1}{n+1/2}}\left(r - \frac{x+iy\cos\theta}{\sin\theta}\right)\right), \tag{8}$$

where H_{2n} is a Hermite polynomial. This gives the 2D space density shown in fig. 1. The nodes of the wave function are located on the major axis (the x-axis) inside the ellipse and are related to the n positive zeros of the Hermite polynomial.

We now derive in a similar way the wave function of the three-dimensional elliptic state. We introduce a set of four coordinates (u_1, u_2, u_3, u_4) related to the (x, y, z) coordinates by the Kustaanhamo-Stiefel transformation [10]:

$$x = u_1 u_3 - u_2 u_4, \qquad y = u_1 u_4 + u_2 u_3, \qquad z = \frac{1}{2}(u_1^2 + u_2^2 - u_3^2 - u_4^2), \tag{9}$$

upon which the Schrödinger equation of the hydrogen atom is transformed into the one of a four-dimensional harmonic oscillator of frequency $\omega_n = \sqrt{-2E_n}$ and energy 2 [11]. There is an additional constraint on the mapping (9) due to the requirement that the wave function be

(1) That is $\langle u|\alpha_u\rangle = \pi^{-1/4}\exp[-(1/2)(|\alpha_u|^2 + u^2 + \alpha_u^2 - 2\sqrt{2}u\alpha_u)$. See, *e.g.*, ref. [9].

(2) This result can be obtained simply by the introduction of the right/left polarisations of the 2D oscillator $a_{d,g} = (a_u \mp ia_v)/\sqrt{2}$ and the associated excitation numbers (n_d, n_g) [9]. The angular momentum L_z becomes $(1/2)(n_d - n_g)$ from which it follows that the circular state is $|n_d = 2n, n_g = 0\rangle$.

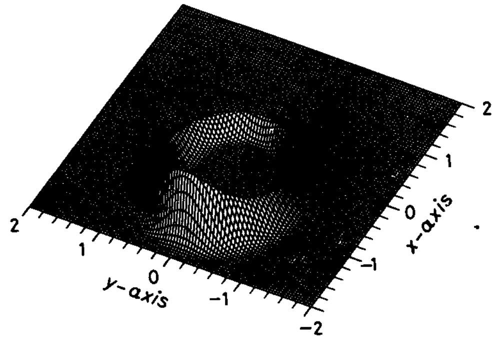

Fig. 1. – Electronic density plot for the 2D elliptic state defined in eq. (1) for $n = 50$, eccentricity $e = 0.6$, coordinate range $\pm 2(n + 1/2)^2 a_0$. It displays a maximum at aphelion and a minimum at perihelion as expected from the classical behaviour. The size of the ellipse scales as n^2 and the of fluctuations as $n^{3/2}$.

single-valued. This leads to the condition

$$(u_1 p_2 - u_2 p_1 + u_4 p_3 - u_3 p_4)|\Psi\rangle = C|\Psi\rangle = 0, \tag{10}$$

where p_i $(i = 1, \ldots, 4)$ are the conjugate momenta of the u_i $(i = 1, \ldots, 4)$. This constraint just expresses that the angular momenta of the (1, 2) and (3, 4) oscillators should be the same. The constraint and all the generators of the $SO(4)$ symmetry group of the hydrogen atom may be put in correspondence with the ones of the $SU(4)$ symmetry group of the 4D oscillator which preserve the constraint (10). Introducing the Fock operators $(a_i;\ i = 1$ to $4)$ as in 2D, this leads in particular to [12]

$$\begin{cases} C = i(a_2^\dagger a_1 - a_1^\dagger a_2 + a_3^\dagger a_4 - a_4^\dagger a_3), \\ L_z = -\dfrac{i}{2}(a_1^\dagger a_2 - a_2^\dagger a_1 + a_3^\dagger a_4 - a_4^\dagger a_3), \\ A_y = -\dfrac{1}{2}(a_1^\dagger a_4 + a_2^\dagger a_3 + a_3^\dagger a_2 + a_4^\dagger a_1), \\ H' = \omega_n(a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3 + a_4^\dagger a_4 + 2), \end{cases} \tag{11}$$

where H' is the Hamiltonian of the oscillator. Introducing the excitation numbers (n_1, n_2, n_3, n_4), one has $n = (1/2)(n_1 + n_2 + n_3 + n_4 + 2)$, where n is the hydrogen principal quantum number.

The circular state has a maximum angular-momentum quantum number L_z and is the direct product of two circular states in the (u_1, u_2) and (u_3, u_4) planes leading to the coherent-state representation:

$$\langle \alpha_1, \alpha_2, \alpha_3, \alpha_4 | \mathrm{Circ}^{(3\mathrm{D})}(n)\rangle = \\ = \frac{1}{(n-1)!}\left(\frac{\alpha_1^* + i\alpha_2^*}{\sqrt{2}}\right)^{n-1}\left(\frac{\alpha_3^* + i\alpha_4^*}{\sqrt{2}}\right)^{n-1} \exp\left[-\frac{1}{2}|\alpha_1|^2 - \frac{1}{2}|\alpha_2|^2 - \frac{1}{2}|\alpha_3|^2 - \frac{1}{2}|\alpha_4|^2\right]. \tag{12}$$

From eq. (1) and the expression of A_y (eq. (11)), we find

$$T_\theta^\dagger|\alpha_1,\alpha_2,\alpha_3,\alpha_4\rangle =$$

$$= \left|\cos\frac{\theta}{2}\alpha_1 - i\sin\frac{\theta}{2}\alpha_4;\ \cos\frac{\theta}{2}\alpha_2 - i\sin\frac{\theta}{2}\alpha_3;\ \cos\frac{\theta}{2}\alpha_3 - i\sin\frac{\theta}{2}\alpha_2;\ \cos\frac{\theta}{2}\alpha_4 - i\sin\frac{\theta}{2}\alpha_1\right\rangle$$

from which we deduce the coherent-state representation of the elliptic state:

$$\langle\alpha_1,\alpha_2,\alpha_3,\alpha_4|\mathrm{Ell}^{(3D)}(n,\theta)\rangle = \frac{1}{(n-1)!}\left(\frac{\alpha_1^*+i\alpha_2^*}{\sqrt{2}}\cos\frac{\theta}{2} - \frac{\alpha_3^*-i\alpha_4^*}{\sqrt{2}}\sin\frac{\theta}{2}\right)^{n-1}\cdot$$

$$\cdot\left(-\frac{\alpha_1^*-i\alpha_2^*}{\sqrt{2}}\sin\frac{\theta}{2} + \frac{\alpha_3^*+i\alpha_4^*}{\sqrt{2}}\cos\frac{\theta}{2}\right)^{n-1}\exp\left[-\frac{1}{2}|\alpha_1|^2 - \frac{1}{2}|\alpha_2|^2 - \frac{1}{2}|\alpha_3|^2 - \frac{1}{2}|\alpha_4|^2\right]. \tag{13}$$

It is *not* the direct product of two 2D elliptic states because the rotation T_θ acts in the (1, 4) and (2, 3) spaces. The wave function is finally deduced using the closure relation on coherent states, yielding

$$[\mathrm{Ell}^{(3D)}(n,\theta)](x,y,z) = \frac{1}{n^2\sqrt{\pi}}\exp[-r/n](\sin\theta)^{n-1}L_{n-1}\left(\frac{1}{n}\left(r - \frac{x+iy\cos\theta}{\sin\theta}\right)\right), \tag{14}$$

where L_{n-1} is a Laguerre polynomial. The nodes of the wave function are located on $n-1$ hyperbolas in the (x, z)-plane, of axis x, of eccentricity $1/\sin\theta$ with focus at the nucleus. Those hyperbolas intersect the major axis inside the ellipse. The probability density in the (x, y)-plane is drawn in fig. 2.

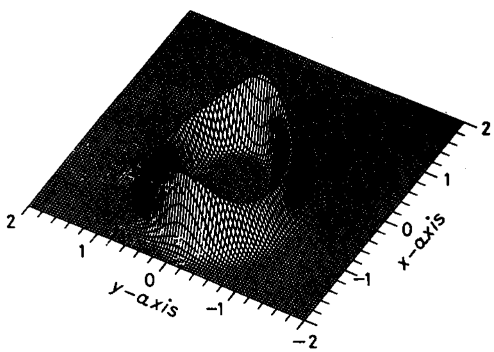

Fig. 2. – Cut of the electronic density in the $z = 0$ plane for the 3D elliptic state ($n = 50$, eccentricity $e = 0.6$ and coordinate range $\pm 2n^2 a_0$). The peaking at the perihelion can be smoothed out by averaging the density over z (this is shown in [5], fig. 2; the axes in this figure are inverted: $(x, y) \to (-x, -y)$). From the comparison with fig. 1, this peaking at perihelion is a consequence the fluctuations of the plane of the orbit.

The wave function of the elliptic state in momentum space can be derived in the same spirit from its coherent-state representation ([3]). The wave function in 2D has a compact

([3]) The wave function can also be calculated by the introduction of the Fock realization of the symmetry group in the momentum space (for more details see [5, 13]).

form:

$$[\mathrm{Ell}^{2D}(n,\theta)](p_x,p_y)=\frac{(-i)^n\sqrt{(2n+1)!}(2n+1)}{\sqrt{2\pi}\,n!}\cdot$$

$$\cdot\frac{1}{(1+(n+1/2)^2p^2)^{3/2}}\left(\frac{(2n+1)(p_x+ip_y\cos\theta)+i(1-(n+1/2)^2p^2)\sin\theta}{2(1+(n+1/2)^2p^2)}\right)^n. \tag{15}$$

The wave functions are peaked on eccentric circles which are the hodographs of the corresponding classical trajectories. In 3D, the momentum wave function is given in [5], eq. (13) and has to be corrected by a factor $(-i)^{n-1}$ to be compatible with the phase factor of (14).

The coherent-state representation $\langle\alpha_u,\alpha_v|\psi\rangle$ of atomic states builds a phase space density where $\alpha_u=(u\sqrt{\omega_n}+ip_u/\sqrt{\omega_n})/\sqrt{2}$ and $\alpha_v=(v\sqrt{\omega_n}+ip_v/\sqrt{\omega_n})/\sqrt{2}$. The squared modulus of this quantity is known as the Husimi distribution [14]. It measures the overlap between ψ and a Gaussian wave packet. For the elliptic states, it is a Poisson distribution ($x^n\exp[-x]$) localized in the vicinity of the classical phase space trajectory which is a circle in the (u,v,p_u,p_v) coordinates with dispersion of order $\sqrt{n}$ at large n.

The elliptic states—which minimalize some Heisenberg uncertainty relations ($\Delta A_x\Delta A_y=1/2|\langle L_z\rangle|$)—are semi-classical from their nearly perfect localization in configuration, momentum and phase space when n tends to infinity. They have very simple representations in configuration and momentum spaces and even simpler coherent-state representation. Aside from their obvious importance in the search for semi-classical states of the hydrogen atom, they build an overcomplete eigenbasis in the n energy shell of the atom leading to direct physical applications to low-energy atomic collisions or atoms interacting with slowly varying electromagnetic fields. For example, they are the first-order quantum solution to the problem of microwave ionization with circularly polarized fields.

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