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LETTER TO THE EDITOR

Coherent states for the hydrogen atom

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Abstract. The long-standing problem of finding coherent states for the (bound state portion of the) hydrogen atom is positively resolved. The states in question (i) are normalized and parametrized continuously, (ii) admit a resolution of unity with a positive measure, and (iii) enjoy the property that the temporal evolution of any coherent state by the hydrogen atom Hamiltonian remains a coherent state for all time.

1. Harmonic oscillator coherent states

In modern terms, the distinguished set of states Schrödinger introduced for the harmonic oscillator [1] are now commonly known as coherent states [2] and are given, for all $z \in \mathbb{C}$, by

$$|z\rangle \equiv \mathrm{e}^{(za^\dagger - z^* a)}|0\rangle = \mathrm{e}^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle \tag{1}$$

where $[a, a^\dagger] = 1$ as usual. Here $|n\rangle, n = 0, 1, 2, \ldots$, denote normalized eigenstates of the number operator N, $N|n\rangle = n|n\rangle$, which may be identified with the eigenstates of the harmonic oscillator Hamiltonian $\mathcal{H}_0 = \omega N = \omega a^\dagger a$ ($\hbar = 1$). As such it follows that

$$\mathrm{e}^{-\mathrm{i}\mathcal{H}_0 t}|z\rangle = \mathrm{e}^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n \mathrm{e}^{-in\omega t}}{\sqrt{n!}} |n\rangle = |\mathrm{e}^{-\mathrm{i}\omega t} z\rangle \tag{2}$$

illustrating the fact that the time evolution of any such coherent state remains within the family of coherent states; we shall refer to the property embodied in (2) as temporal stability of the coherent states under $\mathcal{H}_0$, or, more briefly, just as *temporal stability*. Furthermore, these states are evidently continuous in their label $z = x + \mathrm{i}y$ and admit a resolution of unity given by

$$\mathbb{1} = \int |z\rangle\langle z| \, \mathrm{d}x \, \mathrm{d}y/\pi \tag{3}$$

integrated over $\mathbb{C}$. Continuity in the labels plus a resolution of unity establish that the set $\{|z\rangle\}$ is a set of coherent states in the modern sense of the term [3].

2. Giving up the group

Of course, there exist many other sets of states, which we also refer to as coherent states, that are continuous in their labels and admit a resolution of unity. Such states may, for

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example, take the form, for all $\zeta \in \mathbb{C}$, given by

$$|\zeta\rangle = M(|\zeta|^2) \sum_{n=0}^{\infty} \frac{\zeta^n}{\sqrt{\rho_n}} |n\rangle \tag{4}$$

where M is chosen so that $\langle\zeta|\zeta\rangle = 1$, so long as a positive weight k exists such that when integrated over the plane ($\zeta = \xi + \mathrm{i}\eta$)

$$\mathbb{1} = \int |\zeta\rangle\langle\zeta|\, k(|\zeta|^2)\, \mathrm{d}\xi\, d\eta/\pi\ . \tag{5}$$

Evidently $\mathrm{e}^{-\mathrm{i}\mathcal{H}_0 t}|\zeta\rangle = |\mathrm{e}^{-\mathrm{i}\omega t}\zeta\rangle$ holds for all $\zeta \in \mathbb{C}$ for this alternative set of states just as well. To ensure (5) it suffices to have

$$\begin{aligned} \rho_n &= \int_0^\infty u^n \rho(u)\, \mathrm{d}u \\ \rho(u) &\equiv M^2(u)\, k(u) \end{aligned} \tag{6}$$

and to generate such examples it is easiest to choose ρ first†. As one example of such a set of alternative coherent states for the harmonic oscillator we offer $\rho(u) = \mathrm{e}^{-\sqrt{u}}/2$, with $\rho_n = (2n+1)!$ and $M^2(u) = \sqrt{u}/\sinh\sqrt{u}$. Do not look for a transitively acting group or one up to a factor (as in (1)) that defines the states $|\zeta\rangle$ as unitary tranformations of a fiducial vector; there is no such group [4]. Such states are generally not minimal uncertainty states, of course, but minimal uncertainty states by themselves do not ensure temporal stability as illustrated by the example of squeezed states.

3. Covering-space formulation

As one further generalization we wish to extend the polar coordinates r, θ ($z \equiv r\mathrm{e}^{\mathrm{i}\theta}$), where $0 \leqslant r < \infty$, $-\pi < \theta \leqslant \pi$, to their covering space, namely the domain $0 \leqslant r < \infty$, $-\infty < \theta < \infty$. To this end we introduce

$$|r,\theta\rangle \equiv M(r^2) \sum_{n=0}^{\infty} (r^n \mathrm{e}^{\mathrm{i}n\theta}/\sqrt{\rho_n})|n\rangle \tag{7}$$

and a measure $\nu(r,\theta)$ defined by

$$\int F(r,\theta)\, \mathrm{d}\nu(r,\theta) \equiv \lim_{\Theta\to\infty} \frac{1}{2\Theta} \int_0^\infty \mathrm{d}r^2\ k(r^2) \int_{-\Theta}^{\Theta} \mathrm{d}\theta\ F(r,\theta). \tag{8}$$

It follows that the states $|r,\theta\rangle$ are continuous in r and θ, and admit the resolution of unity

$$\mathbb{1} = \int |r,\theta\rangle\langle r,\theta|\, \mathrm{d}\nu(r,\theta). \tag{9}$$

Evidently $\exp(-\mathrm{i}\mathcal{H}_0 t)\,|r,\theta\rangle = |r,\theta-\omega t\rangle$, which is how temporal stability appears in the present notation.

† We assume ρ is chosen so that all moments exist and that the sum in (4) converges strongly for all $\zeta \in \mathbb{C}$.

4. Relaxing the functional dependence

Prior to considering coherent states for the hydrogen atom, we first analyse a simpler, yet related example. In particular, we consider a single degree of freedom system with a Hamiltonian given by $\mathcal{H}_1 \equiv -\omega/(N+1)^2$, namely one with eigenvalues $E_n \equiv -\omega/(n+1)^2$, $n = 0, 1, 2, \ldots$. As coherent states for this example we choose ($0 \leqslant s < \infty$, $-\infty < \gamma < \infty$)

$$|s, \gamma\rangle \equiv M(s^2) \sum_{n=0}^{\infty} (s^n \mathrm{e}^{\mathrm{i}\gamma/(n+1)^2}/\sqrt{\rho_n}\,)|n\rangle \tag{10}$$

where each state $|n\rangle$ obeys $\mathcal{H}_1|n\rangle = E_n|n\rangle$. Clearly, the states $|s, \gamma\rangle$ are continuous and fulfill

$$\mathbb{1} = \int |s, \gamma\rangle\langle s, \gamma| \; \mathrm{d}\nu(s, \gamma)\,. \tag{11}$$

It is trivial to observe that

$$\mathrm{e}^{-\mathrm{i}\mathcal{H}_1 t}|s, \gamma\rangle = |s, \gamma + \omega t\rangle \tag{12}$$

establishing that the states in question exhibit temporal stability for $\mathcal{H}_1$. The states defined by (10) apply to a wide variety of choices for $\rho(u)$ and its moments ρ_n, $n = 0, 1, 2, \ldots$. Perhaps one of the simplest examples of such coherent states arises when we choose $\rho(u) = \mathrm{e}^{-u}$, $\rho_n = n!$, and $M(s^2) = \exp(-s^2/2)$, in which case

$$|s, \gamma\rangle = \mathrm{e}^{-s^2/2} \sum_{n=0}^{\infty} (s^n \mathrm{e}^{\mathrm{i}\gamma/(n+1)^2}/\sqrt{n!}\,)|n\rangle \tag{13}$$

and

$$\mathbb{1} = \lim_{\Gamma\to\infty} \frac{1}{\Gamma} \int_0^\infty \int_{-\Gamma}^{\Gamma} |s, \gamma\rangle\langle s, \gamma| \; s \; \mathrm{d}s \; \mathrm{d}\gamma\,. \tag{14}$$

5. Hydrogen atom coherent states

We now finally turn to the (bound state part of the) hydrogen atom [5]. We characterize this example by a Hamiltonian $\mathcal{H}$ with spectrum $E_n = -\omega/(n+1)^2$, $n = 0, 1, 2, \ldots$, $\omega = m\mathrm{e}^4/2$, and with a degeneracy of each level given by $(n+1)^2$, which in turn is spanned, for example, by standard angular momentum states $|\ell m\rangle$, $0 \leqslant \ell \leqslant n$, $-\ell \leqslant m \leqslant \ell$, as usual. **N.B.** *In the present usage*, $n = 0, 1, 2, \ldots$, *while the standard usage for the hydrogen atom is* $n = 1, 2, 3, \ldots$ *for the principal quantum number*. Thus the traditional hydrogen atom bound state $|n\ell m\rangle$ becomes $|n + 1\ell m\rangle$. To accomodate the angular momentum states we introduce suitable hydrogen atom adapted angular-momentum coherent states [3, 6]

$$|n, \overline{\Omega}\rangle \equiv \sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} \left[\frac{(2\ell)!}{(\ell+m)!(\ell-m)!}\right]^{\frac{1}{2}} \left(\sin\frac{\overline{\theta}}{2}\right)^{\ell-m} \left(\cos\frac{\overline{\theta}}{2}\right)^{\ell+m}$$
$$\times \mathrm{e}^{-\mathrm{i}(m\overline{\phi}+\ell\overline{\psi})}|n + 1\ell m\rangle\sqrt{2\ell+1} \tag{15}$$

These hydrogen atom adapted angular-momentum coherent states satisfy

$$\int |n, \overline{\Omega}\rangle\langle n, \overline{\Omega}| \sin\overline{\theta} \; \mathrm{d}\overline{\theta} \; \mathrm{d}\overline{\phi} \; \mathrm{d}\overline{\psi}/8\pi^2 = \sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} |n + 1\ell m\rangle\langle n + 1\ell m| = \mathbb{1}_n \tag{16}$$

which for each $n \geqslant 0$ is the unit operator when acting in an angular momentum subspace in which $0 \leqslant \ell \leqslant n$. Observe for all $n \geqslant 1$, that the subspace in question carries a *reducible* representation of the rotation group with a total dimensionality of $\sum_{\ell=0}^{n}(2\ell+1) = (n+1)^2$.

The appropriate coherent states for the hydrogen atom are then given by

$$|s, \gamma, \overline{\Omega}\rangle \equiv M(s^2) \sum_{n=0}^{\infty} (s^n \mathrm{e}^{\mathrm{i}\gamma/(n+1)^2} / \sqrt{\rho_n}\,)|n, \overline{\Omega}\rangle \,. \tag{17}$$

The coherent states in question are evidently continuous and furthermore satisfy ($\mathrm{d}\overline{\Omega} \equiv \sin\overline{\theta}\,\mathrm{d}\overline{\theta}\,\mathrm{d}\overline{\phi}\,\mathrm{d}\overline{\psi}/8\pi^2$)

$$\mathbb{1}_{\mathrm{BS}} = \int |s, \gamma, \overline{\Omega}\rangle\langle s, \gamma, \overline{\Omega}|\;\mathrm{d}\nu(s, \gamma)\;\mathrm{d}\overline{\Omega} \tag{18}$$

where the subscript BS is intended to remind us that this expression is the unit operator only for the bound state portion of the spectrum (and zero for the continuous spectrum). We extend the definition of the number operator N so that

$$N|n, \overline{\Omega}\rangle = n|n, \overline{\Omega}\rangle \tag{19}$$

in which case the hydrogen atom Hamiltonian reads $\mathcal{H} = -\omega/(N+1)^2$, $\omega = m\mathrm{e}^4/2$. It follows that

$$\mathrm{e}^{-\mathrm{i}\mathcal{H}t}|s, \gamma, \overline{\Omega}\rangle = |s, \gamma + \omega t, \overline{\Omega}\rangle \tag{20}$$

demonstrating that the states in question have temporal stability. Thus we have established our goal of exhibiting coherent states with the required continuity and resolution of unity for the hydrogen atom, and which also exhibit temporal stability. Moreover, this goal has been realized for a multitude of possible coherent-state sets based on various choices of the weight $\rho(u)$.

Finally, we turn our attention to exhibiting the hydrogen atom coherent states—at least as much as possible—by way of their configuration-space representation. Recall the standard spherical-coordinate representation of hydrogen atom eigenstates $|n+1\ell m\rangle$ given [7] by

$$\langle r\theta\phi|n+1\ell m\rangle = u_{n+1}^{\ell}(r) Y_{\ell m}(\theta, \phi) \,. \tag{21}$$

Here u_{n+1}^{ℓ} denotes the usual radial hydrogen atom eigenfunctions, while $Y_{\ell m}$ are the standard angular momentum eigenfunctions. In turn,

$$\langle r\theta\phi|n, \overline{\Omega}\rangle \equiv \sum_{\ell=0}^{n} u_{n+1}^{\ell}(r) \sum_{m=-\ell}^{\ell} \left[\frac{(2\ell)!}{(\ell+m)!(\ell-m)!}\right]^{\frac{1}{2}} \left(\sin\frac{\overline{\theta}}{2}\right)^{\ell-m} \left(\cos\frac{\overline{\theta}}{2}\right)^{\ell+m} \times \mathrm{e}^{-\mathrm{i}(m\overline{\phi}+\ell\overline{\psi})} Y_{\ell m}(\theta, \phi)\sqrt{2\ell+1}\,. \tag{22}$$

Finally

$$\langle r\theta\phi|s, \gamma, \overline{\Omega}\rangle = M(s^2) \sum_{n=0}^{\infty} (s^n \mathrm{e}^{\mathrm{i}\gamma/(n+1)^2} / \sqrt{\rho_n}\,) \times \sum_{\ell=0}^{n} u_{n+1}^{\ell}(r) \sum_{m=-\ell}^{\ell} \left[\frac{(2\ell)!}{(\ell+m)!(\ell-m)!}\right]^{\frac{1}{2}} \left(\sin\frac{\overline{\theta}}{2}\right)^{\ell-m} \left(\cos\frac{\overline{\theta}}{2}\right)^{\ell+m} \times \mathrm{e}^{-\mathrm{i}(m\overline{\phi}+\ell\overline{\psi})} Y_{\ell m}(\theta, \phi)\sqrt{2\ell+1}\,. \tag{23}$$

Furthermore, in units where $\omega = 1$, the radial eigenfunctions are given by

$$u_{n+1}^{\ell} = N_{n+1}^{\ell}[2r/(n+1)]^{\ell} F(-n+\ell, 2\ell+2, 2r/(n+1))\mathrm{e}^{-r/(n+1)} \tag{24}$$

where

$$N_{n+1}^{\ell} \equiv \frac{1}{(2\ell+1)!}\sqrt{\frac{(n+\ell+1)!}{2(n+1)(n-\ell)!}}\left(\frac{2}{n+1}\right)^{\frac{3}{2}} \tag{25}$$

and

$$F(-n+\ell, 2\ell+2, z) = 1 + \frac{(\ell-n)}{(2\ell+2)}\frac{z}{1!} + \frac{(\ell-n)(\ell-n+1)}{(2\ell+2)(2\ell+3)}\frac{z^2}{2!} + \frac{(\ell-n)(\ell-n+1)(\ell-n+2)}{(2\ell+2)(2\ell+3)(2\ell+4)}\frac{z^3}{3!} + \cdots \tag{26}$$

which has a last non-vanishing coefficient for $z^{n-\ell}$.

Armed with this coordinate-space representation of the coherent states one may, if desired, begin to choose an 'optimal' weight function ρ, e.g. by minimizing the uncertainty product for $\langle(r-\langle r\rangle)^2\rangle\langle(p_r-\langle p_r\rangle)^2\rangle$ for given values of s and γ, etc. Since different problems may well require different, problem-specific optimizations, we shall not pursue this question further. Instead we conclude by making explicit one example of hydrogen atom coherent states, namely, those with $\rho_n = n!$, $n \geqslant 0$. In that case

$$\langle r\theta\phi|s,\gamma,\overline{\Omega}\rangle = \mathrm{e}^{-s^2/2}\sum_{n=0}^{\infty}(s^n \mathrm{e}^{\mathrm{i}\gamma/(n+1)^2}/\sqrt{n!}\,) \times \sum_{\ell=0}^{n} u_{n+1}^{\ell}(r)\sum_{m=-\ell}^{\ell}\left[\frac{(2\ell)!}{(\ell+m)!(\ell-m)!}\right]^{\frac{1}{2}}\left(\sin\frac{\overline{\theta}}{2}\right)^{\ell-m}\left(\cos\frac{\overline{\theta}}{2}\right)^{\ell+m} \times \mathrm{e}^{-\mathrm{i}(m\overline{\phi}+\ell\overline{\psi})}Y_{\ell m}(\theta,\phi)\sqrt{2\ell+1}\,. \tag{27}$$

We re-emphasize that the coherent states we have introduced only span the bound state subspace of the hydrogen atom. Therefore, it follows that

$$\langle r\theta\phi|r'\theta'\phi'\rangle \neq \int \langle r\theta\phi|s,\gamma,\overline{\Omega}\rangle\langle s,\gamma,\overline{\Omega}|r'\theta'\phi'\rangle\,\mathrm{d}\nu(s,\gamma)\,\mathrm{d}\overline{\Omega}\,. \tag{28}$$

6. Summary

In equation (23), and more specifically in (27), we propose a set of coherent states appropriate to the bound state portion of the hydrogen atom. In the definition adopted, these states involve five real parameters, namely s, γ, and $\overline{\Omega} = (\overline{\theta}, \overline{\phi}, \overline{\psi})$. The coherent states (i) are continuous in these five parameters, (ii) admit a resolution of unity, equation (18), as a positive integral over one-dimensional projection operators, and (iii) evolve into one another under time evolution with the Hamiltonian of the bound-state hydrogen atom, equation (20). There is some arbitrariness in the definition in (23) that would permit optimization of some additional feature(s) of the coherent states.

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