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LETTER TO THE EDITOR

Dispersion of Klauder's temporally stable coherent states for the hydrogen atomPaolo Bellomo[†] and C R Stroud JrRochester Theory Center for Optical Science and Engineering and The Institute of Optics,
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Abstract. We study the dispersion of the 'temporally stable' coherent states for the hydrogen atom introduced by Klauder. These are states which under temporal evolution by the hydrogen atom Hamiltonian retain their coherence properties. We show that in the hydrogen atom such wavepackets do not move quasiclassically; i.e. they do not follow, with no or little dispersion, the Keplerian orbits of the classical electron. The poor quantum–classical correspondence does not improve in the semiclassical limit.

1. Temporally stable coherent states for the hydrogen atom

Recently accurate experimental results have generated renewed interest [1–13] in a long standing problem of quantum physics, which was addressed, albeit unsuccessfully, in 1926 by Schrödinger [14]: that is the problem of constructing localized, non-spreading wavepackets in the hydrogen atom which travel along the classical trajectories (Keplerian ellipses) of the electron. A partial solution to the problem has only been found recently [3–5], in the form of wavepackets which are superpositions of coherent states of the angular momentum [15] and minimize quantum fluctuations, confining the bound electron (for high quantum numbers) to a Keplerian ellipse. Such wavepackets, however, do not remain localized in the angular variable and spread along the classical ellipse. Eventually they display interference fringes as the front of the packet catches up with its tail, and finally they also show quantum revivals and super-revivals [1–3, 16, 17].

More recently, two alternative solutions to this fundamental problem have been proposed by Klauder [18] and Majumdar and Sharatchandra [19], who modelled the properties of their coherent states for the hydrogen atom on those of the more familiar coherent states for the harmonic oscillator [20]. More precisely, those authors constructed states which enjoy the property of *temporal stability* [18]. Under the action of the harmonic propagator a coherent state for the harmonic oscillator remains a coherent state; by a judicious choice of the coefficients in the expansion over the eigenstates of the hydrogen atom Hamiltonian, Klauder [18] and also Majumdar and Sharatchandra [19] constructed wavepackets which satisfy exactly the same property (i.e. temporal stability) retaining their 'coherence' under the action of the hydrogenic propagator. This is done by extending the parameter space of the wavepacket from the polar coordinates r, θ where $0 \leq r < \infty$, $-\pi < \theta \leq \pi$, to their covering space, namely the domain $0 \leq r < \infty$, $-\infty < \theta < \infty$, with an appropriately

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modified measure, which is identical to the classical phase space measure [18, 19]. In this new space the temporally stable coherent states are parametrized continuously and also admit a resolution of unity (limited to the bound part of the spectrum), very much like the coherent states for the harmonic oscillator.

However, in the case of the hydrogen atom, the question of the relation between quasiclassical dynamics and the temporal stability of coherent states remained unanswered. The harmonic spectrum, with its equally spaced levels, occupies a very special place in physics (for example, its spacings distribution is not Poissonian [21], in contrast with most other integrable systems) and therefore it is not obvious that temporal stability is equivalent to quasiclassical dynamics also in the case of the hydrogenic spectrum. In fact, in this letter we study precisely the dynamical properties of temporally stable coherent states for the hydrogen atom, and we find that they *do not move along classical Keplerian ellipses with little or no dispersion*. We also demonstrate that in the semiclassical limit the poor correspondence between the dynamics of temporally stable states and classical orbits does not improve. Therefore, the well known wavepackets which confine the electron on a Kepler ellipse [3–5], but not in the angular variable, remain the most accurate solution to the problem of non-spreading wavepackets in the hydrogen atom.

2. The autocorrelation function

The most natural way to study the dynamics of any quantum state is to solve the time-dependent Schrödinger equation and actually observe the time evolution of the state. In principle this is particularly simple if the projections of the state on the eigenstates of the Hamiltonian are known exactly. Unfortunately, in the hydrogen atom each eigenenergy corresponds to a very large manifold of degenerate eigenstates, and the actual calculation of the temporal evolution of a wavepacket which spans several (in principle infinitely many) high-energy eigenstates becomes computationally overwhelming.

However, there is an alternative way to extract information about the dynamics of a wavepacket $|\phi\rangle$, and that is to calculate its autocorrelation function, which in atomic units (which we use throughout this paper) is defined as [4, 22]:

$$C(t) = |\langle \phi | \exp^{-i\hat{H}t} | \phi \rangle|^2. \quad (1)$$

The autocorrelation function carries information about when and how a state returns to its original configuration; this is precisely the information necessary to determine whether temporal stability warrants quasiclassical dynamics in the hydrogen atom as it does in the harmonic oscillator. The classical dynamics of the hydrogen atom is obviously periodic and a normalized wavepacket which travels along a Keplerian ellipse with little or no dispersion yields an autocorrelation function which returns to 1 (i.e. its maximum value), or very close to 1, at every Kepler period [4]. We study the autocorrelation function of temporally stable coherent states (we discuss here the states proposed by Klauder [18], and study the particulars of a similar proposal by Majumdar and Sharatchandra [19] elsewhere [23]), and we demonstrate that in the hydrogen atom temporal stability is not equivalent to quasiclassical dynamics.

The expansion of temporally stable states on the hydrogenic eigenbasis reads [18]:

$$|s\gamma\bar{\Omega}\rangle = e^{-s^2/2} \sum_{n=1}^{\infty} \frac{s^{n-1} e^{i\gamma/n^2}}{\sqrt{(n-1)!}} |n\bar{\Omega}\rangle \quad (2)$$

where s , γ and $\bar{\Omega} = (\bar{\theta}, \bar{\phi}, \bar{\psi})$ are continuous parameters and the states $|n\bar{\Omega}\rangle$ are defined

as [18]:

$$|n\bar{\Omega}\rangle = \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} \left[\frac{(2\ell+1)!}{(\ell+m)!(\ell-m)!} \right]^{\frac{1}{2}} \left(\sin \frac{\bar{\theta}}{2} \right)^{\ell-m} \left(\cos \frac{\bar{\theta}}{2} \right)^{\ell+m} e^{i(m\bar{\phi}+\ell\bar{\psi})} |n\ell m\rangle. \quad (3)$$

The states $|n\bar{\Omega}\rangle$ are normalized to the degeneracy of the hydrogenic n -manifold:

$$\langle n\bar{\Omega}|n'\bar{\Omega}\rangle = \delta_{n,n'} \sum_{\ell=0}^{n-1} (2\ell+1) \sum_{m=-\ell}^{\ell} \frac{(2\ell)!}{(\ell+m)!(\ell-m)!} \left(\sin^2 \frac{\bar{\theta}}{2} \right)^{\ell-m} \left(\cos^2 \frac{\bar{\theta}}{2} \right)^{\ell+m} \quad (4)$$

and setting $k = \ell + m$ one obtains:

$$\begin{aligned} \langle n\bar{\Omega}|n'\bar{\Omega}\rangle &= \delta_{n,n'} \sum_{\ell=0}^{n-1} (2\ell+1) \sum_{k=0}^{2\ell} \frac{(2\ell)!}{k!(2\ell-k)!} \left(\sin^2 \frac{\bar{\theta}}{2} \right)^{2\ell-k} \left(\cos^2 \frac{\bar{\theta}}{2} \right)^k \\ &= \delta_{n,n'} \sum_{\ell=0}^{n-1} (2\ell+1) \left(\sin^2 \frac{\bar{\theta}}{2} + \cos^2 \frac{\bar{\theta}}{2} \right)^{2\ell} = n^2 \delta_{n,n'}. \end{aligned} \quad (5)$$

Therefore the normalization coefficient of the state in equation (2) is:

$$\langle s\gamma\bar{\Omega}|s\gamma\bar{\Omega}\rangle = e^{-s^2} \sum_{n=1}^{\infty} \frac{n^2 s^{2(n-1)}}{(n-1)!} = e^{-s^2} \left[\frac{\partial}{\partial (s^2)} s^2 \right]^2 e^{s^2} = (s^2 + 1)^2 + s^2 \quad (6)$$

where the square of the operator between brackets indicates that the operator must be applied twice.

We are now in the position to calculate the autocorrelation function of temporally stable coherent states:

$$C(t) = |\langle s\gamma\bar{\Omega} | \exp^{-i\hat{H}t} |s\gamma\bar{\Omega}\rangle|^2 = \frac{e^{-2s^2} \left| \sum_{n=1}^{\infty} \frac{n^2 s^{2(n-1)}}{(n-1)!} e^{it/2n^2} \right|^2}{[(s^2 + 1)^2 + s^2]^2}. \quad (7)$$

The sum in equation (7) can be evaluated numerically with great efficiency. Clearly, we evaluated a finite sum, however, only relatively few terms in the sum of equation (7) yield a non-negligible contribution. We only neglected terms which are $< 10^{-100}$, so that our results are an extremely accurate approximation. We also tested our results by repeating the calculations with increasingly stringent constraints on the terms to be neglected, and we did not notice any significant changes in the final results. In figure 1 we plot our results for two states; in figure 1(a) we show the autocorrelation function for a temporally stable state with $s = 5$, whereas in figure 1(b) we set $s = 20$. In both cases the dispersion of the wavepacket is very different from that of a quasiclassical packet, moving periodically and with little or no dispersion along a Kepler ellipse [4]. Surprisingly, the peaks of figure 1(a), which imply at least some partial recurrences on part of the temporally stable wavepacket, disappear almost completely in figure 1(b), where one would expect the wavepacket to behave more classically, as we explain next.

The coefficients of the sum in equation (7) are (including normalization):

$$c_n = \frac{n^2 s^{2(n-1)}}{(n-1)! [(s^2 + 1)^2 + s^2]} \quad (8)$$

and are determined by the constraint that the integration over the parameter space yields a resolution of the unity for the bound part of the spectrum [18]. Although the c_n 's are not exactly Poissonian they still enjoy to a good approximation many properties of the Poisson distribution. For example, they satisfy the following recursion relation:

$$c_{n+1} = \frac{(n+1)^2}{n^3} s^2 c_n \quad (9)$$

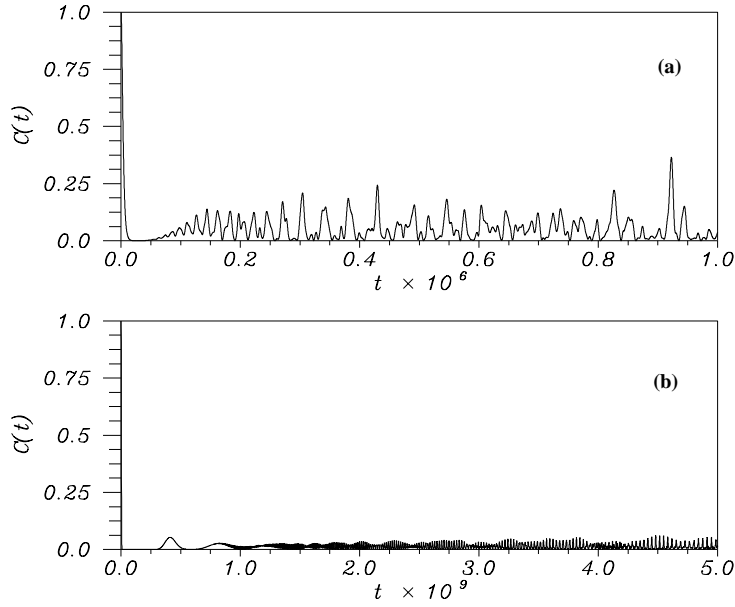


Figure 1. The autocorrelation function for temporally stable coherent states: in (a) we set $s = 5$ and in (b) we set $s = 20$. The small recurrence peaks of (a) essentially disappear in (b), i.e. for a wavepacket with a much larger average principal quantum number.

and the distribution is centred around a principal quantum number \bar{n} such that:

$$\frac{(\bar{n} + 1)^2}{\bar{n}^3} s^2 = 1 \Rightarrow \bar{n} \approx s^2. \quad (10)$$

Therefore the results of figures 1(a) and 1(b) refer to wavepackets in which the eigenstate carrying the largest weight has a principal quantum number of $\bar{n} \approx 25$ and $\bar{n} \approx 400$ respectively. Therefore one would expect a closer quantum–classical correspondence in the second wavepacket, whereas the evaluation of the autocorrelation function yields exactly the opposite result. This unexpected finding can be understood by further studying the properties of the coefficients c_n , and in figures 2(a) and 2(b) we plot the natural logarithm of the most significant coefficients (times the e^{-2s^2} factor) in the expansion of equation (7) for the states of figure 1. In the state centred around $\bar{n} \approx 25$ only ~ 100 states offer a significant contribution, whereas in the second state ($\bar{n} \approx 400$) one needs ~ 600 states. Similar results hold for all our other extensive calculations and the explanation is that in the limit $s^2 \gg 1$ the variance of the distribution of the coefficients c_n approaches the Poissonian limit:

$$\langle n^2 \rangle - \langle n \rangle^2 = \frac{e^{-s^2} \left(\frac{\partial}{\partial (s^2)} s^2 \right)^4 e^{s^2}}{(s^2 + 1)^2 + s^2} - \left[\frac{e^{-s^2} \left(\frac{\partial}{\partial (s^2)} s^2 \right)^3 e^{s^2}}{(s^2 + 1)^2 + s^2} \right]^2 = s^2 + 6 + \mathcal{O}\left(\frac{1}{s^2}\right). \quad (11)$$

Therefore in the semiclassical limit temporally stable coherent states involve an ever increasing number of hydrogenic n -manifolds, which prevent an accurate equivalence between the dynamics of wavepackets and classical trajectories.

More precisely, the separation of two hydrogenic energy levels with quantum numbers

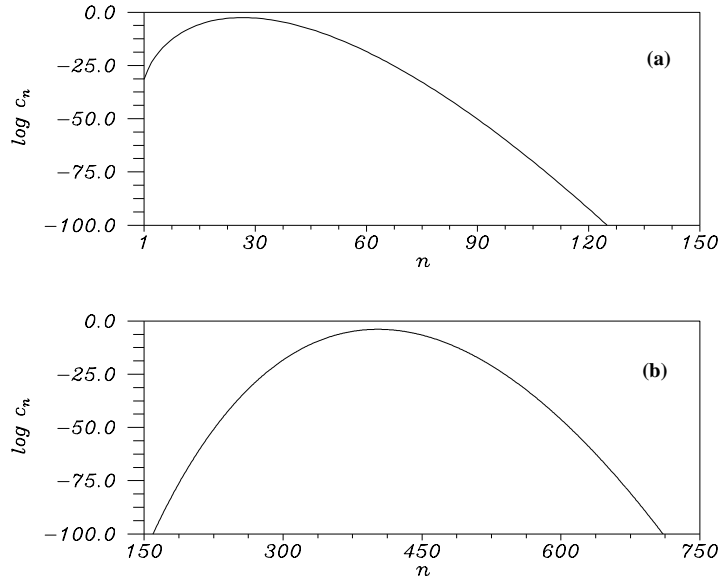


Figure 2. The natural logarithm of the coefficients of the autocorrelation function. In (a) we set $s = 5$ and in (b) we set $s = 20$. For a larger s more states yield a non-negligible contribution to the dynamics of the wavepacket.

$\bar{n} \approx s^2 \gg 1$ and $n = \bar{n} + \Delta$ is:

$$E_n - E_{\bar{n}} = \frac{2\bar{n}\Delta + \Delta^2}{2\bar{n}^2n^2} = \Delta \frac{1}{\bar{n}^3} - \frac{3\Delta^2}{2\bar{n}} \frac{1}{\bar{n}^3} + O\left(\frac{\Delta^3}{\bar{n}^2}\right) \frac{1}{\bar{n}^3}. \quad (12)$$

For a narrowly peaked distribution, and in the semiclassical limit the hydrogenic spectrum is approximately harmonic. That is, the spacings between adjacent energy levels are well approximated by an integer multiple of a fundamental frequency (i.e. $1/\bar{n}^3$), which is the Kepler frequency of the eigenstate at the centre of the expansion. That is why it is possible to construct wavepackets which follow classical trajectories with little dispersion for at least a few Kepler periods [3–5]. However, for temporally stable coherent states in the semiclassical limit the distribution over the eigenmanifolds becomes flatter, and the anharmonic corrections of equation (12) *cannot be neglected*. For example, any term in the autocorrelation function with $n = \bar{n} + \Delta$ and $\Delta \approx \sqrt{\bar{n}/3}$ is well within the root mean square deviation of the distribution (i.e. $\sqrt{\bar{n}}$) and yet after a period $T = 2\pi\bar{n}^3$ is already $\approx 180^\circ$ out of phase with the \bar{n} -term. Therefore recurrences and even quasirecurrences become impossible for timescales comparable with the average Kepler period of the wavepacket.

3. Conclusions

In this paper we have studied the dispersive properties of Klauder's temporally stable coherent states for the hydrogen atom by calculating their autocorrelation function. We have found that in the hydrogen atom (in contrast to the harmonic oscillator) temporally stable wavepackets do not follow the trajectories of the classical electron remaining well localized; instead they spread significantly even within a Kepler period. Such poor quantum-classical equivalence does not improve in the semiclassical limit, i.e. when the expansion of the wavepacket is dominated by high-energy eigenstates. The explanation of this surprising

result resides in the properties of the distribution over the eigenmanifolds of the hydrogen atom, which in the semiclassical limit approaches a Poisson distribution. For large quantum numbers the variance of the distribution is also very large, and the anharmonic corrections dominate the dynamics, so that full or even partial recurrences become impossible.

In the harmonic oscillator temporal stability, coherence and quasiclassical dynamics are all properties of the same set of states: this is not true in the hydrogen atom, and therefore one should always state clearly the specific properties that a set of atomic 'coherent states' satisfies. In fact, in the hydrogen atom temporally stable coherent states are *not* a viable solution to the problem of finding non-spreading, quasiclassical wavepackets, and one has to resort either to wavepackets which remain localized only for a few Kepler periods [3–5] or to modified Hamiltonians [7–12] in which external fields bring about the desired localization of the wavepacket.

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