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# Comment on ‘‘Coherent states for the hydrogen atom’’

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Majumdar and Sharatchandra recently proposed a set of ‘‘coherent states’’ for the hydrogen atom [Phys. Rev. A **56**, R3322 (1997)]. These states satisfy some of the typical properties of coherent states, such as, for example, continuity in the parameters. The time evolution of these states is given by the classical evolution of the angle variables, and the expectation values of the quantum observables behave quasiclassically. However, those authors also claimed that, although one does not obtain exactly the same state after a Kepler period, the gross features of their wave packets do not change. We show that this is not correct, and that these wave packets do not remain localized on the classical variables, but spread rapidly over the Keplerian orbit. The localization properties of these states do not improve in the limit of large quantum numbers.
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In a recent paper Majumdar and Sharatchandra [1] (hereafter referenced as MS) offered a solution to a long-standing problem of modern physics [2], i.e., the construction of ‘‘coherent states for the hydrogen atom.’’ The properties of the coherent states for the harmonic oscillator are uniquely defined [3]: (i) coherent states are continuous in their label; (ii) they yield a resolution of unity; (iii) under time evolution a coherent state remains within the family of coherent states; (iv) coherent states are well localized (i.e., minimum uncertainty), *nonspreading* wave packets which are peaked on the classical coordinates. On the other hand, the properties of coherent states for atomic systems are not so clearly set, and in principle one should always spell out clearly what are the properties which a proposed set of atomic ‘‘coherent states’’ must satisfy.

In any case, MS [1] constructed states labeled by the classical phase-space variables which satisfy some of the properties which one expects of ‘‘coherent states;’’ i.e., they are continuous in the parameters and yield a resolution of the identity by integrating over the parameter space with the classical phase-space measure. The time evolution of these states is given by the classical evolution of the angle variables, and under time evolution a state of the set is mapped into another state within the same set. Moreover, these states yield quantum expectation values which approximately follow the corresponding classical variables.

However, MS also concluded that although one does not obtain exactly the same state after a period, the ‘‘gross features do not change’’ [1]. Furthermore, those authors claimed that asymptotically their wave packets are peaked around position, momenta, etc., corresponding to the action-angle variables labeling them, and also become minimum uncertainty states [1]. All these conclusions, however, appear to be incorrect.

The best way to study the properties of the states proposed by MS is visualizing the dynamics of those states, but in the limit of very large quantum numbers this is almost impossible because of the overwhelming number of basis states involved (the degeneracy of a hydrogenic manifold equals the square of its principal quantum number). However, the problem can still be addressed effectively by studying the autocorrelation function of the states proposed by MS. In atomic units ($\hbar=1$) the autocorrelation function of a state $|\psi\rangle$ is defined as [4]

$$C(t)=|\langle\psi|e^{-i\hat{H}t}|\psi\rangle|^2. \tag{1}$$

For a normalized wave packet moving along a Kepler orbit with no or little dispersion, $C(t)$ must return to a value close to one (i.e., its maximum value) every Kepler period, and therefore it is an optimal probe to test the dynamics of a wave packet when direct inspection of its properties is impossible.

Using Eq. (17) of Ref. [1], we evaluated the autocorrelation function of the states proposed by MS,

$$C(t)=\left|\sum_{n=1}^{\infty} e^{-R}\frac{R^{n-1}}{(n-1)!}e^{it/2n^2}\right|^2, \tag{2}$$

where $R$ is the parameter of the state corresponding to the total classical action and one has

$$\overline{n}\approx R, \tag{3}$$

where $\overline{n}$ is the principal quantum number which carries the largest weight in the expansion, and is approximately equal to the average principal quantum number of the state. We have relabeled the original sum of Ref. [1] in terms of the principal quantum number $n$, to make the Poissonian nature of the distribution more evident. The sum in Eq. (2) can be computed numerically with great efficiency up to times which are much longer than the expected Kepler period $T_K=2\pi R^3$. Obviously we evaluated a finite sum; however, we neglected only terms $<10^{-100}$, and therefore our results are an extremely accurate approximation to the exact sum. In Fig. 1 we show our results for $R=10$ and 200; there is no recurrence close to 1, and the peaks of the autocorrelation function become smaller for a larger $R$, as we also observed in many other extensive calculations.

Clearly, the results of Fig. 1 strongly indicate that the wave packets constructed by MS [1] *do not travel along Keplerian orbits with no or little dispersion* and most im-

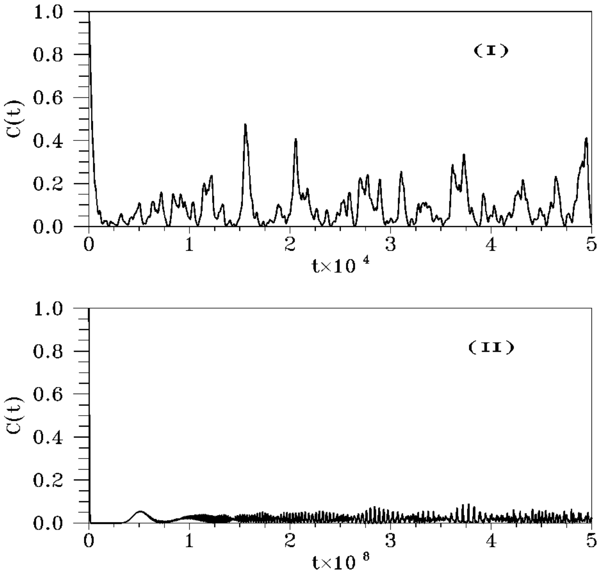

FIG. 1. The autocorrelation function or the coherent states of Ref. [1]: in panel (I) we set $R=10$ and in panel (II) we set $R=200$. In both cases the largest time considered is approximately equal to ten Kepler periods.

portantly the quantum-classical correspondence, i.e., the localization of the wave packets around the classical variables, does not improve in the semiclassical limit.

The properties of the autocorrelation function can be understood by considering the Poissonian nature of the distribution over the eigenstates of the hydrogen atom. As $R$ grows larger, the distribution is peaked (but not sharply) around a large principal quantum number $\overline{n}\approx R$, but the variance of the distribution is also equal to $R$ [5], which is a large number. Therefore as one approaches the semiclassical limit the distribution over the hydrogenic eigenmanifolds becomes increasingly flatter. It is well known that in the hydrogen atom, and for a distribution centered around a principal quantum number $\overline{n}$, the deviations from the harmonic spectrum are proportional to $(n-\overline{n})^2$ [4,6] so that a Poissonian distribution yields an ever-increasing number of anharmonic frequencies which carry a non-negligible weight. A purely harmonic spectrum permits the construction of quasiclassical, nonspreading wave packets [2,3] by using a Poissonian superposition of energy eigenstates: in the hydrogen atom the deviations from the harmonic spectrum are non-negligible and recurrences or quasirecurrences for times comparable to the Kepler period become impossible.

Note that the vanishing of the autocorrelation function does not necessarily imply the spreading of the wave packet. In principle, after a Kepler period the wave packet could come back to its original location still being sharply localized, and yet it could also be orthogonal to its original copy (for example, consider two wave packets consisting of the same Gaussian envelope, but of a sine and cosine carrier wave, respectively). However, this is *not* the case for the states constructed by MS [1] and the vanishing of the autocorrelation function is due precisely to the ultrafast spreading of their wave packets, as we demonstrate next.

We start from Eq. (9) of Ref. [1], which gives the states proposed by MS $|\psi(0)\rangle$ at time $t=0$:

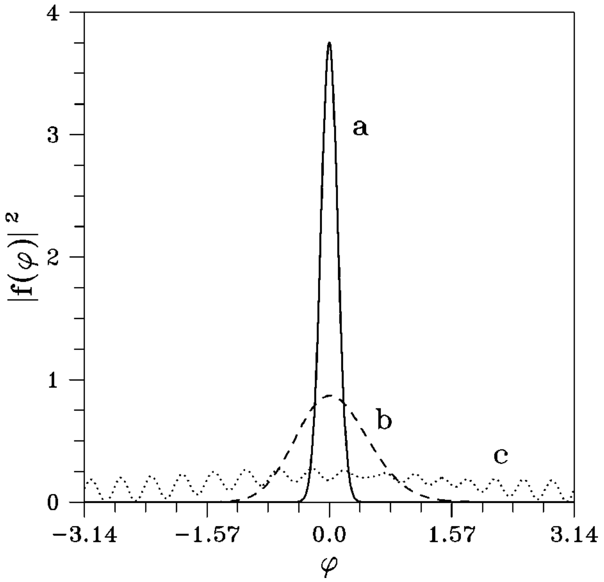

FIG. 2. The reduced wave packet for $R=200$ and with $\overline{r}=R(R-1)$ and $\overline{\theta}=\pi/2$. Line *a*—continuous—shows the reduced wave packet at time $t=0$; line *b*—dashed—shows the same wave packet after a Kepler period; line *c*—dotted—shows the reduced wave packet after four Kepler periods, and the reduced state has completely spread along the orbit.

$$|\psi(0)\rangle=\sum_n C_n(R)e^{-\imath\omega_1\hat{J}_z}e^{-\imath\omega_4\hat{J}_y}e^{-\imath\omega_2\hat{J}_z}$$
$$\times e^{-\imath\omega_5\hat{a}_y}e^{\imath\omega_3R^3/2n^2}|n,n-1,n-1\rangle, \qquad (4)$$

where $C_n(R)$ is the Poissonian weight, the $\hat{J}_i$'s are components of the angular momentum operator, and we have used the more standard notation $\hat{a}_y$ for the $y$ component of the scaled Runge-Lenz vector operator; finally the $|n,n-1,n-1\rangle$'s are the usual circular eigenstates of the hydrogen atom.

The first three exponentials are nothing other than an Euler rotation, and because the hydrogenic Hamiltonian is spherically symmetric one can set $\omega_1=\omega_4=\omega_2=0$ without loss of generality. Also, it is easy to see that the factor $\omega_3R^3$ in the last exponential is just equivalent to an initial time $t_0$, and one can also set $\omega_3=0$ again without loss of generality. Therefore, the states proposed by MS are just a Poissonian superposition of elliptic states [7,8]. The idea of constructing localized wave packets in the hydrogen atom by a superposition of elliptic states is not new [8]. Nauenberg did it by using a Gaussian distribution over the eigenmanifolds, and his wave packets slowly spread within a few Kepler periods [8,4].

In any case, one can further analyze the states constructed by MS [1] by setting $\omega_5=0$, i.e., by considering a wave packet moving along a circular orbit, which greatly reduces the complexity of the problem because only one eigenstate per eigenmanifold is needed. Moreover, in a circular orbit the dynamics is confined to the azimuthal angle $\phi$, and one can further reduce the problem by choosing particular values for the radial coordinate and the polar angle. That is, one can define a one-dimensional ''reduced'' wave function as follows:

$$f(\phi,t)=\psi(\overline{r},\overline{\theta},\phi,t)=\sqrt{\frac{1}{N}}\sum_n e^{-(R/2+\overline{r}/n)}\sqrt{\frac{(R\overline{r^2}\sin^2\overline{\theta})^{n-1}}{\pi n^{2n-1}(n!)^3}}e^{\imath(n-1)\phi-\imath E_n t}, \tag{5}$$

where we have used the usual coordinate representation of the spherical eigenstates of the hydrogen atom [9] and where $N$ is a normalization coefficient:

$$N=\int_0^{2\pi}|f(\phi,t)|^2 d\phi=2\sum_n e^{-(R+2\overline{r}/n)}\frac{(R\overline{r^2}\sin^2\overline{\theta})^{n-1}}{n^{2n-1}(n!)^3}. \tag{6}$$

The circular eigenstates of the hydrogen atom are well localized in the $xy$ plane, and so we set $\overline{\theta}=\pi/2$. Moreover, it is easy to show that

$$\frac{d\mathcal{R}_{n,n-1}}{dr}=0\Leftrightarrow r=n(n-1), \tag{7}$$

that is, the radial wave function $\mathcal{R}_{n,n-1}$ of a circular eigenstate with principal quantum number $n$ is peaked at $r=n(n-1)$. The eigenstate which carries the largest weight in the Poissonian distribution has $n=\overline{n}\approx R$, and therefore we set $\overline{r}=R(R-1)$.

We present the results of our calculations for $R=200$ in Fig. 2, where we plot the magnitude of $f(\phi,t)$ at three different times. Line $a$—continuous—shows the sharply peaked reduced wave packet at the initial time ($t=0$); line $b$—dashed—shows the same wave packet after a Kepler period ($t=2\pi R^3$); finally, line $c$—dotted—shows the reduced wave packet after four Kepler periods ($t=8\pi R^3$). Clearly, the reduced wave packet spreads very rapidly, and after just a Kepler period its height has decreased to $\approx 20\%$ of its original value. We have carried out several other calculations for increasing values of $R$, and the ratio of the height of the initial reduced wave packet to its copy after a Kepler period remains the same as in Fig. 2. Most importantly, after only four Kepler periods the reduced wave packet has spread completely along the orbit, and it does not show any remnant of quasiclassical localization.

However, the spreading of the whole wave packet proposed by MS [1] is actually *much faster* than it appears from Fig. 2. This can be easily understood by considering the same reduced wave function as before, but with a different value of $\overline{r}$, as we explain next.

Choosing a different $\overline{r}$ means evaluating the whole wave packet at a new radial coordinate, which maximizes the radial amplitude $\mathcal{R}_{n,n-1}$ of an eigenstate with $n\neq\overline{n}$. At the same time, the radial wave function of the state $|\overline{n},\overline{n}-1,\overline{n}-1\rangle$ (the state at the center of the Poissonian distribution) can be very small when is evaluated at the new $\overline{r}$. The choice of a different $\overline{r}$ is then equivalent to skewing the Poissonian distribution in favor of a principal quantum number smaller (or larger) than $\overline{n}$. Therefore, the new reduced wave packet will oscillate with a period which may be significantly different from the Kepler period of the whole state, as we illustrate very clearly in Fig. 3.

In panel (I) we set $R=200$ and $\overline{r}=0.9R(R-1)$, and compute the evolution of the new reduced state. Line $a$—continuous—shows the new reduced wave packet at $t=0$, and line $b$—dashed—shows the same wave packet after a Kepler period ($t=2\pi R^3$, i.e., the Kepler period of the whole state proposed by MS). The new wave packet spreads as expected; moreover, its distribution over the quantum numbers is centered on $n_1<\overline{n}$, and so the new wave packet oscillates with a shorter period. Therefore after a Kepler period not only the new wave packet has completed a full oscillation, but it has also gone further, moving beyond its original location. In panel (II) we show the same for a state with $\overline{r}=1.1R(R-1)$, that is, a reduced state with a longer period: line $c$—continuous—shows the wave packet at $t=0$, and line $d$—dashed—shows the wave packet after a Kepler period. The reduced state spreads as expected, but it has not completed a full oscillation and has not returned yet to its original location.

Because of the Poissonian distribution over the eigenmanifolds, the whole wave packet proposed by MS [1] is not sharply peaked in the radial direction. Indeed, using well-known results for the expectation values of $r$ and $r^2$ over circular states of the hydrogen atom [10], it is easy to show that

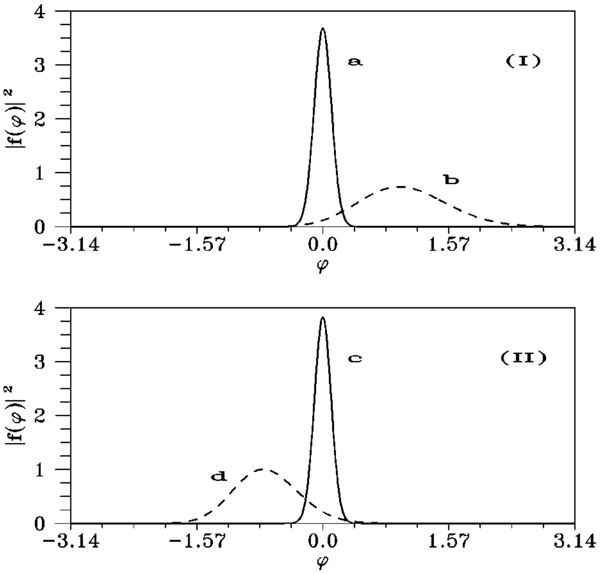

FIG. 3. The reduced wave packet for $R=200$, with $\overline{\theta}=\pi/2$ and two different choices for $\overline{r}$. In panel (I) we set $\overline{r}=0.9R(R-1)$, and the period of the reduced packet is shorter than the Kepler period of the whole state. After a Kepler period (line $b$—dashed) the reduced packet has already moved beyond its original location (line $a$—continuous). In panel (II) we set $\overline{r}=1.1R(R-1)$, which implies a longer period. After a Kepler period (line $d$—dashed) the reduced packet has not returned yet to its original location (line $c$—continuous).

$$\langle\psi|r^2|\psi\rangle-\langle\psi|r|\psi\rangle^2=\frac{9}{2}R^3\left[1+O\left(\frac{1}{R}\right)\right]. \tag{8}$$

Therefore reduced states like the ones in Fig. 3 constitute a significant part of the overall wave packet. This leads to a much faster spreading of the state than it appears from Fig 2, as it is well demonstrated by our calculations based on the autocorrelation function, which take automatically into account all the reduced states which make up the whole wave packet. Obviously, an identical argument holds also for different choices of $\overline{\theta}$.

Finally, although we have derived our analysis of reduced wave packets in the case of circular orbits, we can extend its results to all elliptic orbits, and so we can fully confirm our calculations based on the autocorrelation function, which are general and do not depend on the eccentricity of the orbit. More precisely, the Runge-Lenz vector commutes with the hydrogenic Hamiltonian, and one is free to apply first the hydrogenic propagator, and second the pseudorotation operator which maps circular states into elliptic states of arbitrary eccentricity. It is well known [7,8] that such an operator does not bring about any localization, although the amplitude of an elliptic state is somewhat larger at the aphelion, reflecting the longer time which the classical electron spends away from the nucleus. Therefore wave packets which have spread along a circular orbit, like the ones proposed by MS [1], will be mapped into wave packets which are spread along the desired Keplerian ellipse.

In conclusion we have shown that the ‘‘coherent states for the hydrogen atom’’ which were recently proposed by MS [1] are not sharply localized wave packets which move along the classical trajectories with no or little dispersion, as the more familiar coherent states of the harmonic oscillator do. The states constructed by MS [1] do possess some of the properties which one typically expects of coherent states: that is, they are continuous in the parameter, yield a resolution of the unity, and under time evolution a state of the set is mapped into another state within the same set. Also, they yield quantum expectation values which approximately follow their classical counterparts. However, these states are *not* quasiclassical, nonspreading wave packets, and the claim by MS that after a Kepler period ‘‘the gross features [of the wave packet] do not change’’ [1] is incorrect, because such wave packets do spread almost immediately, and their localization properties change dramatically even over a single Kepler period. Also, the ultrafast spreading of these wave packets means that soon the wave packets are not peaked on the classical variables in any physically significant way, and therefore they cannot remain minimum uncertainty states.

The reason for the breakdown of the classical-quantum correspondence (in the sense of minimum uncertainty localization of the wave packet around the classical variables) is due to the choice of a Poissonian distribution over the energy levels. In the semiclassical limit the Poissonian distribution becomes increasingly flatter, and the anharmonic corrections of the hydrogenic spectrum (which scale with the variance of the distribution, not its root-mean-square deviation) remain non-negligible, and therefore these wave packets spread rapidly also in the regime of ultralarge principal quantum numbers.

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[1] P. Majumdar and H. S. Sharatchandra, Phys. Rev. A **56**, R3322 (1997).

[2] E. Schrödinger, Naturwissenschaften **14**, 664 (1926).

[3] J. R. Klauder and B. S. Skagerstam, *Coherent States* (World Scientific, Singapore, 1985).

[4] M. Nauenberg, J. Phys. B **23**, L385 (1990).

[5] A. Rényi, *Probability Theory* (North-Holland, Amsterdam, 1970).

[6] P. Bellomo and C. R. Stroud, Jr., J. Phys. A. **31**, L445 (1998).

[7] J. C. Gay, D. Delande, and A. Bommier, Phys. Rev. A **39**, 6587 (1989).

[8] M. Nauenberg, Phys. Rev. A **40**, 1133 (1989).

[9] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electrons Atoms* (Plenum, New York, 1977).

[10] T. F. Gallagher, *Rydberg Atoms* (Cambridge University Press, Cambridge, 1994).