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Large quantum-number states and the correspondence principle

G. G. Cabrera
Instituto de Física "Gleb Wataghin," Universidade Estadual de Campinas (UNICAMP), 13.081 Campinas, São Paulo, São Paulo, Brazil

Miguel Kiwi
Facultad de Física, Universidad Católica, Casilla 6177, Santiago 22, Chile
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The large principal-quantum-number limit is investigated. Several concrete examples are worked out and the correspondence principle is reexamined under the light shed by these calculations. In particular, it is shown that a simple linear combination of three one-dimensional harmonic-oscillator eigenstates leads to results at variance with classical physics, in the high quantum-number limit. The possibility of actually observing these phenomena is also briefly discussed.

I. INTRODUCTION

The first statement of the correspondence principle can be traced to Max Planck.[1] In 1906, he inferred, from his radiation law, that in the $h \rightarrow 0$ limit classical physics is rederived. In fact, in this limit Planck's result reduces to the Rayleigh-Jeans Law.

The connection between classical and quantum physics is precisely the objective of the correspondence principle. However, intriguing problems remain unsettled in connection with it, in spite of the elapsed time and the interest and attention attracted by the subject. Moreover, the assertation that quantum mechanics reduces to classical mechanics in the large quantum-number limit, which is found in most textbooks, does not hold in general.

The degree of acceptance of the correspondence principle is well illustrated by the evolution of popular quantum-mechanics textbooks. Schiff[2] in 1955, when examining the probability density associated with the harmonic oscillator (HO), concludes that, "The agreement between classical and quantum probability densities improves rapidly with increasing *n*." In 1977, Cohen-Tannoudji, Diu, and Laloe[3] commenting on the same evidence say, "In a stationary state $|n\rangle$, the behavior of a harmonic oscillator is totally different from that predicted by classical mechanics, even if *n* is very large." More recently, Segre,[4] in 1980, states that the correspondence principle,"... is most useful as a guide to intuition, but it cannot be formulated rigorously.... Rather, it may be described, with some exaggeration, as a way of saying: Bohr would have proceeded in this way."

Close examination of the correspondence principle has attracted renewed interest during the last few years. Home and Sengupta[5] constructed a superposition of odd- and even-parity eigenfunctions of a one-dimensional modified Coulomb potential which leads to inconsistency with classical mechanics. Liboff[6] probed in depth the relation between the $h \rightarrow 0$ and $n \rightarrow \infty$ limits, showing that they are not universally equivalent. More recently, Bohm and Hiley,[7] in a profound study of the connection between quantum realism and macroscopic levels, emphasized that "high quantum numbers are not a universally valid criterion for the classical limit." In spite of this evolution, we can find, in as recent a publication[8] as a 1987 Letter, the following opening statement: "Bohr's correspondence principle indicates that the classical description of a physical system is adequate in the limit of large quantum number." We will show below that this is not always the case.

In this contribution we show that it is not necessary to look for elaborate special cases to illustrate the statements mentioned above. We construct a simple superposition of a few eigenstates of the ordinary one-dimensional harmonic oscillator (HO) and employ it to investigate the large quantum-number limit. This way we obtain, in a very direct and transparent fashion, an insight into how quantum effects persist for arbitrarily large values of the principal quantum number. These results are contrasted with classically expected values.

This contribution is organized as follows: after the Introduction, Sec. II contains the explicit presentation of calculations and results. In Sec. III these results are analyzed in the light of their possible experimental observation. Conclusions are drawn to close this paper.

II. CALCULATIONS AND RESULTS

We now carry out explicit calculations to evaluate a few representative physical objects: the probability density $\rho(x,t)$, the spatial correlation function, and the density matrix. Since our main concern is the large quantum-number limit we do compare our results with their classical analogs, whenever feasible.

A. Probability density

In classical mechanics the probability density is given by $\rho(x) = N/v(x)$, where v is the speed and N a normalization constant. For the HO it yields $\rho(x) = 1/[\pi(A^2 - x^2)^{1/2}]$, where $A = (2E/m^2)^{1/2}$ is the amplitude, E is the total energy, m the mass, and ω the angular frequency of the classical HO.

In quantum mechanics, ρ is directly related to the wave function $\psi(x,t)$, by $\rho(x,t) = |\psi(x,t)|^2$. The particular wave function one does consider is thus of paramount importance. If a semiclassical coherent[2] state $\psi(x,t) = \langle x \mid \alpha(t)\rangle$ is chosen, where

$$|\alpha(t)\rangle = \exp(-|\alpha|^2/2) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle , \qquad (1)$$

with $|n\rangle$ denoting an eigenstate of the one-dimensional HO and

$$\alpha(t) = (m\omega/2\hbar)^{1/2} A \exp[-i(\omega t - \phi)] ,$$

then the classical result is rederived for the *center* of the wave packet. This comes as no surprise when one recalls the motivation for constructing the quasiclassical coherent states.[2]

On the other hand, if pure eigenstates are used to evaluate the probability density for large quantum numbers, we obtain strong oscillations and many nodes displaying a highly nonclassical behavior.[6] For $n \gg 1$, the probability density can be approximated by the expression[9]

$$\rho_n(x) \cong \frac{2/\pi}{(A_n^2 - x^2)^{1/2}} \cos^2 \left[\frac{1}{2} \beta x (A_n^2 - x^2)^{1/2} + \frac{1}{2} \beta A_n^2 \sin\left(\frac{x}{A_n}\right) - \frac{\pi n}{2} \right] \qquad (2)$$

for $|x| < A_n$, where $\beta = m\omega/\hbar$ and $A_n^2 = (2n+1)/\beta$. The quantity A_n becomes the classical amplitude for $n \to \infty$. For large but finite n, $\rho_n(x)$ is not infinite at $x = A_n$, and it is not zero for $|x| > A_n$. Nodes are always present for arbitrarily large quantum numbers, and recovering of the classical result implies an average process in formula (2). We can justify this latter process arguing that macroscopic probes are insensitive over length scales of the order of several de Broglie wavelengths.

Nodes can be eliminated if we consider a linear superposition of eigenfunctions which are close in energy, as we show in our example below. But now results which are at variance with classical mechanics are obtained in the $n \to \infty$ limit, due to nonvanishing quantum coherence in the large quantum-number regime.

If we adopt a superposition of HO eigenstates with successive quantum numbers, $\{|n-1\rangle, |n\rangle, |n+1\rangle\}$, and form the following orthonormal basis set to span the pertinent three-dimensional Hilbert space:

$$|\eta_1\rangle = \frac{1}{\sqrt{3}} (|n-1\rangle + |n\rangle + |n+1\rangle) , \qquad (3a)$$

$$|\eta_2\rangle = \frac{-1}{2\sqrt{3}} [(1+i\sqrt{3})|n-1\rangle - 2|n\rangle + (1-i\sqrt{3})|n+1\rangle] , \qquad (3b)$$

$$|\eta_3\rangle = \frac{-1}{2\sqrt{3}} [(1-i\sqrt{3})|n-1\rangle - 2|n\rangle + (1+\sqrt{3})|n+1\rangle] , \qquad (3c)$$

then several interesting consequences do result. First, we notice the HO Hamiltonian $H = \hbar\omega(a^+a + \frac{1}{2})$ has the diagonal matrix elements

$$\langle \eta_1 | H | \eta_1 \rangle = \langle \eta_2 | H | \eta_2 \rangle = \langle \eta_3 | H | \eta_3 \rangle = E_n = (n + \tfrac{1}{2})\hbar\omega . \qquad (4)$$

Next, we observe that if at time $t=0$ the system is prepared in state $|\psi(0)\rangle = |\eta_1\rangle$, then

$$\left| \psi\left(mT + \frac{j-1}{3} T \right) \right\rangle = |\eta_j\rangle , \qquad (5)$$

where $m = 0, \pm 1, \pm 2, \pm 3, \ldots$ and $T = 2\pi/\omega$ is the *classical* period of the HO. Thus, the system is found every one-third of a period in one of the orthonormal states $\{|\eta_j\rangle\}$, no matter how large the value of the principal quantum-number n. The associated time evolution of the probability density $\rho(x,t)$ is displayed in Fig. 1. The persistency of quantum coherence, which originates in the equal spacing of the HO energy eigenstates, is completely independent of the quantum-number n and holds even in the $n \to \infty$ limit.

We note that the center of the wave packet for the time-dependent state

$$|\psi(t)\rangle = \frac{1}{\sqrt{3}} (e^{-iE_{n-1}t/\hbar} |n-1\rangle + e^{-iE_n t/\hbar} \times |n\rangle + e^{-iE_{n+1}t/\hbar} |n+1\rangle) \qquad (6)$$

performs harmonic oscillations with frequency ω, given by the formula

$$\langle x \rangle_{\psi(t)} = \frac{2}{3} \left(\frac{\hbar}{2m\omega} \right)^{1/2} (\sqrt{n} + \sqrt{n+1}) \cos\omega t , \qquad (7)$$

and the $n \to \infty$ limit yields $\langle x \rangle = \frac{2}{3} A \cos\omega t$, i.e., the amplitude of the oscillation for large quantum numbers is $\frac{2}{3}$ of the classical value.

B. Spatial correlations

Now we focus our attention on the spatial autocorrelation function $\langle x(t)x(0)\rangle$. Actually, in order to compare with classical physics we have to evaluate the symmetrized form

$$\chi(t) \equiv \tfrac{1}{2} \langle x(t)x(0) + x(0)x(t) \rangle ,$$

which is easily obtained and reads

$$\langle x(t)x(0)\rangle_{\rm Cl} = \frac{A^2}{2} \cos\omega t = \frac{E}{m\omega^2} \cos\omega t . \qquad (8)$$

This expression is derived either using the classical probability density, or through an average procedure over the ensemble of classical HO with the same energy and different phases.

As before, we also evaluate the correlation function using the coherent states of Eq. (1). After some algebra one obtains

$$\langle x(t)x(0)\rangle_\alpha = \frac{E_\alpha}{m\omega^2} \cos\omega t + \frac{\hbar}{m\omega} \times {\rm Re}(\alpha^2 e^{-i\omega t}) - \frac{i\hbar}{m\omega} \sin\omega t , \qquad (9)$$

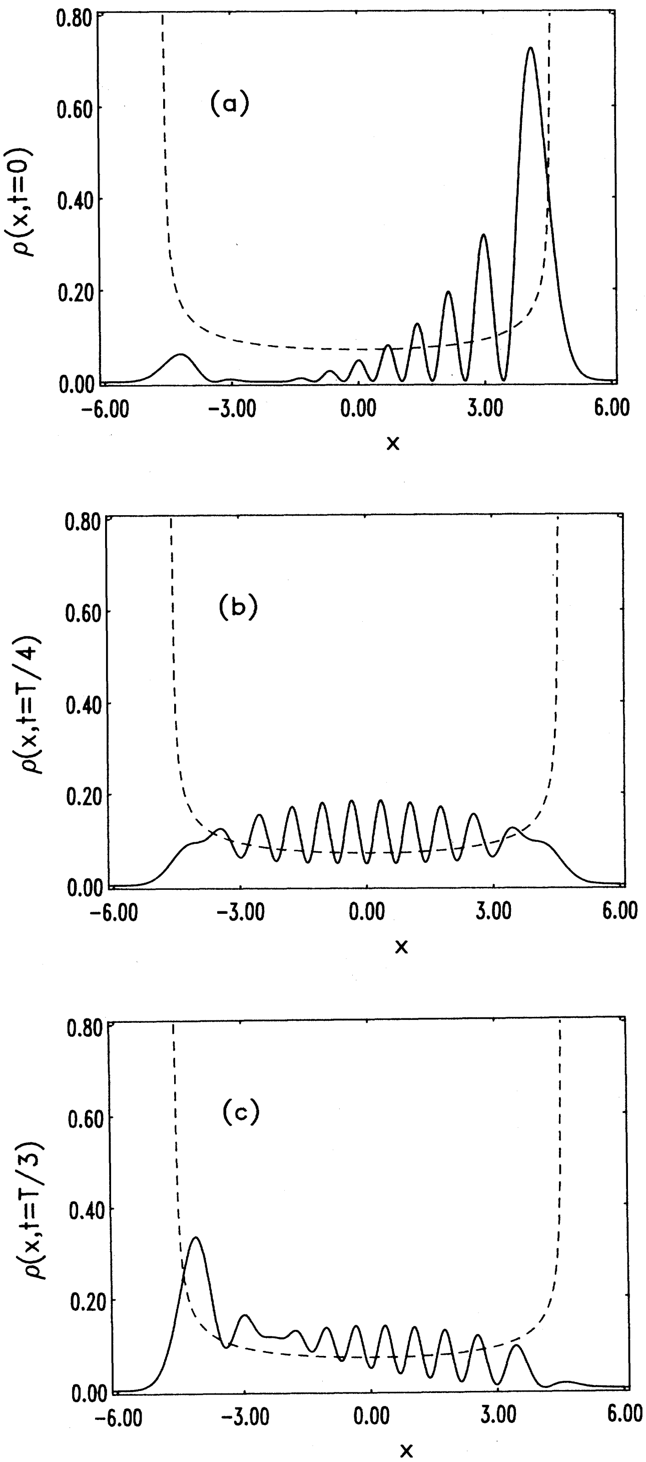

FIG. 1. (a) Probability density $\rho(x,t=0)$ for $n=10$. x is in units of $(\hbar/m\omega)^{1/2}$. The dashed line is the classical result. The mirror image of $\rho(x,t=0)$ applies to $\rho(x,t=T/2)$. (b) Same as (a), but for $\rho(x,t=T/4)$ and $\rho(x,t=3T/4)$. (c) Same as (a), but for $\rho(x,t=T/3)$, which turns out to be identical with $\rho(x,t=2T/3)$; the former is associated with $|\eta_2\rangle$ and the latter with $|\eta_3\rangle$. Inspection of these plots shows that the center of gravity of $\rho(x,t)$ just bounces back and forth with period T, without loss of coherence.

and for the symmetric form

$$\chi_\alpha(t) \equiv \tfrac{1}{2}\langle x(t)x(0)+x(0)x(t)\rangle = \frac{E_\alpha}{m\omega^2}\cos\omega t + \frac{\hbar}{m\omega}\,\mathrm{Re}(\alpha^2 e^{-i\omega t}) \; . \qquad (10)$$

The fact that in Eq. (9) we obtained a complex expression for $\langle x(t)x(0)\rangle_\alpha$ underscores the need to symmetrize, that is to introduce $\chi(t)$, in order to evaluate physically meaningful quantities. In expressions (9) and (10) the energy E_α of the coherent state is

$$E_\alpha = \langle\alpha|H|\alpha\rangle = \hbar\omega(|\alpha|^2+\tfrac{1}{2}) \; . \qquad (11)$$

The classical result of Eq. (8) is recovered by means of a two-step process: (i) writing $\alpha=|\alpha|e^{i\phi}$, and averaging the phase ϕ over the total angle 2π; (ii) taking the limit $|\alpha|\gg 1$. If the pure HO eigenstates $|n\rangle$ are used, one obtains a result formally equal to the classical one for any n; of course the classical correlation is obtained in the large quantum-number limit.

We now compute with the states introduced in Eqs. (3). A straightforward calculation yields

$$\chi_{\eta_1}(t) = \frac{\hbar}{m\omega}\{n+\tfrac{1}{2}+\tfrac{1}{3}[n(n+1)]^{1/2}\}\cos\omega t \; , \qquad (12a)$$

$$\chi_{\eta_2} = \chi_{\eta_3}(t) = \frac{\hbar}{m\omega}\{n+\tfrac{1}{2}+\tfrac{1}{6}[n(n+1)]^{1/2}\}\cos\omega t \; . \qquad (12b)$$

Once more, only the symmetrized form $\chi(t)$ yields real expressions.

We do observe that in the high-quantum-number limit $n\to\infty$ the square root on the right-hand side of Eqs. (12) yields a nonvanishing contribution over and above the classical result. In fact, for $n\gg 1$, one obtains

$$\chi_{\eta_1}(t) = \tfrac{4}{3}\langle x(t)x(0)\rangle_{\mathrm{Cl}} \; , \qquad (13a)$$

$$\chi_{\eta_2}(t) = \chi_{\eta_3}(t) = \tfrac{7}{6}\langle x(t)x(0)\rangle_{\mathrm{Cl}} \; . \qquad (13b)$$

Since all the results given by formulas (13) are overcorrelated, not even the average can yield the classical expression; in fact, one obtains $\frac{11}{9}$ of it. Furthermore, because of the properties that are inferred from Eq. (5), it is clearly the case that time and ensemble averages are identical for our example.

C. Density matrix

The density matrix for the states of Eq. (3) is readily obtained and reads

$$[\rho(t)] = \begin{array}{c} \\ (n-1) \\ (n) \\ (n+1) \end{array} \begin{array}{ccc} (n-1) & (n) & (n+1) \\ \frac{1}{3} & \frac{1}{3}e^{i\omega t} & \frac{1}{3}e^{2i\omega t} \\ \frac{1}{3}e^{-i\omega t} & \frac{1}{3} & \frac{1}{3}e^{i\omega t} \\ \frac{1}{3}e^{-2i\omega t} & \frac{1}{3}e^{-i\omega t} & \frac{1}{3} \end{array} \; , \qquad (14)$$

with all remaining matrix elements being identically zero. The process of taking the limit of $n\to\infty$ only slides the (3×3) nonzero block "down" the diagonal, without modification of the matrix elements. Thus, the classical limit, given by a matrix identical to (14), except that all off-diagonal elements are equal to zero, is never attained.

Having provided all these pieces of evidence we turn to the discussion of their significance and physical implications.

III. DISCUSSION AND CONCLUSION

Since as simple a state as a superposition of a few HO eigenstates retains quantum effects, even for arbitrarily high quantum numbers, we have to carefully examine the possibility of actually observing such phenomena.

The first question that naturally emerges is this: Can these states, i.e., the ones of Eq. (3) for example, be prepared in a laboratory? Next, one has to address the issue of how to observe the macroscopic quantum effects derived in Sec. II. As far as the preparation of arbitrary quantum states is concerned Lamb[10] has provided a general procedure in *principle*. The difficulty that comes up right away is that the potential for which the states $\{|\eta_i\rangle\}$ of Eq. (3) are eigenstates, is highly singular. However, Lamb[10] manages to circumvent this problem through a simple, idealized three-step scheme which unfortunately seems extremely improbable to implement in a laboratory.

In spite of these hard facts, let us pursue our argument even further. Having somehow succeeded in the preparation of state $|\eta_1\rangle$, for example, presumably the best way to observe the macroscopic quantum effects derived above would be to allow the state to tunnel in and out of a HO potential well. This way one could determine if quantum coherence is retained or not. However, at this stage we would be faced with the subtle difficulties pointed out by Leggett.[11] He showed that only a selected class of states are likely candidates for the observation of these macroscopic quantum phenomena.

Consequently, the main conclusion of our work is that simple examples of states which exhibit macroscopic effects in the large quantum-number limit, can be constructed analytically in a straightforward way. In particular, a simple linear combination of three HO eigenstates suffices to illustrate our argument. Of course, experiments to observe these phenomena are much more difficult to carry out. However, the very recent work by Cary, Ruso, and Skodje[8] allows for some hope that the observation of the predicted macroscopic quantum effects may be implemented in a Penning trap.

Many other examples with similar properties can be envisaged. However, what is relevant in ours is that macroscopic quantum coherence is ascribed to a one-particle state, not to a condensate of a many-particle system. So we are referring to a system of high energy ($E \gg \hbar\omega$), but with few degrees of freedom (as in the case of wave packets constructed in neutron interferometry, which may have sizes of the order of 1 cm, with coherence[12] length as long as 0.1 mm). Those are systems which are likely candidates to visualize Schrödinger's cat experiment.

In conclusion, if quantum mechanics is the correct theory to describe physical reality, the correspondence principle has only heuristic value: Quantum and classical mechanics only partially overlap in the macroscopic domain.

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