Exact classical limit of the quantum bouncer

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Abstract In this paper, we develop a systematic approach to determine the classical limit of periodic quantum systems and we applied it successfully to the problem of the quantum bouncer. It is well known that, for periodic systems, the classical probability density does not follow the quantum probability density. Instead, it follows the local average in the limit of large quantum numbers. Guided by this fact, and expressing both the classical and quantum probability densities as Fourier expansions, here we show that local averaging implies that the Fourier coefficients approach each other in the limit of large quantum numbers. The leading term in the quantum Fourier coefficient yields the exact classical limit, but subdominant terms also emerge, which we may interpret as quantum corrections at the macroscopic level. We apply this theory to the problem of a particle bouncing under the gravity field and show that the classical probability density is exactly recovered from the quantum distribution. We show that for realistic systems, the quantum corrections are strongly suppressed (by a factor of $\sim 10^{-10}$) with respect to the classical result.

1 Introduction

The correspondence principle states that any new theory in physics should reduce, in the appropriate limit, to preceding theories that have been proven to be valid. Besides, the new theory should also explain new phenomena beyond the validity of the older theory. For example, special relativity reduces to classical mechanics for velocities small as compared with the velocity of light in vacuum. Similarly, general relativity reduces to Newtonian gravitation in the limit of weak gravitational fields. The quantum-to-classical correspondence is much more subtle, so much that after a century of the inception of the quantum theory it remains problematic. Put simply, it refers to that any model describing the behaviour of quantum systems must yield the same results as classical physics in the macroscopic limit.

Although its conceptual and technical importance is largely undisputed, still there is no agreement concerning how the quantum-to-classical correspondence should be defined, and the main difficulty is perhaps that the conceptual framework of both theories is quite different. In classical mechanics we deal with quantities that are directly observable, such as the position and momentum, which indeed define the classical trajectory of the particle. In quantum mechanics, however, we are concerned with the probability density, which specifies the probability of finding the particle at some position or bearing some momentum. By many other aspects like this, the quantum-to-classical transition remains a difficult task.

There are two different formulations of the correspondence principle between quantum and classical physics [1]. One is due to Planck, who postulated that the quantum theory reduces to the classical theory in the limit $h \to 0$. The other, due to Bohr, asserts that the classical behaviour emerges from the quantum world for large energy quantum number $n$. As shown by Liboff, when applied to transition frequencies, these two formulations of the correspondence principle are not universally equivalent [2]. A combination of both has also been proposed to characterize the classical limit: taking simultaneously $h \to 0$ and $n \to \infty$ subject to the constraint that $J = nh$ is finite, where $J$ is the appropriate classical action [3]. There are a few proposals, all of them rooted in the Planck and Bohr correspondence principles, addressing the intricate connection between the classical and quantum worlds.

For example, as Wentzel, Kramers and Brillouin found, an approximate solution to the Schrödinger equation (for slowly varying potentials) yields, in the limit $h \to 0$, to the Hamilton-Jacobi equation of classical physics [4–6]. Planck’s limit has also been used to characterize the classical limit of the Feynman path integral formulation of quantum mechanics [7]. As we shall discuss later, neither the WKB approximation nor the Lagrangian formulation yields the complete classical limit when $h \to 0$. An additional form of the quantum–classical correspondence is given by Ehrenfest’s theorem [8], which states that the quantum–mechanical averages of the position and momentum operators obey the classical equations of motion. However, as discussed in Ref. [9], this is not true at all if the width of the probability distribution in position space is not negligible.

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In a less sophisticated level, many textbooks [10, 11] and articles [12–17] compare the quantum mechanical and classical probability densities and conclude, by inspection, that they approach each other in a locally averaged sense in the limit of large energy quantum number \( n \). Nevertheless, it has been argued that this comparison is unsuitable when applied to a pure energy eigenstate, since it is an inherently oscillating state; rather, it should be applied to a mixed ensemble of quantum coherent states [18]. The local averaging required to show that the oscillatory quantum probability density approaches the smooth classical distribution is technically quite difficult. It can actually be done analytically only for a particle in a box because of the simplicity of the involved quantum and classical distributions [12], but its application to more intricate periodic quantum systems is still lacking. Our main goal in this paper is to reformulate the local averaging process in a simpler and manageable fashion. The method is based on some simple assumptions, such as the periodicity of the classical motion, the highly oscillatory behaviour of the quantum distribution for large energy quantum number, and that they converge each other when averaged locally over a finite interval. This allows us to express the quantum–classical correspondence in the Fourier space as follows: in the limit of large energy quantum number \( n \), the quantum Fourier coefficient asymptotically behaves as the classical Fourier coefficient. A series of subleading terms (in inverse powers of \( n \)) may emerge, which can be interpreted as quantum corrections at the macroscopic level. This method has been successfully applied to the infinite square well potential, the harmonic oscillator and the hydrogen atom [19–21]. Here we shall apply this theory to the finite interval, approaches to the classical distribution sense. Namely, for every smooth function \( \phi \) representations of the wave function are related each other via a Fourier transformation, i.e.

\[
\rho_{\text{cl}}(x) = \frac{2}{\pi \tau(x)} \int_{v(x)}^{v(x)+\tau(x)} \rho_{\text{qm}}(y) \, dy,
\]

where \( \tau \) and \( v(x) \) are the classical period and the local speed, respectively. The comparison between these is not satisfactory at all, since in the limit of large quantum number \( n \), the highly oscillatory quantum distribution \( \rho_{\text{qm}}(x) \) does not converge pointwise to the smooth classical probability density \( \rho_{\text{cl}}(x) \). Instead, the classical limit should be understood in a distributional sense. Namely, for every smooth function \( f(x) \), the integral \( \int f(x) \rho_{\text{qm}}(x) \, dx \) must converge to \( \int f(x) \rho_{\text{cl}}(x) \, dx \). Any function \( f(x) \) provides averaging over rapid oscillations of the quantum probability density, so speaking about the classical limit is justified. To say that \( \rho_{\text{qm}}(x) \) converges in distribution to \( \rho_{\text{cl}}(x) \) we write \( \rho_{\text{qm}}(x) \xrightarrow{d} \rho_{\text{cl}}(x) \). Distributional convergence is widely discussed in many textbooks [22, 23]. The convergence in distribution means that the quantum distribution \( \rho_{\text{qm}}(x) \), if averaged locally in a finite interval, approaches to the classical distribution \( \rho_{\text{cl}}(x) \) provided the principal quantum number \( n \) is sufficiently large. A more formal statement of this might be that

\[
\rho_{\text{cl}}(x) = \lim_{n \to \infty} \frac{1}{2\epsilon_n} \int_{x-\epsilon_n}^{x+\epsilon_n} \rho_{\text{qm}}(y) \, dy,
\]

where the interval \( \epsilon_n \) decreases with increasing the quantum number \( n \). Local averaging (1) can be analytically evaluated only for the most familiar of all quantum mechanical bound state problems: the infinite well. However, it is impractical for more intricate bound-state systems for which wave functions involve special functions (e.g. the harmonic oscillator, the quantum bouncer and the hydrogen atom), and have at best can be treated numerically. The main goal of this section is to reformulate the local averaging process of Eq. (1) in a simpler and manageable fashion. The method is based on the following simple and well-known assumptions:

(i) the classical motion is periodic, i.e. the particle bounces back and forth between the turning points,
(ii) the quantum probability density rapidly oscillates in the limit of large energy quantum number \( n \),
(iii) for large \( n \), the classical and quantum distributions approach each other when averaged locally over a finite interval.

Assumptions (i) and (ii) imply that both the quantum and classical probability densities can be expressed as Fourier expansions:

\[
\rho_{\text{cl}}(x) = \int \varphi_{\text{cl}}(p) e^{ipx/\hbar} \, dp, \quad \rho_{\text{qm}}(x) = \int \varphi_{\text{qm}}(p) e^{ipx/\hbar} \, dp,
\]

where \( \varphi_{\text{cl}}(p) \) and \( \varphi_{\text{qm}}(p) \) are the classical and quantum Fourier coefficients, respectively. Recall that the position and momentum representations of the wave function are related each other via a Fourier transformation, i.e. \( \phi_n(p) = \frac{1}{2\pi\hbar} \int \psi_n(x) e^{-ipx/\hbar} \, dx \). This implies that the Fourier coefficients in Eq. (2) do not correspond to the momentum space probability densities, i.e. \( \varphi_{\text{qm}}(p) \neq \rho_{\text{qm}}(x) \).
Rather, they have the same information content than the probability distributions in position space, just encoded in a different way.

We now take for granted assumption (iii). Substituting the Fourier expansions of Eq. (2) into Eq. (1) we obtain

\[ \int \varrho_{\text{cl}}(p) e^{ipx/\hbar} dp = \lim_{n \to \infty} \int \varrho_{n}^{\text{qm}}(p) \left[ \frac{1}{2\epsilon_n} \int_{x-\epsilon_n}^{x+\epsilon_n} e^{ipy/\hbar} dy \right] dp. \]  

(3)

This integral is quite simple. Retaining only the leading-order term, which is \( \epsilon_n \)-independent, we find

\[ \int \varrho_{\text{cl}}(p) e^{ipx/\hbar} dp \sim \lim_{n \to \infty} \int \varrho_{n}^{\text{qm}}(p) e^{ipx/\hbar} dp. \]  

(4)

Finally, due to the linearity of Fourier expansions (2), Eq. (4) implies that the quantum Fourier coefficient \( \varrho_{n}^{\text{qm}}(p) \) approaches, asymptotically, to the classical Fourier coefficient \( \varrho_{\text{cl}}(p) \) for \( n \gg 1 \), i.e.

\[ \varrho_{n}^{\text{qm}}(p) \sim \varrho_{\text{cl}}(p) + O(1/n). \]  

(5)

This is an alternative manner to rewrite the local averaging process of Eq. (1), but expressed in the Fourier space. As evinced by Eq. (5), the leading term of the asymptotic expansion corresponds exactly with the classical Fourier coefficient \( \varrho_{\text{cl}}(p) \), but subleading terms (in inverse powers of the quantum number \( n \)) may arise. Evidently, the correction terms vanish when \( n \) tends to infinity, thus implying that the quantum Fourier coefficient converges pointwise to its classical analogue. It then seems natural to ask the question, Is the \( n \to \infty \) limit a classical limit? We answer this question in the negative by the following reason. Let us consider as a guiding system the quantum harmonic oscillator.

If an eigenstate is used to evaluate the quantum probability density, in the limit of large quantum number \( n \), we obtain strong oscillations and many nodes. As increasing \( n \), the quantum distribution confines progressively in a finite region, defined by \( |x| < A_n \), and is small but nonzero for \( |x| > A_n \), where \( A_n = \sqrt{(\hbar/m\omega)(2n + 1)} \). So, the quantity \( A_n \) becomes the amplitude of the corresponding classical oscillator. Since no special assumption concerning the size, mass or \( \hbar \) is made, the limit \( n \to \infty \) implies an infinite amplitude, which is nonsense. Thus, in the classical limit, \( n \) has to be large, but finite. All in all, our result of Eq. (5) suggests that, strictly speaking, quantum mechanics do not converge to classical mechanics, but rather in the limit of large energy quantum number \( n \), the quantum correction terms will be finite, and they may be interpreted as small quantum corrections at the macroscopic level. In next Section 3 we apply this theory to the quantum bouncer and demonstrate that the leading-order term yields the exact classical probability density.

The above formulation was introduced in the position-space representation of the probability distribution; however, we can generalize it to the momentum-space representation. To see this we appeal to the special symmetry inherent in the harmonic oscillator problem, in which \( x \) and \( p \) play similar roles. This imply that the energy eigenfunctions in momentum-space representation can be obtained from that in position-space representation by replacing \( x \to p \) and \( m \to \frac{m}{\hbar\omega} \). So, the results we reported in Ref. [19] for the classical limit of the quantum harmonic oscillator in the position space guarantee that the classical momentum distribution is exactly recovered from the quantum–mechanical solution. Of course, the formulation in momentum-space representation requires a deeper analysis as well as the application to other simple periodic quantum systems.

In addition to position and momentum representations of quantum mechanics, a joint position-momentum representation has proven to be useful in different branches of physics as well. For example, the Wigner function has been used to describe quantum transport in quantum optics and quantum chaos [24, 25]. It is natural to wonder whether the procedure we introduce here can be extended to the phase-space probability distribution. In fact, the applicability of the procedure separately to the position and momentum representations does not imply its suitability for the phase-space representation. In this regard, it is worth to mention that in Ref. [26], the authors showed that for the harmonic oscillator, the classical limit of the Wigner function for highly excited states (i.e. coherent and WKB states) yields the microcanonical ensemble. Once formulated the above procedure in the phase-space representation, it would be interesting to compare the results with the ones obtained in Ref. [26]. We left these problems for future investigations.

### 3 Classical limit of the quantum bouncer

The problem of a particle in a constant field force is more than a simple conceptual model. It has found many applications in different branches of physics, for example, it models a particle in a constant electric field, the quantum chromodynamics of quark–antiquark pair at some separation [27], and it is often used in modulation-doped semiconductors [28]. The quantum bouncer is a variation of the constant force problem which adds an infinite wall at the ground level. It has been used to model the quantum states of neutrons in the Earth’s gravitational field [29]. Thus the study of a particle in a constant field should be of wide interest. We shall now apply the theory developed above to the quantum bouncer.
We begin our discussion by reviewing briefly the classical problem. Let us consider a point particle of mass \( m \) bouncing on a perfectly reflecting surface, at \( z = 0 \), under the influence of the gravitational acceleration \( g \). The corresponding potential energy function is given by

\[
V(z) = \begin{cases} 
mgz & z \geq 0 \\
\infty & z < 0 
\end{cases}.
\]

(6)

Assuming that the particle is initially at rest and dropped from a height \( h \), the classical probability density is easily found to be

\[
\rho_{\text{cl}}(z) = \frac{1}{2\sqrt{h(h - z)}} H(h - z),
\]

(7)

where \( H(x) \) is the Heaviside step function. Note that probability density \( \rho_{\text{cl}}(z) \) does not depend on neither the gravitational acceleration \( g \) nor the mass \( m \). Besides, it has a divergence at \( z = h \), where the particle slows down and reverses direction, but is finite at \( z = 0 \) where the particle simply bounces, reversing direction, but with no change in speed.

The associated quantum mechanical problem, the so-called quantum bouncer, is much more difficult. It has been extensively discussed in a number of pedagogical articles and textbooks [30, 31]. The normalized wave function \( \psi_n(z) \) which properly decays for \( z \to \infty \) and satisfies the boundary condition \( \psi_n(z = 0) = 0 \) (i.e. the ground is impenetrable), is

\[
\psi_n(z) = \frac{1}{\sqrt{l_g}} \frac{\text{Ai}(a_n + z/l_g)}{\text{Ai}'(a_n)},
\]

(8)

where \( \text{Ai}(x) \) is the Airy function [32], \( a_n \) is the \( n \)-th zero of the Airy function \( \text{Ai}(x) \), and \( l_g = \left( \frac{h^2}{2mg} \right)^{1/3} \) is the gravitational length. Another linearly independent solution to the Schrödinger equation exists, the Airy function \( \text{Bi}(x) \), which is eliminated as a physical solution since it diverges when the argument becomes large. The corresponding quantized energies \( E_n \) are

\[
E_n = -mg l_g a_n, \quad n = 1, 2, 3, \ldots
\]

(9)

An exact analytical expression for the zeros \( a_n \) of the Airy function is not available, but a good approximation can be given, especially for large \( n \). Using the asymptotic expansion of the Airy function \( \text{Ai}(x) \) for large negative argument one finds \( a_n \approx -[(3\pi/2)(n - 1/4)]^{2/3} \) [32]. This yields an approximate expression for energy levels \( E_n \), which indeed coincides with the WKB quantized spectrum.

We are now able to verify visually that the quantum probability density, when locally averaged, approaches the classical result for large values of \( n \). To this end, we first recall that the quantum distribution exhibits strong oscillations and confines bit by bit between the ground level (at \( z = 0 \), under the influence of the gravitational acceleration \( g \)), while it is small for large quantum numbers (e.g. \( P_{10} \approx 0.25 \) and \( P_{20} \approx 0.20 \)), whereas it is small for large quantum numbers (e.g. \( P_{10} \approx 0.016 \), \( P_{30} \approx 0.0077 \)).

We now follow the theory developed in the previous section and calculate the classical limit of the quantum bouncer. We first proceed to the evaluation of the quantum Fourier coefficient \( \varrho_n^{\text{qm}}(p) \), defined by Eq. (2). It requires the evaluation of the integral

\[
\varrho_n^{\text{qm}}(p) = \frac{1}{2\pi \hbar l_g} \frac{1}{\text{Ai}'(a_n)} \int_0^\infty \text{Ai}^2(a_n + z/l_g) e^{-ipz/h} dz.
\]

(12)

Up to the best of our knowledge, an exact analytical expression for this integral is still absent in the literature. However, for the purposes of this paper, we only need its asymptotic behaviour for \( n \gg 1 \). We achieve this by using the method of Albright [33], since some basic primitives of the Airy functions allow us to express Fourier coefficient (12) as a series in inverse powers of \( a_n \). To
which produces a corresponding quantum number is \( n \). For example, the corresponding gravitational length for a neutron is \( \sim n \). The resulting integral can be evaluated by means of the method of Albright [33]. Using the following properties \( \text{Ai}(x) \), we can simply iterate the above result. Indeed, we can simply iterate the above result. After one iteration we obtain

\[
\mathcal{Q}^{\text{qm}}(p) \approx \frac{1}{2\pi h} e^{-ipx/h} \sum_{k=0}^{\infty} (-i p h / k !) \int_{a_n}^{\infty} x^k \text{Ai}^2(x) dx.
\]

We observe that this expression is a series in inverse powers of \( a_n \). Recalling that \( |a_n| > |a| = 2.33811 \) for \( n > 1 \), the second term in braces is smaller than the first one by a factor of \( a_n^{-3} \), and the third one will be smaller than the second one by an additional factor of \( a_n^{-3} \) and so on. We can perform iterations indefinitely; however, for the purposes of this paper, it is sufficient to keep only the leading terms. In order to justify this assumption, let us estimate how large the quantum number is in a realistic classical situation. From Eq. (10), for a given classical height \( h \), it can be estimated as \( n \sim \frac{h}{\sqrt{\pi}} (l_q)_{a_n^3} \), where we used the asymptotic form of the zeros of the Airy function. For reference, for a Caesium atom one finds \( l_q = 0.226 \mu m \), such that, if released from 1mm, the corresponding quantum number is \( n \sim 62,500 \) and hence \( 1/a_n^3 \sim 10^{-11} \). For the much lighter Na atom one finds \( l_q = 0.727 \mu m \), which produces \( n \sim 10,000 \) so that \( 1/a_n^3 \sim 10^{-10} \). To obtain smaller values for \( n \), the gravitational length has to be larger, and this is achieved with light particles. For example, the corresponding gravitational length for a neutron is \( l_q = 5.87 \mu m \), which implies \( n \sim 470 \) such that \( 1/a_n^3 \sim 10^{-7} \). These results imply that we can safely disregard the subleading terms in asymptotic expansion (15) and retain only the leading term, i.e.

\[
\mathcal{Q}^{\text{qm}}(p) \sim \frac{1}{2\pi h} e^{-ipQ} \sum_{k=0}^{\infty} \frac{(i Q)^k}{k !(2k + 1)}.
\]

where \( Q = ph_n/h \). This summation can be performed in an analytical fashion. The result is

\[
\mathcal{Q}^{\text{qm}}(p) \sim \frac{1}{4\sqrt{\pi} \sqrt{Q}} e^{-iQ - \pi/4} \text{erf}\left[ e^{-\pi/4 \sqrt{Q}} \right].
\]

where \( \text{erf}(x) \) is the error function, defined as \( \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \), that in turn can also be expressed in terms of the Fresnel integrals [34]. The summations of the subdominant terms can also be performed analytically; they are however not relevant for the purposes of this paper.
According to the theory developed in the previous section, to obtain the asymptotic behaviour of the quantum probability density in position space, we have to compute the Fourier transformation of the coefficient $\varrho_n^{\text{qm}}(p)$, given by Eq. (17), as defined in Eq. (2). This yields

$$\varrho_n^{\text{qm}}(z) \sim \frac{1}{4\sqrt{\pi} h_n} e^{-z^2/4} \int_{-\infty}^{\infty} \text{erf} \left[ e^{-\pi/4 \sqrt{Q}} \right] e^{-iQ(1-z)/h_n} \frac{dQ}{\sqrt{Q}} = \frac{1}{2\sqrt{h_n(h_n-z)}} H(h_n-z),$$

(18)

which is exactly the classical probability density, $\rho_{\text{cl}}(z)$, given by Eq. (7), with the classical height $h$ replaced by the turning point $h_n$ of Eq. (10). Following the same procedure, in Refs. [19–21] we successfully applied this method to other periodic systems, such as the harmonic oscillator, the infinite square well potential and the hydrogen atom.

We close this section by commenting some previous works related to the classical limit of the quantum bouncer. Many pedagogical articles show the comparison between the classical and quantum distributions for this system, asserting that they approach each other in a locally averaged sense when the energy quantum number is large. However, none of them have computed the local averages to confirm this claim, either analytically or numerically. In a recent paper [35], the authors consider a particle in a homogeneous field and analyse the expectation values of the position, momentum and their moments up to fourth order (without restoring to numerical or graphical techniques), to confirm that they reduce to the corresponding classical values for large quantum numbers. Note that all the results reported in Ref. [35] are just particular cases of our findings in this paper. For example, having showed that the quantum distribution $\varrho_n^{\text{qm}}(z)$ converges to its classical analogue $\rho_{\text{cl}}(z)$ for large quantum number $n \gg 1$, then the expectation value of any observable $f$ depending on the position $z$ correctly yields the classical result:

$$\langle f(z) \rangle_{\text{qm}} = \int_0^{\infty} dz f(z) \varrho_n^{\text{qm}}(z) \sim \int_0^{\infty} dz f(z) \rho_{\text{cl}}(z) = \langle f(z) \rangle_{\text{cl}}.$$

(19)

In a similar fashion, the expectation value of any observable $g$ depending on the momentum $p$ reduces to the classical result. To demonstrate this claim, we consider that the observable $g$ can be written as a power series, i.e. $g(p) = \sum_{k=0}^{\infty} c_k p^k$. Because of parity considerations, the expectation value of the odd terms vanishes, so we are left only the even terms in the power expansion. However, using the quantum Hamiltonian $H = \frac{p^2}{2m} + mgz$, it is clear that

$$\int_0^{\infty} dz \psi_n^*(z) p^{2k} \psi_n(z) = \int_0^{\infty} dz [2m(H-mgz)]^{2k} \rho_n^{\text{qm}}(z),$$

(20)

which is simply evaluated by using the result of Eq. (19). Therefore, all the results reported in Ref. [35] are easily reproduced with our method.

Finally, in Ref. [18] the authors pointed out that comparison between classical and quantum probability densities is unwarranted when applied to pure energy eigenstates. Instead, they claim that it should be applied to a mixed ensemble of quantum coherent states, and hence they compare the quantum distribution with an ensemble of classical systems (each with the same initial conditions). A similar analysis was undertaken in Ref. [36], where the authors investigate the large quantum number behaviour of a quantum state which consists of a superposition of a few successive energy eigenstates for the harmonic oscillator. Their conclusions are the same: quantum effects persist for arbitrarily large quantum number, and they do not recover the exact classical distribution. There are important conceptual differences between these approaches and the one introduced in this paper: while they consider an ensemble of classical systems [18] or a superposition of energy eigenstates [36], here we apply the correspondence principle to a single-particle energy eigenstate and obtain the exact classical result in an analytical fashion. Interestingly, the classical limit of the harmonic oscillator in the phase-space representation of quantum mechanics has been reported by using highly excited states [26]. It would be interesting to extend the procedure we introduced to include the analysis of energy averages as well, not only eigenfunctions.

### 4 Discussion and outlook

Our results have interesting implications in the understanding of the classical limit. To better understand the scope and limitations of our approach, we shall discuss briefly various formulations of the classical limit, by critically reviewing their main advantages and drawbacks. As discussed in Sect. 1, there are two different formulations of the correspondence principle. The first is traced back to Planck, in 1906, which asserted that classical physics is recovered from quantum physics in the limit $h \to 0$. Planck originally introduced this limit to show that his energy density for blackbody radiation,

$$\rho(v, T) = \frac{8\pi h v^3}{c^3} \frac{1}{e^{hv/k_B T} - 1},$$

(21)

reduces in the limit $h \to 0$ to the classical Rayleigh-Jeans energy density,

$$\rho_{\text{cl}}(v, T) = \lim_{h \to 0} \rho(v, T) = \frac{8\pi v^2}{c^3} k_B T.$$

(22)

In these expressions $k_B$ is the Boltzmann constant and $T$ is the temperature. Clearly, Planck applied the correspondence principle to a statistical average of the energy eigenvalues over a canonical probability distribution, without appealing to any quantum number.

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Years later, in 1913, Bohr postulated that quantum mechanics reduces to classical mechanics when the energy quantum number is large, $n \gg 1$. Bohr first enunciated this formulation to show that in his model of the hydrogen atom the transition frequency between neighbouring energy levels,

$$v = \frac{me^4}{64\pi^3 \epsilon_0^2 h^3} \left[ \frac{1}{n^2} - \frac{1}{(n+1)^2} \right], \quad (23)$$

in the limit of large quantum numbers $n \gg 1$, tends to the classical orbital frequency of the electron

$$v_{\text{cl}} = \frac{1}{2\pi} \sqrt{\frac{e^2}{4\pi \epsilon_0 m r_n^3}}, \quad (24)$$

where $r_n = n^2 r_B$ is the radius of stationary orbits and $r_B$ is the Bohr radius. So, Bohr applied his correspondence principle to a single atom, not to an statistical ensemble of them. The inadequacy of Bohr’s correspondence principle to connect quantum and classical theory has been extensively discussed in Refs. [37–39]. Also, as shown in Refs. [40, 41], Planck and Bohr correspondence principles are not universally equivalent when applied to transition frequencies. This is clearly seen for a particle in a box, for which the transition frequency between adjacent energy levels is $v = \frac{b}{2m a^2} (2n - 1)$, such that the separate limits $h \to 0$ and $n \to \infty$ give zero and infinity, respectively. However, as suggested in Ref. [3], taking simultaneously the limits $h \to 0$ and $n \to \infty$ but keeping finite the classical action $J = nh$, the classical frequency is exactly recovered.

It is worth mentioning that both Planck and Bohr formulations of the correspondence principle were introduced before the development of wave mechanics by Schrödinger and matrix mechanics by Heisenberg, Born and Jordan in 1925, and so they did not make any allusion to the classical limit of quantum dynamics. Therefore, it was not clear how to apply these correspondence principles to whether the wave function or the matrix elements of an operator. Along the years, a few methods addressing the quantum-to-classical correspondence have been proposed within modern quantum mechanics, all of them rooted in the old Planck and Bohr correspondence principles, namely, the WKB method, the path integral formulation and the Ehrenfest’s theorem. As we shall discuss in the following, these methods are not universally reliable for investigating the classical limit of quantum dynamics in a general way, and at the end all of them require of a very narrowly peaked probability density.

- The WKB method, also called the semiclassical approximation, is important as a practical means of approximating solutions to the Schrödinger equation for slowly varying potentials compared to the de Broglie wavelength $\lambda = h/p$ of the particle [4–6]. The basic idea is that the wave function can be written as the exponential of a complex function $S(x)$, i.e. $\psi_{\text{WKB}}(x) = e^{iS(x)/\hbar}$.

Plugging this ansatz into the Schrödinger equation leaves us with the nonlinear differential equation

$$i\hbar \frac{\partial \psi}{\partial x} = \left( \frac{\partial S}{\partial x} \right)^2 + p^2(x) = 0, \quad (25)$$

where $p(x) = \sqrt{2m[E - V(x)]}$ is the momentum. Inserting the so-called WKB expansion $S = S + (h/i)S_1 + (h/i)^2 S_2 + \cdots$ into Eq. (25) we then find that the function $S$ satisfies the Hamilton-Jacobi equation, whose solution is the Hamilton’s principal function $S(x) = \pm \int x \ p(x')dx'$. At $O(\hbar)$ one finds $S_1(x) = -\frac{1}{2} \ln p(x)$. Putting these together gives us the WKB wave function,

$$\psi_{\text{WKB}}(x) \sim \frac{1}{\sqrt{p(x)}} \exp \left[ \pm \frac{i}{\hbar} \int x \ p(x')dx' \right]. \quad (26)$$

Clearly, WKB wave function (26) diverges near the turning points of the classical motion, where the velocity component vanishes. Even though the WKB method sheds light about the classical limit of the Schrödinger equation, it suffers from some difficulties that indicate its lack of generality for calculating the classical limit of quantum mechanics. For example, superposition of WKB wave functions, such as $\psi(x) = e^{iS(x)/\hbar} + e^{-iS(x)/\hbar}$, does not lead to the classical Hamilton-Jacobi equation. Besides, there are physical systems which cannot be described by WKB wave functions. For example, it is not adequate to describe the circular orbits in the hydrogen atom, since the electron is always at a turning point, where the WKB method breaks down [42–44]. This would mean that the circular orbits in the hydrogen atom do not have classical limit, which is clearly nonsense. Interestingly, the WKB wave function has been used to study the classical limit of the Wigner function for the harmonic oscillator, converging to the microcanonical ensemble [26].

- Feynman path integral formulation of nonrelativistic quantum mechanics provides a different conceptual framework which is completely equivalent to that given by Schrödinger’s equation. It passes from standard Hamiltonian formulation to a Lagrangian description in which there are only commuting objects, not operators. In this approach, the quantum nature arises because to compute a quantum amplitude, one considers not a unique classical trajectory, but a sum (or functional integral) over an infinity of possible trajectories. The contribution of a path is proportional to $e^{iS(x(i))/\hbar}$, where $S(x(i)) = \int x(i) \ L(x, \dot{x})dt$ is the action given by the time integral of the Lagrangian $L(x, \dot{x})$ along the path $x(t)$. If $S \gg \hbar$, the exponential in the Feynman’s kernel

$$K(x, t : x', t') \sim \int_{x, t}^{x', t'} d[x(t)] \ \exp \left\{ \frac{i}{\hbar} S(x(t)) \right\}, \quad (27)$$

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oscillates rapidly and the path integral will be dominated by contributions from the extrema of the action (by the usual stationary phase approximation), i.e. precisely by those paths that are solutions to the Lagrange's equation \[7\]. However this cannot be regarded as a complete description of the classical limit. To get a full classical limit, one needs to specify the initial and final positions of the particle. In the quantum formalism instead we are able to provide only the amplitudes for a particle to be in a given position at a given time and at best a sharply peaked probability density with well-defined position and momentum. Consequently, although the Planck's limit correctly gives to the Lagrange's equations in the path integral formalism, it does not say how to obtain the required sharply peaked distribution to classically define the initial and final points.

- Many textbooks discuss the classical limit in terms of Ehrenfest's theorem. The essential points of the theorem can be illustrated for a particle moving in a one-dimensional potential \( V(x) \). The Heisenberg equations of motion for position and momentum, averaged in some quantum state, are

\[
\frac{d\langle p \rangle}{dt} = \langle F(x) \rangle, \quad \frac{d\langle x \rangle}{dt} = \frac{\langle p \rangle}{m},
\]

where \( F(x) = -\partial V(x)/\partial x \) is the force operator. At first glance, it might appear that Ehrenfest's theorem says that the mean position and momentum obey Hamilton's equations of motion, but this is not actually the case. If they were to satisfy Hamilton's equations, the right-hand side of the first equation would have to be \( F(\langle x \rangle) \) instead of \( \langle F(x) \rangle \), which are quite different in general. Consequently, Ehrenfest's theorem does not say that the quantum motion follows a classical trajectory. At best, it ensures that if the uncertainties \( \Delta x \) and \( \Delta p \) are both sufficiently small, the quantum motion will approximate the classical trajectory. Corrections to Ehrenfest's theorem can be derived as follows. Taylor expanding the force operator \( F(x) \) around the mean position \( \bar{x} = \langle x \rangle \) one gets \[9\]

\[
\frac{d\bar{p}}{dt} \approx F(\bar{x}) + \frac{1}{2}(\delta x)^2 \frac{\partial^2 F(\bar{x})}{\partial x^2} + \cdots,
\]

where \( \bar{p} = \langle p \rangle \) is the mean momentum and \( \delta x = x - \bar{x} \) is an operator for the deviation from the mean value. Clearly, \( \bar{x} \) and \( \bar{p} \) obey the classical equations only if the correction terms in Eq. (29) are negligible, for which a very narrowly peaked probability density is needed. Therefore, although Ehrenfest's theorem does not resort directly to Planck or Bohr correspondence principles, one needs to appeal to some of them to get the required sharp narrow probability density. All in all, Ehrenfest's theorem cannot be regarded as a general description of the classical limit of the quantum theory.

From all of the above we have learned that the probability density plays a fundamental role to the fulfillment of the classical limit within the different approaches. However, none of them tackles the problem of how a narrowly peaked distribution can be obtained from the quantum one. In this regard, many textbooks and articles make direct comparisons between the quantum and classical probability densities for periodic systems. The former, defined by \( \rho_{\text{qm}}(x) = |\langle x | \psi_n(x) \rangle|^2 \), is intrinsic within quantum mechanics, while the latter, given by \( \rho_{\text{cl}}(x) = \frac{1}{2\pi\hbar} \int H(x,\tau) d\tau \), is intuitively derived by the argument of how much time spent the particle in a given interval. These quantities are fundamentally different: while the quantum distribution is defined in the whole real line and is oscillatory, the classical distribution is a smooth function defined between the turning points. Therefore, it is clear that \( \rho_{\text{cl}}(x) \) cannot be obtained from \( \rho_{\text{qm}}(x) \) by taking directly the Bohr's limit \( n \gg 1 \). However what is relevant in the comparison between the distributions is that, for a large energy quantum number, the quantum distribution follows its classical counterpart in a locally averaged sense, as defined by Eq. (1). In principle, one could use the WKB wave function to do this, but it diverges near the turning points. An exact wave function instead does not actually diverge there, but become sharply peaked around, thus resembling to the classical turning points, but smoothed out by the uncertainty principle, which also causes some of the wave function to spill over into the classically forbidden region. In general, local averaging exact quantum distributions in position space are a difficult task due to its highly oscillatory behaviour. To fill in this gap, in this paper we develop a systematic approach to determine the classical limit of periodic quantum systems.

Our method lies in three simple assumptions: (i) the classical motion is periodic, (ii) the quantum probability density rapidly oscillates for large quantum numbers, and (iii) the classical and quantum distributions approach each other for large \( n \). Assumptions (i) and (ii) allow us to express the quantum probability density as Fourier expansion (2), and the latter (iii) implies that, for large quantum numbers, the Fourier coefficient converges to its classical counterpart (5). In fact, the classical Fourier coefficient is just the leading term in the asymptotic expansion of the quantum Fourier coefficient, and hence, quantum corrections may arise in inverse powers of the quantum number \( n \) (or equivalently in powers of the WKB ratio \( h/S \ll 1 \), where \( S \) is the classical action). Clearly, we assume that both \( h \) and \( n \) have to be finite, which is consistent with the fact that Planck constant is a nonzero universal constant of nature (and is unwarranted to make it exactly zero) and that the energy of a classical system, although large as compared with the quantum of energy, must be finite.

Following our method, we obtain the exact classical limit of a particle bouncing in the presence of the gravitational field. In this case, the quantum probability distribution is related to the Airy function, so the computation of the exact Fourier coefficient can be treated numerically, at best. However, our method requires only its asymptotic behaviour for large quantum number, which can be obtained analytically by means of the method of Albright, as showed. As expected, we obtain a series in inverse powers of \( a_n \), the zeros of the Airy function. Our estimations showed that for large \( n \), the first subdominant term is strongly suppressed with respect to the leading term. Retaining only the dominant term and going back again to the position space (through the inverse Fourier
transformation), we obtain the exact classical probability density. This is precisely the main result of this paper. In a forthcoming publication we will report the analysis of the quantum corrections, which as discussed, is small at the macroscopic level but nonzero. Indeed, they consist of small oscillations enveloping the classical distribution, whose amplitude is of the order of $a_n^{-3}$ [45]. Physically, this seems that, by a conspiracy of nature, the quantum nature of the world is hidden at the macroscopic level, leaving us with an apparent world described consistently by classical physics.

Finally, we suggest some possible avenues of research and open problems, amenable to explore. First, we encourage the calculation of the exact classical limit of other well-known periodic quantum systems in a given energy eigenstate, such as the Morse and Pöschl-Teller potentials, which are quite important in physics. As widely discussed, the leading term in the asymptotic expansion of the quantum Fourier coefficient yields the exact classical probability distribution. However, subleading terms may arise which we interpret as small quantum corrections at the macroscopic level. These correction terms remain unexplored and deserve further investigations. Also, we suggest the analysis of the classical limit of quantum systems described by wave-packets constructed by superposition of energy eigenstates, i.e. $\Psi(x) = \sum_n c_n |\psi_n(x)\rangle$. According to our classical experience we expect the quantum probability density $|\Psi(x)|^2$ to converge to $\sum_n |c_n|^2 \rho_{cl}(x)$, while the nondiagonal terms of the form $\sum_{n,m} c_n^* c_m \langle \psi_n(x) \psi_m^*(x) \rangle$ should be strongly suppressed in the high energy limit. A mandatory extension of this procedure should be its formulation in the momentum-space representation of quantum mechanics as well as in the phase-space representation. It would be interesting also to analyse the inclusion of the spin in the classical limit procedure. We leave all of these problems for future investigations.

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Declarations

Conflict of interest The authors declare no conflict of interest.

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