The Fejér Average and the Short Term Behaviors of a Wave Packet in Infinite Square Well

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The first two period behaviors of a quantum wave packet in an infinite square well potential is studied. First, the short term behavior of expectation value of a quantity on an equally weighted wave packet (EWWP) is in classical limit proved to reproduce the Fejér average of the Fourier series decomposition of the corresponding classical quantity. Second, in order to best mimic the classical behavior, a nice relation between number $N$ of stationary states in the EWWP with the average quantum number $n$ as $N \approx \sqrt{n}$ is revealed. Third, since the Fejér average can only approximate the classical quantity, it carries an uncertainty which in large quantum number case is almost the same as the quantum uncertainty.

03.65.-w Quantum mechanics; 02.30.Nw Fourier analysis

Introduction In quantum mechanics, wave packet is a basic concept having broad applications [1]. During the past few years, the dynamics of the wave packets has become a very active field of research [2]. Intensive theoretical and experimental studies show that only the short term, one or two periods for precise, behaviors of an initially localized wave packet prove to be like those of an appropriate ensemble of classical orbits. Its long term behaviors such as collapse, (super-)revival etc. are inevitable and of purely quantum mechanical origin [1]. However, an outstanding problem remains open: In what sense can or can not the quantum mechanics recover the classical mechanics for a single orbit in classical limit?

As stated in standard textbook [3], in order to obtain a definite classical orbit in classical limit, we must start from a semiclassical wave packet of a particular form $\sum m c_m \psi_m$, where the coefficients $c_m$ are noticeably different from zero only in some range $\delta m$ of values of the quantum number $n$ such that $1 \ll \delta m \ll n$; the numbers $n$ are supposed large and the superposed states $\psi_m$ have nearly the same energy $E_n$ [4]. The mostly utilized wave packet $\sum m c_m \psi_m$ is the Gaussian wave packet in which the distribution of $m$ in $c_m$ is Gaussian. As believed, the expectation value of a quantity in such a wave packet must become, in the classical limit, simply the classical value of the quantity; and the expectation value in the classical limit was “proved” to be the Fourier series form of the classical quantity [3]. In fact, the proof given in [3] is not rigorous in mathematics, as recently shown in [5]. In fact, if thing is really so simple, some arguments in quantum-to-classical correspondence would have been settled long before. There are indeed many delicate problems awaiting to be resolved.

Even the form is quite simpler than the Gaussian wave packet, the equally weighted wave packet (EWWP) covers the essence of the semiclassical wave packet [3]. By EWWP, we mean that there are only $2N + 1$ stationary states around the $n$th superposed into the wave packet with the same weight $1/\sqrt{2N + 1}$. Explicitly the EWWP $|\psi(t)\rangle$ is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2N + 1}} \sum_{m=-N}^{N} \psi_{n+m}(x) \exp\left(-\frac{iE_{n+m}t}{\hbar}\right), \quad (N < n).$$

We recently proved that in the constraint classical limit $\hbar \to 0$, $n\hbar = \text{an appropriate classical action}$, the quantum mechanical average of a quantity on the EWWP goes over to the classical quantity. But the form is Fejér average [3] rather than the Fourier series of the classical quantity [3]. In general, for a piecewise smooth function $f(x)$ on a circle, the Fejér average, denoted by $F(f)$, converges to the usual sense (i.e., $\lim_{x \rightarrow x_0} f(x) = f(x_0)$) to, while the truncated Fourier series of $f(x)$ converges in the mean to, $(f(x + 0) + f(x - 0))/2$ [3]. However, the choice of $N$ is not arbitrary: It is determined by the minimizing the uncertainty relation $\Delta x \Delta p$. The relation between $N$ and $n$ can be reasonably assumed to be given by

$$N \sim n^m, \quad m < 1,$$

where $m$ is a constant; and the value of $m$ depends on the form of potential. For instance, the analytical calculation can give for a harmonic oscillator $m = 2/3$, whereas the numerical calculation in this Letter will show for the infinite square well potential $m = 1/2$. The quantum motion of a single particle in an infinite square well is worthy of paying...
special attention, not only because it is a fundamental model in quantum mechanics and insights into the dynamics exhibited in it speak immediately to a widely range of physical systems \[6\] but also the classical position \(x\) and momentum \(p\) against time \(t\) give the sawtooth and square wave respectively (cf. the Fig. 2), which are indispensable in elementary discussion of Fourier analyses relevant to Fejér average \[4\] that offers the base of our exact treatment. This Letter dedicates to the study of the quantum motion of EWWP in the well.

This Letter starts with a direct illustration that the quantum motion of the EWWP in an infinite square potential well and its classical limit, where the Fejér averages come out in the following classical limit \[4\]. Next with the value of the Planck’s constant remaining invariant, the behaviors of the EWWP in first two period are studied. Since EWWP

\[
\text{This Letter dedicates to the study of the quantum motion of EWWP in the well.}
\]

\[\text{Basic results For the quantum motion of a particle of mass } \mu\text{ in the one dimension infinite square well with width } a, \text{ the normalized stationary state function is } \psi_n(x) \exp(-iE_n t / \hbar) = (2/a)^{1/2} \sin(k_n x) \exp(-ip_n x / (2\mu \hbar)), \text{ where } k_n = n\pi / a, E_n = p_n^2 / (2\mu) \text{ is the energy and the momentum } p_n = \pm \hbar k_n \text{ are equally probable. In classical mechanics, the particle moves to and fro within the two impenetrable walls. The classical position } x = p \mu / \omega, \text{ when } 0 < t < T / 2, \text{ and } 2a - \omega t / \pi, \text{ when } T / 2 < t < T, \text{ where } T = 2\mu / p_n \text{ is the time of one period, } p_n = \text{ the magnitude of momentum, and } \omega = 2\pi / T \text{ is the frequency. The derivative of position } x \text{ with respect to time } t \text{ gives the velocity } p / \mu. \text{ The } m\text{th partial sum of its Fourier series representing } x, \text{ or simply called the } m\text{th truncated Fourier series of } x \text{, is given by } x_m \text{ as}
\]

\[
x_m = a^2 / 2 - 4a / \pi^2 \sum_{r=0}^{m} \cos((2r+1)\omega t) / (2r+1)^2.
\]

Its Fejér average \(F(x)\) is

\[
F(x) = a^2 / 2 - 8a / \pi^2 \sum_{r=0}^{N-1} \sum_{r=0}^{l} \sum_{r=0}^{t} \cos((2r+1)\omega t) / (2r+1)^2.
\]

Similarly, we have \(F(f)\) for \(f = x^2, p, p^2\) (cf. the following Eqs. \[5\]–\[8\]). To note that there is the famous Gibb’s phenomenon when using truncated Fourier series to approximate the classical momentum \(p\), while \(F(p)\) has not such a phenomenon \[4\]. The calculation of \(\langle f \rangle\) in the EWWP for \(f = x, x^2, p, p^2\) is straightforward, and they are

\[
\langle x^2 \rangle = a^2 / 3 - 2a^2 / (2N+1) \sum_{=m-N}^{N} \frac{1}{(n+m)^2}
\]

\[
+ 4a^2 / \pi^2 \sum_{l=0}^{2N} \sum_{r=1}^{l} (-1)^r \frac{1}{\pi^2} - \frac{1}{(2n-2N+2l-r)^2} \cos \left[ r \left(1 - \frac{2N-2l+r}{2n} \right) \omega_n t \right].
\]

\[
\langle p \rangle = \mu \frac{d}{dt} \langle x \rangle;
\]

\[
\langle p^2 \rangle = \frac{1}{2N+1} \left( \frac{\pi \hbar}{a} \right)^2 \sum_{m=-N}^{N} (n+m)^2 = \left( \frac{n\pi \hbar}{a} \right)^2 (1 + \frac{N+N^2}{3n^2}) = p_n^2 (1 + \frac{N+N^2}{3n^2}),
\]

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where \( \omega_n = \pi p_n / (\mu a) = n \hbar \pi^2 / (\mu a^2) \). Strictly speaking, only the following set of classical limits
\[
n \to \infty, \ N \to \infty, \ N/n \to 0, \ n \hbar \to p_c a / \pi = \omega (a / \pi)^2 \quad (i.e., \ |p_n| \to p_c, \ or, \ \omega_n \to \omega),
\]
is necessary and sufficient to make the quantum mechanical averages (5)-(8) exactly equal to the following Fejér averages respectively
\[
\langle x \rangle = F(a) = \frac{a}{2} - \frac{8a}{\pi^2} \frac{1}{2N + 1} \sum_{l=0}^{N-1} \sum_{r=0}^{l} \frac{\cos[(2r + 1)\omega t]}{(2r + 1)^2};
\]
\[
\langle x^2 \rangle = F(a^2) = \frac{a^2}{3} + \frac{4a^2}{\pi^2} \frac{1}{2N + 1} \sum_{l=1}^{2N} \sum_{r=1}^{l} \frac{(-1)^l \cos(r\omega t)}{r^2};
\]
\[
\langle p \rangle = F(p) = \mu \frac{d}{dt} F(a);
\]
\[
\langle p^2 \rangle = \left( \frac{n \pi \hbar}{a} \right)^2 (1 + \frac{N + N^2}{3n^2}) \equiv (9) p_n^2.
\]

In fact, we have recently proved in general that the classical limit of mean value of every quantity on an EWWP can exactly give the Fejér average of the Fourier series expansion of its corresponding classical quantity. So far, we can draw with safety the following conclusion: In conformity with mathematical rigor, quantum mechanics can never reproduce the exact classical mechanics unless in the nonphysical limit \( \hbar \to 0 \). This situation is not new to us. The special relativity can also not reduce to the classical Newtonian mechanics unless in the nonphysical limit the speed of light \( c \to \infty \).

**Large quantum number limit only is not sufficient to reproduce the classical mechanics from quantum mechanics**

In the previous section, we have demonstrated that the single classical orbit can not be recovered unless in the limit involving the nonphysical limit \( \hbar \to 0 \). In physical sense, this limit \( \hbar \to 0 \) can only be viewed as the comparably small to the classical action, which is essentially the large quantum number case. But the large quantum number alone is not sufficient to reproduce the classical mechanics from quantum mechanics. Its long term behaviors such as collapse, (super- or fractional-) revival etc. are doomed to appear. Even in the short term, a finite \( n \) means a finite \( N \) as well; and a EWWP with finite \( 2N + 1 \) stationary states approaches to the Fejér average of \( 2N + 1 \) partial sums of the Fourier series decomposition of the classical quantity only. The finite term Fejér average can in essence approximate the classical quantity. Therefore the large quantum number limit is in general not sufficient to reproduce the classical mechanics from quantum mechanics. In this section, we will study these problems in detail. In all numerical calculations, the natural units are used in which \( a = \mu = \hbar = 1 \).

To give the relation between \( N \) and \( n \) is easy, which can be obtained by minimizing the uncertainty relation \( \Delta x \Delta p \). To note that \( \langle p \rangle \) is a continuous function of \( t \); it is zero when the center of EWWP starts to return from either of the two walls. Since the expectation of \( p^2 \) is a constant of time, \( \Delta p = \sqrt{\langle p^2 \rangle} \) when the \( \langle p \rangle = 0 \). At this instant, minimizing \( \Delta x \Delta p \) amounts to minimizing \( \Delta x \). Numerical result as given in Fig. 1 shows that \( N \equiv \sqrt{n} \), e.g., \( N = 23 \) when \( n = 500 \). In Fig.2-Fig.4, various quantities in first two periods are plotted when \( n = 500 \quad (N = 23) \), \( p_c = 500\pi \), \( T = 0.00127 \).

As shown in Fig. 2, there is little difference between \( F(f) \) and \( f \) for \( f = x, \ p \) respectively. In order to yield a marked difference between the quantum mechanical expectation value, Fejér average and the represented function, a reduced uncertainty \( \delta f \) defined as \( \delta f = \sqrt{1 - (F(f))^2 / \langle f^2 \rangle} \) and the classical one \( \delta f \) defined as \( \delta f = \sqrt{1 - (F(f))^2 / F(f^2)} \) are introduced. In Fig.3 and Fig.4, we compare the behaviors of \( \delta f \) and \( \delta f \) for \( f = x, \ p \) respectively. We use solid lines to plot the reduced classical uncertainties, and the dotted for either the pure quantum mechanical quantities or the quasi-quantum mechanical ones. By the quasi-quantum mechanical quantities, we mean those constructed from the pure quantum mechanical ones in which the quantum mechanical matrix elements \( f_{n+r,n} = \int \psi_n(x) \psi_{n+r}(x) dx \) are replaced with the \( r \)th Fourier amplitudes \( f_r \) of the classical quantity \( f \), while the time factors \( \exp \{(E_{n+r} - E_n)t / \hbar \} \) remain unchanged. From Eqs. (3)-(5), the pure quantum mechanical quantities and the quasi-ones have little difference when \( n \) is large and \( t \) is small, e.g. \( n = 500 \), \( t \leq 0.0025 \). Therefore when we speak of one of them, both are practically referred to. Thus, the difference between solid and dotted lines comes from the inequality of energy level spacing. The longer the time evolves, the bigger the quantum mechanics deviates from the classical mechanics.
In classical mechanics, there is no uncertainty; and the reduced uncertainty is zero except when \( x = 0 \). In Figs. 3-4, for \( f = x \), \( p \) respectively, \( \delta f \) and \( \delta' f \) are almost the same and are not zero at all. It means that the wave nature can be described by Fejér average; namely, Fejér average accompanies an uncertainty. But this uncertainty is entirely different from the standard deviation in ensemble statistics. In current statistical interpretation of quantum mechanics, the uncertainty is usually interpreted to have a statistical origin. This assertion holds true because a wave packet usually corresponds to an ensemble of classical orbit. In our approach, the uncertainty exists because the incomplete description of Fejér average approximation of the classical quantity. This uncertainty is unrevealed before because we have seldom tried to carefully examine the relation between wave packet and a single classical orbit.

**Conclusion** The Fejér average was firstly an intellectual creation in pure mathematics is successfully demonstrated to exist in physics that reflects the objective structure of nature. The quantum mechanical average of a quantity on the EWWP in the classical limit goes over to the Fejér average of Fourier series expansion of the classical quantity, rather than the Fourier series itself as widely accepted. In the limit of large quantum number, the inequality of the energy level spacing accounts for the small difference between the quantum mechanical expectation value of a quantum quantity and the Fejér average of the classical quantity. The short term behaviors of reduced quantum motion uncertainty are almost identical to the reduced classical ones defined via the Fejér average approximation of classical quantity. This uncertainty is entirely different from either the classical one (zero) or the statistical standard deviation in the statistical interpretation of quantum mechanics.

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[4] Fourier series had not come to mathematician as a reliable and convenient tool until the discovery of the convergence of Fejér average of its partial sums in 1900. The Fejér’s theorem is: The Fejér average of the partial sums of the Fourier series \( S_n = \sum_{k=-n}^{n} \exp(ik\pi x/l) \) as \( \sigma_n = (S_0 + S_1 + S_2 + \ldots S_{n-1})/n \) approximate the given function \( f \) at each point where \( f(x+0) \) and \( f(x-0) \) exit and \( f(x) = \frac{1}{2}[f(x+0) + f(x-0)] \), and uniformly when \( f \) is continuous on the circle. As a consequence, the Gibbs phenomenon does not occur with the Fejér average. On its history, see, Kahane J.-P. and Lemarie-Rieusset P.-G., Fourier series and wavelets, (Gordon and Breach, Luxembourg, 1995). On its fundamentals, see, for example, Hardy G. H., and Rogosinski W. W., Fourier Series (3rd ed),(Cambridge University Press, Cambridge, 1956). On its applications, see, Jerri A. J., The Gibbs phenomenon in Fourier Analysis, Splines and Wavelet Approximations, (Kluwer, London,1998). On its modern developments, see a recent review: Gottlib D., and Shu C. W., SIAM review, 39, (1997)644. Nearly every university student in mathematics department knows the theorem and its importance. But when I (Liu) asked ten theoretical physics professors if they heard of this terminology before, only one with mathematical background told me that he did.

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FIG. 1. Corresponding to each \( n \) ranging from 10 to 500, there is a unique value of \( N \) (dotted curve) minimizing the uncertainty \( \Delta x \Delta p \). The smooth curve is \( \sqrt{n} \). Since \( N = \lfloor \sqrt{n} \rfloor \pm 1 \) with \( [x] \) the integer part of \( x \), \( N \approx \sqrt{n} \) give a nice fit.

FIG. 2. When \( N = 23, p_n = \pm p_c = \pm 500\pi \), i.e., \( n = 500 \), and taking 500\( \pi \) as the unit of the momentum, the Fejér average approximations \( F \langle x \rangle \) (solid sawtooth wave), \( F \langle p \rangle \) (solid square wave), and the quantum mechanical averages \( \langle x \rangle \) (dotted sawtooth curve), and \( \langle p \rangle \) (dotted square curve) in the EWWP. In the first period, \( \langle x \rangle \) and \( F \langle x \rangle \) are almost the same, and so are \( \langle p \rangle \) and \( F \langle p \rangle \). In some intervals two curves completely coincide, only one curve is possibly visible.
FIG. 3. The difference between $\langle x \rangle$ and $F \langle x \rangle$ viewed from the “magnifier” the reduced uncertainty $\delta x$ (dotted curve) and the classical one $\delta' x$ (solid curve). The difference between $\langle x \rangle$ and $F \langle x \rangle$ comes from the inequality of energy level spacing. Both curves are entirely different from classical result $\delta x = 0 \ (x \neq 0)$.

FIG. 4. The difference between $\langle p \rangle$ and $F \langle p \rangle$ viewed from the “magnifier” the reduced uncertainty $\delta p$ (dotted curve) and the classical one $\delta' p$ (solid curve). Both are entirely different from classical result $\delta p = 0 \ (p \neq 0)$. 