The Classical Limit of Quantum Mechanics and the Fejér Sum of the Fourier Series Expansion of a Classical Quantity

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(August 3, 2000)

In quantum mechanics, the expectation value of a quantity on a quantum state, provided that the state itself gives in the classical limit a motion of a particle in a definite path, in classical limit goes over to Fourier series form of the classical quantity. Different from this widely accepted point of view, a rigorous calculation shows that the expectation value on such a state in classical limit exactly gives the Fejér’s arithmetic mean of the partial sums of the Fourier series.

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I. INTRODUCTION

It is widely accepted that the expectation value of a quantity in any quantum state must become, in the classical limit, simply the classical value of the quantity, provided that the state itself gives, in the limit, a motion of a particle in a definite path [1]. And the expectation value in the classical limit gives the Fourier series form of the classical quantity [1]. In this Letter, we would like to point out that the expectation value on such a state in classical limit is exactly the Fejér’s arithmetic mean of the partial sums of the Fourier series. The Fourier series itself and the Fejér’s arithmetic mean of the partial sums of the Fourier series are different. Even through both of them can be used to represent a periodic function, conceptually they are totally different from each other. Furthermore, the former is worse than the latter in convergence [2].

In our approach, the classical limit will refer to the following mathematically well-established one [3]:

\[ n \to \infty, \hbar \to 0, \hbar n = an\text{ appropriate classical action}. \tag{1}\]

In order to obtain a definite classical path in classical limit, we must start from a wave function of a particular form [1]. A routine way to construct such a wave function is \( \sum_n c_n \psi_n \), where the coefficients \( c_n \) are noticeably different from zero only in some range \( \delta n \) of values of the quantum number \( n \) such that \( 1 \ll \delta n \ll n \); the numbers \( n \) are supposed large and the superposed states \( \psi_n \) have nearly the same energy. This particular wave function, commonly called wave packet, suffices to discuss the classical limit of quantum mechanics. To note that the choice of a set of coefficients \( c_n \) is a matter of convenience. The only requirement on the distributions of \( c_n \) among \( n \) is that they must be equal to each other in classical limit, otherwise we would give results rather than correct classical mechanical ones (we will come back to this point in Section IV). For example, the commonly used Gaussian distribution or Poisson distribution meets this requirement in classical limit, for both give the same thing: the distribution of \( c_n \) among \( n \) being approximately equal. So, the characteristic of the classical limit of quantum mechanics is involved in the classical limit of the following wave packet, which is a linear combination of energy eigenfunctions of large quantum number with equal weight (equally-weighted wave packet, for abbreviation) of the following form:

\[ |\psi(t)\rangle = \frac{1}{\sqrt{2N+1}} \sum_{m=-N}^{N} |n + m\rangle \exp(-iE_{n+m}t/\hbar), \tag{2}\]

where \( n \) and \( N \) are positive integers and \( N > 0, n - N > 0 \). In fact, this wave packet not only does the job well but also is very easy to handle. As we will see later, for matching with the exact classical result in classical limit, \( n \) and the parameter \( N \) are necessarily large in physics, or approach infinity in terms of mathematics. It is what

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we expected. However, in the following section II, the expectation value on the equally-weighted wave packet in the classical limit will be shown to be the Fejér’s arithmetic mean of the partial sums of the Fourier series, rather than the Fourier series itself. In section III, an example will be given. In section IV, a brief discussion and conclusion will be presented.

II. CLASSICAL LIMIT OF EQUALLY-WEIGHTED WAVE PACKET

The expectation of a physical observable \( f \) on the wave packet is

\[
<\psi(t)|f|\psi(t)> = \frac{1}{2N+1} \sum_{m'=-N}^{N} \sum_{m=-N}^{N} <n+m'|f|n+m> \exp[i(E_{n+m'} - E_{n+m})t/\hbar].
\]

(3)

For the simple and integrable quantum systems having classical correspondence, the Bohr’s correspondence principle holds true. It asserts that in classical limit \((E_{n+m'} - E_{n+m})/\hbar = (m'-m)\omega\), with \(\omega\) denoting the classical frequency \([1]\). Also in the classical limit, the matrix element \(<n+m'|f|n+m> = f_{m'-m}\) is the \((m'-m)\)th Fourier component of the corresponding classical quantity \(f(t)\) in terms of the ordinary Fourier series \([4]\). The latter relation appears trivial to some, Landau and Lifshitz for instance \([1]\), and is quite new to others. It should be emphasized that the two relations above are generally applicable only in the classical limit \([4]\). One should not confuse the Bohr’s correspondence principle, \((E_{n+m'} - E_{n+m})/\hbar = (m'-m)\omega\), with the difference of energy eigenvalues for a harmonic oscillator. One can easily verify that the Bohr’s correspondence principle is valid for hydrogen atom, rigid rotators and particles in an infinite square-well potential, etc. Then we have:

\[
<\psi(t)|f|\psi(t)> = \frac{1}{2N+1} \sum_{m'=-N}^{N} \sum_{m=-N}^{N} f_{m'-m} \exp[i(m-m')\omega t]
\]

\[
= \frac{1}{2N+1} \sum_{l=0}^{2N-1} \sum_{s=-l}^{l} f_{s} \exp[is\omega t]
\]

\[
= \frac{1}{2N+1} \sum_{l=0}^{2N} \Sigma(2N-l, -l),
\]

(4)

where we have made variable transformations as

\(s = m - m', \quad l = m + N,\)

(5)

and used the symbol \(\Sigma(\alpha, \beta)\) which is defined by

\[
\Sigma(\alpha, \beta) = \sum_{\beta} f_{s} \exp(is\omega t).
\]

(6)

Our aim is to show that the equation given by the last line of Eq.(4) and the RHS of following Eq.(12) are identical although they look different from each other. The following is a proof.

We study the sum in Eq.(4) and find that

\[
\sum_{l=0}^{2N} \Sigma(2N-l, -l) = \sum_{l=0}^{N-1} \Sigma(2N-l, -l) + \Sigma(N, -N) + \sum_{l=N+1}^{2N} \Sigma(2N-l, -l).
\]

(7)

Breaking the term \(\Sigma(2N-l, -l)\) in the first sum on RHS of above equation into two parts as \(\Sigma(l, -l) + \Sigma(2N-l, l+1)\), the RHS becomes:

\[
\sum_{l=0}^{N} \Sigma(l, -l) + \sum_{l=0}^{N-1} \Sigma(2N-l, l+1) + \sum_{l=N+1}^{2N} \Sigma(2N-l, -l).
\]

(8)

The last term in Eq.(8) can be changed into the following form with transformation \(2N-l \rightarrow l\):

\[
\sum_{l=0}^{N} \Sigma(l, -l) + \sum_{l=0}^{N-1} \Sigma(2N-l, l+1) + \sum_{l=N+1}^{2N} \Sigma(2N-l, -l).
\]
\[ \sum_{l=-N+1}^{2N} \Sigma(2N - l, -l) = \sum_{l=0}^{N-1} \Sigma(l, -2N + l). \]  

(9)

Then Eq.(8) becomes:

\[
\begin{align*}
\sum_{l=0}^{N} \Sigma(l, -l) + \sum_{l=0}^{N-1} \Sigma(2N - l, l + 1) + \sum_{l=0}^{N-1} \Sigma(l, -2N + l) \\
= \sum_{l=0}^{N} \Sigma(l, -l) + \sum_{l=0}^{N-1} \Sigma(2N - l, -2N + l) \\
= \sum_{l=0}^{N} \Sigma(l, -l) + \sum_{l=N+1}^{2N} \Sigma(l, -l) \\
= \sum_{l=0}^{2N} \Sigma(l, -l),
\end{align*}
\]

(10)

where we have used the transformation $2N - l \rightarrow l$. Thus we finally obtain:

\[ \sum_{l=0}^{2N} \Sigma(2N - l, -l) = \sum_{l=0}^{2N} \Sigma(l, -l). \]

(11)

From the definition of $\Sigma(\alpha, \beta)$, Eq.(6), we immediately know that $\Sigma(l, -l)$ is the $l$-th partial sum of the ordinary Fourier series of the classical quantity $f(t)$. We know that in the classical limit (1) together with limit $N \rightarrow \infty$, $\Sigma(N, -N)$ converges to the classical quantity $f(t)$. In fact, according to the Fejér’s summation theorem [2], in the same limit, the following arithmetic mean of the partial sums

\[ <\psi(t)|f|\psi(t)> = \frac{1}{2N+1} \sum_{l=0}^{2N} \Sigma(l, -l), \]

(12)

converges uniformly to the classical quantity $f(t)$ provided the quantity $f(t)$ is continuous [2]. This means that for every observable $f$, the expectation value in the equally-weighted wave packet in the classical limit gives the corresponding classical quantity $f(t)$. This also means that, in the same limit, the equally-weighted wave packet gives a motion of the particle in a definite classical path. Thus, our proof is complete.

### III. EQUALLY-WEIGHTED WAVE PACKET FOR A SINGLE ONE-DIMENSIONAL HARMONIC OSCILLATOR

The wave packet is

\[ |\psi(t)\rangle = \frac{1}{\sqrt{2N+1}} \sum_{m=-N}^{N} |n + m\rangle \exp(-iE_{n+m}t/\hbar). \]

(13)

We have the expectation values for quantities $H, H^2, x, x^2, p, p^2$ in the following.

\[ <\psi(t)|H|\psi(t)> = (n + \frac{1}{2})\hbar\omega. \]

(14)

\[ <\psi(t)|H^2|\psi(t)> = [(n + \frac{1}{2})\hbar\omega]^2 + (n\hbar\omega)^2 \frac{2(N+1)}{3n^2}. \]

(15)

\[ <\psi(t)|x|\psi(t)> = (\frac{2}{2N+1})^2 \sqrt{\frac{\hbar}{2\mu \omega}} \sum_{m=-N+1}^{N} \sqrt{n + m} \cos\omega t. \]

(16)

\[ <\psi(t)|x^2|\psi(t)> = \frac{2}{2N+1} \sqrt{\frac{\hbar}{2\mu \omega}} \sum_{m=-N+1}^{N} \sqrt{n + m} \cos\omega t. \]

(17)
\[ (n + \frac{1}{2}) \mu \frac{\hbar}{\omega} + \frac{\hbar}{\mu \omega} \sum_{m=-N+1}^{N} \sqrt{(n+m)(n+m-1)} \cos 2 \omega t. \]

\[ <\psi(t)|p|\psi(t)> = (\frac{2}{2N+1}) \sqrt{\frac{\hbar \mu \omega}{2}} \sum_{m=-N+1}^{N} \sqrt{n+m} \sin \omega t. \]

\[ <\psi(t)|p^2|\psi(t)> = (n + \frac{1}{2}) \mu \hbar - \mu \hbar \frac{1}{2N+1} \sum_{m=-N+2}^{N} \sqrt{(n+m)(n+m-1)} \cos 2 \omega t. \]

It is easy to see that these results in the classical limit \( N \to \infty, \quad N/n \to 0. \)

are exactly the classical quantities. And they are respectively

\[ <\psi(t)|H|\psi(t)> = E. \]

\[ <\psi(t)|H^2|\psi(t)> = E^2. \]

\[ <\psi(t)|x|\psi(t)> = \sqrt{\frac{2E}{\mu \omega^2}} \cos(\omega t). \]

\[ <\psi(t)|p|\psi(t)> = \sqrt{2 \mu E \sin(\omega t)}. \]

\[ <\psi(t)|x^2|\psi(t)> = \frac{E}{\mu \omega^2} + \frac{E}{\mu \omega^2} \cos(2 \omega t) \]

\[ = <\psi(t)|x|\psi(t)>^2. \]

\[ <\psi(t)|p^2|\psi(t)> = \mu E - \mu E \cos(2 \omega t) \]

\[ = <\psi(t)|p|\psi(t)>^2. \]

**IV. DISCUSSION AND CONCLUSION**

Before enclosing this Letter, the following points should be mentioned.

1. One should not confuse the classical state, the coherent state, Gaussian or Poisson wave packet for instance, with the classical limit of quantum mechanics. The Planck's constant \( \hbar \) can not be treat as zero in classical state of quantum mechanics while in classical mechanics it is practically zero.

2. If one starts a wave packet of following from

\[ |\psi(t)> = \sum_{m=-N}^{N} c_m |n+m> \exp(-iE_{n+m}t/\hbar), \]

where in classical limit both \( n \) and the parameter \( N \) are necessarily large, but the coefficients \( c_m \) do not be equally distributed among \( m \) even in classical limit, the dependence of the expectation values \( <\psi(t)|f|\psi(t)> \) on \( n \) will be different. It means that, for a specific system, the dependence of classical equation of motion on the classical action would be different if the action is different. It is not the case in classical mechanics. Thus, the characteristic of the classical limit of quantum mechanics is indeed involved in the classical limit of the equally-weighted wave packet.

3. The expectation value of a quantity in the equally-weighted wave packet in the classical limit goes over to the Fejér's arithmetic mean of the partial sums of Fourier series form of the classical quantity, not the Fourier series itself as widely accepted. The ordinary Fourier series differs from its Fejér sum in convergence, for some cases the former does not converge, whereas the latter does \[2\]. In comparing with our proof, the usual proof involves some approximations \[1\], and is not rigorous. We are confident that Fejér's arithmetic mean of the partial sums of Fourier decomposition of the classical quantity is the only possible form representing a single classical orbit from classical limit of quantum mechanics.
4. In our approach, we used a prerequisite that classical limit of the matrix element $< n + m' | f | n + m > = f_{m' - m}$ is the $(m' - m)\text{th}$ Fourier component of the corresponding classical quantity $f(t)$ in terms of the ordinary Fourier series [1,4]. In fact, this prerequisite is not necessary. To note that the Fejér sums can also be used to represent a periodic function [2], as does the usual Fourier series, and we can then write the classical quantity directly in the form of the Fejér sums. Because the expectation value $< \psi(t) | f | \psi(t) >$, Eq.(12), in classical limit gives nothing but a classical quantity, a comparison of the Fejér sums form of the classical quantity with the classical limit of $< \psi(t) | f | \psi(t) >$ given by Eq.(12) directly leads to the prerequisite.

5. Our study implies that one may study that physical significance of a constructed quantity $\sum_m f_{m} \exp[i(E_m - E_n)t/\hbar]$ or its like for it in classical limit corresponds to the physical quantity in terms of ordinary Fourier series. In fact there is already such a theory [5].

6. Our approach is straightforward and simple, but the results appear exact and new. Obviously, our results do not support the assertion that pure-state quantum mechanics in classical limit only reduces to classical statistical mechanics then nothing more to it [6–8].

V. ACKNOWLEDGMENT

I am indebted to Profs. Huan-Wu Peng, Ou-Yang Zhong-Can and Zu-Sen Zhao for enlightening discussions, to Dr. Zhou Haijun for useful comments and to Prof. V. Srivastava for critical reading of the manuscript. This subject is supported by Grant No: KJ952-J1-404 of Chinese Academy of Science.