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**LETTER TO THE EDITOR**

# The classical limit of quantum mechanics and the Fejér sum of the Fourier series expansion of a classical quantity

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**Abstract.** 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 the classical limit goes over to a Fourier series form of the classical quantity. In contrast to this widely accepted point of view, a rigorous calculation shows that the expectation value on such a state in the classical limit exactly gives the Fejér arithmetic mean of the partial sums of the Fourier series.

## 1. 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]. Also, 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 the classical limit is exactly the Fejér arithmetic mean of the partial sums of the Fourier series. The Fourier series itself and the Fejér arithmetic mean of the partial sums of the Fourier series are different. Even though 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]:

$$n \to \infty \qquad \hbar \to 0 \qquad n\hbar = \text{an appropriate classical action.} \tag{1}$$

In order to obtain a definite classical path in the classical limit, we must start from a wavefunction of a particular form [1]. A routine way to construct such a wavefunction 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 wavefunction, commonly called a wavepacket, 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 the classical limit, otherwise we would give results other than the correct classical mechanical ones (we will return to this point in section 4). For example, the commonly used Gaussian distribution or Poisson

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distribution meets this requirement in the 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 wavepacket, which is a linear combination of energy eigenfunctions of large quantum number with equal weight (equally-weighted wavepacket, for abbreviation) of the following form:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2N+1}} \sum_{m=-N}^{N} |n+m\rangle \exp(-\mathrm{i}E_{n+m}t/\hbar) \tag{2}$$

where $n$ and $N$ are positive integers and $N > 0$, $n - N > 0$. In fact, this wavepacket not only does the job well but is also very easy to handle. As we will see later, for matching with the exact classical result in the classical limit, $n$ and the parameter $N$ are necessarily large in physics, or approach infinity in terms of mathematics. It is what we expected. However, in section 2, the expectation value on the equally-weighted wavepacket in the classical limit will be shown to be the Fejér arithmetic mean of the partial sums of the Fourier series, rather than the Fourier series itself. In section 3, an example will be given. In section 4, a brief discussion and conclusion will be presented.

## 2. Classical limit of equally-weighted wavepacket

The expectation of a physical observable $f$ on the wavepacket is

$$\langle\psi(t)|f|\psi(t)\rangle = \frac{1}{2N+1} \sum_{m'=-N}^{N} \sum_{m=-N}^{N} \langle n+m'|f|n+m\rangle \exp[\mathrm{i}(E_{n+m'} - E_{n+m})t/\hbar]. \tag{3}$$

For the simple and integrable quantum systems having classical correspondence, the Bohr correspondence principle holds true. It asserts that in the 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 $\langle n+m'|f|n+m\rangle = f_{m'-m}$ 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 above two relations are generally only applicable in the classical limit [4]. One should not confuse the Bohr 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 correspondence principle is valid for hydrogen atom, rigid rotators and particles in an infinite square-well potential, etc. Then we have:

$$\begin{aligned}\langle\psi(t)|f|\psi(t)\rangle &= \frac{1}{2N+1} \sum_{m'=-N}^{N} \sum_{m=-N}^{N} f_{m'-m} \exp[\mathrm{i}(m-m')\omega t] \\ &= \frac{1}{2N+1} \sum_{l=0}^{2N} \sum_{s=-l}^{2N-l} f_s \exp[\mathrm{i}s\omega t] \\ &= \frac{1}{2N+1} \sum_{l=0}^{2N} \Sigma(2N-l, -l)\end{aligned} \tag{4}$$

where we have made variable transformations as

$$s = m - m' \qquad l = m + N \tag{5}$$

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

$$\Sigma(\alpha, \beta) = \sum_{\beta}^{\alpha} f_s \exp(\mathrm{i}s\omega t). \tag{6}$$

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

**Proof.** We study the sum in equation (4) and find that

$$\sum_{l=0}^{2N} \Sigma(2N-l,-l) = \sum_{l=0}^{N-1} \Sigma(2N-l,-l) + \Sigma(N,-N) + \sum_{l=N+1}^{2N} \Sigma(2N-l,-l). \tag{7}$$

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

$$\sum_{l=0}^{N} \Sigma(l,-l) + \sum_{l=0}^{N-1} \Sigma(2N-l,l+1) + \sum_{l=N+1}^{2N} \Sigma(2N-l,-l). \tag{8}$$

The last term in equation (8) can be changed into the following form with transformation $2N-l \to l$:

$$\sum_{l=N+1}^{2N} \Sigma(2N-l,-l) = \sum_{l=0}^{N-1} \Sigma(l,-2N+l). \tag{9}$$

Then equation (8) becomes:

$$\begin{aligned} &\sum_{l=0}^{N} \Sigma(l,-l) + \sum_{l=0}^{N-1} \Sigma(2N-l,l+1) + \sum_{l=0}^{N-1} \Sigma(l,-2N+l) \\ &\quad = \sum_{l=0}^{N} \Sigma(l,-l) + \sum_{l=0}^{N-1} \Sigma(2N-l,-2N+l) \\ &\quad = \sum_{l=0}^{N} \Sigma(l,-l) + \sum_{l=N+1}^{2N} \Sigma(l,-l) \\ &\quad = \sum_{l=0}^{2N} \Sigma(l,-l) \end{aligned} \tag{10}$$

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

$$\sum_{l=0}^{2N} \Sigma(2N-l,-l) = \sum_{l=0}^{2N} \Sigma(l,-l). \tag{11}$$

From the definition of $\Sigma(\alpha,\beta)$, equation (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 $N \to \infty$, $\Sigma(N,-N)$ converges to the classical quantity $f(t)$. In fact, according to the Fejér summation theorem [2], in the same limit, the following arithmetic mean of the partial sums

$$\langle\psi(t)|f|\psi(t)\rangle = \frac{1}{2N+1} \sum_{l=0}^{2N} \Sigma(l,-l) \tag{12}$$

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 wavepacket in the classical limit gives the corresponding classical quantity $f(t)$. This also means that, in the same limit, the equally-weighted wavepacket gives a motion of the particle in a definite classical path. □

## 3. Equally-weighted wavepacket for a single one-dimensional harmonic oscillator

The wavepacket is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2N+1}} \sum_{m=-N}^{N} |n+m\rangle \exp(-\mathrm{i}E_{n+m}t/\hbar). \tag{13}$$

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

$$\langle\psi(t)|H|\psi(t)\rangle = (n+\tfrac{1}{2})\hbar\omega \tag{14}$$

$$\langle\psi(t)|H^2|\psi(t)\rangle = \left[\left(n+\frac{1}{2}\right)\hbar\omega\right]^2 + (n\hbar\omega)^2\frac{N(N+1)}{3n^2} \tag{15}$$

$$\langle\psi(t)|x|\psi(t)\rangle = \left(\frac{2}{2N+1}\sqrt{\frac{\hbar}{2\mu\omega}} \sum_{m=-N+1}^{N} \sqrt{n+m}\right)\cos\omega t \tag{16}$$

$$\langle\psi(t)|x^2|\psi(t)\rangle = \left(n+\frac{1}{2}\right)\left(\frac{\hbar}{\mu\omega}\right) + \left(\frac{\hbar}{\mu\omega}\right)\frac{1}{2N+1}\sum_{m=-N+2}^{N}\sqrt{(n+m)(n+m-1)}\cos 2\omega t \tag{17}$$

$$\langle\psi(t)|p|\psi(t)\rangle = \left(\frac{2}{2N+1}\sqrt{\frac{\hbar\mu\omega}{2}} \sum_{m=-N+1}^{N} \sqrt{n+m}\right)\sin\omega t \tag{18}$$

$$\langle\psi(t)|p^2|\psi(t)\rangle = \left(n+\frac{1}{2}\right)\mu\hbar\omega - \mu\hbar\omega\frac{1}{2N+1}\sum_{m=-N+2}^{N}\sqrt{(n+m)(n+m-1)}\cos 2\omega t. \tag{19}$$

It is easy to see that these results in the classical limit (1) in conjunction with the limit

$$N \to \infty \qquad N/n \to 0. \tag{20}$$

are exactly the classical quantities. And they are respectively,

$$\langle\psi(t)|H|\psi(t)\rangle = E \tag{21}$$

$$\langle\psi(t)|H^2|\psi(t)\rangle = E^2 \tag{22}$$

$$\langle\psi(t)|x|\psi(t)\rangle = \sqrt{\frac{2E}{m\omega^2}}\cos(\omega t) \tag{23}$$

$$\langle\psi(t)|p|\psi(t)\rangle = \sqrt{2mE}\sin(\omega t) \tag{24}$$

$$\begin{aligned}\langle\psi(t)|x^2|\psi(t)\rangle &= \frac{E}{m\omega^2} + \frac{E}{m\omega^2}\cos(2\omega t)\\ &= (\langle\psi(t)|x|\psi(t)\rangle)^2\end{aligned} \tag{25}$$

$$\begin{aligned}\langle\psi(t)|p^2|\psi(t)\rangle &= mE - mE\cos(2\omega t)\\ &= (\langle\psi(t)|p|\psi(t)\rangle)^2.\end{aligned} \tag{26}$$

## 4. Discussion and conclusion

Before closing this letter, the following points should be mentioned.

(1) One should not confuse the classical state, the coherent state, or the Gaussian or Poisson wavepacket, for instance, with the classical limit of quantum mechanics. The Planck constant $\hbar$ cannot be treated as zero in the classical state of quantum mechanics while in classical mechanics it is practically zero.

(2) If one starts a wavepacket of the following form

$$|\psi(t)\rangle = \sum_{m=-N}^{N} c_m |n+m\rangle \exp(-\mathrm{i}E_{n+m}t/\hbar) \tag{27}$$

where in the classical limit both $n$ and the parameter $N$ are necessarily large, but the coefficients $c_m$ are not equally distributed among $m$ even in the classical limit, the dependence of the expectation values $\langle\psi(t)|f|\psi(t)\rangle$ on $n$ will be different. It means that, for a specific system, the dependence of the classical equation of motion on the classical action would be different if the action is different. This 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 wavepacket.

(3) The expectation value of a quantity in the equally-weighted wavepacket in the classical limit goes over to the Fejér 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 comparison 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 the classical limit of the matrix element $\langle n+m'|f|n+m\rangle = f_{m'-m}$ is the $(m'-m)$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. Note that Fejér sums can also be used to represent a periodic function [2], as does the usual Fourier series, and that we can then write the classical quantity directly in the form of the Fejér sums. Because the expectation value $\langle\psi(t)|f|\psi(t)\rangle$, equation (12), in the classical limit gives nothing but a classical quantity, a comparison of the Fejér sums form of the classical quantity with the classical limit of $\langle\psi(t)|f|\psi(t)\rangle$ given by equation (12) directly leads to the prerequisite.

(5) Our study implies that one may study that the physical significance of a constructed quantity $\sum_m f_{mn} \exp[\mathrm{i}(E_m - E_n)t/\hbar]$ or its like for it in the 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 the classical limit only reduces to classical statistical mechanics and that there is nothing more to it [6–8].

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