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Classical Limit of Expectation Values in a Wave Packet Involving Few Stationary States

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Expectation values of physical quantities in a wave packet involving few stationary states in an infinite square well are calculated. Explicit results show that the expectation values in the classical limit go over to the corresponding classical quantity in the form of the arithmetic mean (in mathematical term, the Fejér's average) of the partial Fourier series converging to the classical quantity. The number of the stationary states is that of the partial Fourer series in the Fejér's average. The quantum uncertainty is then demonstrated to have a classical counterpart.

KEY WORDS: quantum mechanics; uncertainty relation; classical correspondence; Fejér's average.

1. INTRODUCTION

What is the classical limit of expectation values of a quantity on a wave packet? The following two opposite extremes are fully understood. The first is that the so-called quasiclassical wave packet in the classical limit involves a large number of terms such that the expectation value of any quantity on it gives sufficiently accurate classical quantity (Gea-Banacloche, 1999; Landau and Lifshitz, 1987). The second is that the wave packet involves only one stationary state on which the expectation value of any quantity is in the classical limit nothing but the constant term of the Fourier series form of the classical quantity (Heisenberg, 1994; Liu and Hu, 2001). Then, what about a wave packet involving only a couple of stationary states?

For our purpose, the following "rectangular wave packet" (RWP) $|\psi(t)\rangle$ is studied,

$$|\psi(t)\rangle = \frac{1}{\sqrt{2N+1}} \sum_{m=-N}^{N} |n+m\rangle \exp(-iE_{n+m}t/\hbar), \quad (N \ll n), \qquad (1)$$

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in which there are $2N + 1$ successive stationary states centered at the nth, populated in the RWP with equal weight $\sqrt{2N+1}$. The expectation value of any quantity in the RWP is in the classical limit found to converge as $N \to \infty$ the classical quantity (Liu, 1999; Liu *et al.*, 2002). In this paper, the expectation value of quantities on the RWP with the finite Ns for a single particle in an infinite square well is explicitly calculated. The classical limit of the quantum uncertainty is given and its classical meaning is clearly illustrated. This paper consists of five sections. In Section 2, the classical motion of a particle in an infinite square well is given. The arithmetic mean (or Fejér's average) of $2N + 1$ partial sums of the Fourier series is explicitly shown. In Section 3, the quantum motion of the particle in the RWP involving only $2N + 1$ stationary states is studied. In Section 4, the meaning of the classical limit of the uncertainties Δx and Δp are investigated. In final Section 5, a short conclusion will be given.

2. CLASSICAL SOLUTION FOR A PARTICLE IN THE INFINITE SQUARE WELL

For a particle of mass μ moving in an infinite square well along x-axis, the Newtonian equation gives its solution as

$$x = \begin{cases} p_c t/\mu = a\omega t/\pi, & 0 < t < T/2 \\ 2a - a\omega t/\pi, & T/2 < t < T' \end{cases} \tag{2}$$

where p_c is the magnitude of the particle's momentum, a is the width of the potential, $T = 2a\mu/p_c$ is the duration of one period, and $\omega = 2\pi/T$ is the frequency.

A Fourier analysis of this periodic motion is given by

$$x = \frac{a}{2} - \frac{4a}{\pi^2}\sum_{r=0}^{\infty}\frac{\cos[(2r+1)\omega t]}{(2r+1)^2}, \tag{3}$$

which can be rewritten as

$$x = \sum_{l=0}^{\infty} c_l \cos(l\omega t), \tag{4}$$

where

$$c_l = \begin{cases} a/2, l = 0 \\ 0, l = \text{even positive number} \\ -4(4a/\pi^2)1/l^2, l = \text{odd positive number} \end{cases} \tag{5}$$

The $(n + 1)$th partial sum S_n of the Fourier series is then,

$$S_n = \sum_{l=0}^{n} c_l \cos(l\omega t). \tag{6}$$

It is evident that the $(2n+1)$th partial sum S_{2n} and the $(2n)$th are identical, i.e.,

$$S_{2n} = S_{2n-1}, \qquad \text{for } n > 0. \tag{7}$$

The arithmetic mean of the first $2N+1$ partial sums $S_n (n = 0, 1, 2, \ldots 2N)$ is the so-called Fejér's average which is given by

$$\begin{aligned} \sigma_{2N+1}(x) &= \frac{1}{2N+1}\sum_{n=0}^{2N} S_n(x) \\ &= \frac{a}{2} - \frac{8a}{\pi^2}\frac{1}{2N+1}\sum_{l=0}^{N-1}\sum_{r=0}^{l}\frac{\cos[(2r+)\omega t]}{(2r+1)^2}. \end{aligned} \tag{8}$$

According to the Fourier series theory, the sequence $\sigma_{2N+1}(x)$, $N = 1, 2, 3 \ldots$, uniformly converges to x (see Appendix A). In fact, the Fejér's average is a crucial intellectual invention in the development of the Fourier series theory for its uniform convergence, and a short introduction to it is available in Appendix A.

3. QUANTUM SOLUTION OF A PARTICLE IN THE INFINITE SQUARE WELL

The Schrödinger equation for the problem allows a discrete set of normalized eigenfunctions belonging to energies E_n,

$$\begin{cases} \psi_n(x,t) = \sqrt{\frac{2}{a}}\,\sin(k_n x)\,\exp\left(\frac{-iE_n t}{\hbar}\right)\theta(x)\theta(a-x), \\ k_n = \frac{n\pi}{a}, \quad E_n = \frac{\hbar^2 k_n^2}{2\mu}, \quad n = 1, 2, 3 \ldots \end{cases} \tag{9}$$

where $\theta(x)$ is the step function and $\theta(x)\theta(a-x) = 1$ only in the closed interval $[0, a]$ and $\theta(x)\theta(a-x) = 0$ otherwise. The matrix element of the position operator x between mth and nth states is computed as

$$\langle x\rangle_{mn} = \begin{cases} \frac{a}{2} & m-n=0 \\ 0 & m-n = \text{nonzero even integer} \\ \frac{2a}{\pi^2}\left(\frac{1}{(m+n)^2} - \frac{1}{(m-n)^2}\right)\exp\left(\frac{i(E_m-E_n)t}{\hbar}\right) & m-n = \text{odd integer} \end{cases} \tag{10}$$

In our problem, the RWP takes the following form:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2N+1}}\sum_{m=-N}^{N}|n+m\rangle\exp(-iE_{n+m}t/\hbar), \tag{11}$$

where n and N are two positive integers and $n - N > 0$. From it we know that there are $(2N+1)$ energy eigenstates superposed in RWP. The quantum number of these states ranges from $(n-N)$ to $(n+N)$ with n being the middle, the average quantum number.

Then the expectation value of position x is

$$\begin{aligned}\langle x\rangle &= \langle\psi(t)|x|\psi(t)\rangle = \frac{1}{2N+1}\sum_{m'=-N}^{N}\sum_{m=-N}^{N}\langle x\rangle_{n+m',n+n}\\ &= \frac{a}{2}+\frac{2a}{\pi^2}\frac{1}{2N+1}\sum_{m'=-N}^{N}\sum_{m=-N}^{N}\left[\frac{1}{(2n+m'+m)^2}-\frac{1}{(m'-m)^2}\right]\\ &\quad\times\exp\left[\frac{i(m'-m)(2n+m'+m)\omega_n t}{2n}\right],\end{aligned} \tag{12}$$

where we used result (10), and introduced two symbols ω_n and p_n which are defined by:

$$\omega_n \equiv \frac{\pi P_n}{\mu a} = \frac{n\hbar\pi^2}{\mu a^2}, \qquad p_n \equiv \sqrt{2\mu E_n} = \frac{n\hbar\pi}{a}. \tag{13}$$

Since only the terms satisfying $m' - m =$ odd integer contribute into the double sum (12), we have from (12):

$$\langle x\rangle = \frac{a}{2}+\frac{4a}{\pi^2}\frac{1}{2N+1}\mathrm{Re}(I_1+I_2) \tag{14}$$

where (a derivation is available in Appendix B),

$$\begin{aligned}I_1 &= \sum_{l=0}^{N-1}\sum_{r=0}^{l}\left[\frac{1}{(2n+2N-4l+2r-1)^2}-\frac{1}{(2r+1)^2}\right]\\ &\quad\times\exp\left[i(2r+1)\left(1+\frac{2N-4l+2r-1}{2n}\right)\omega_n t\right],\end{aligned} \tag{15}$$

$$\begin{aligned}I_2 &= \sum_{l=0}^{N-1}\sum_{r=0}^{l}\left[\frac{1}{(2n+2N-4l+2r-3)^2}-\frac{1}{(2r+1)^2}\right]\\ &\quad\times\exp\left[i(2r+1)\left(1+\frac{2N-4l+2r-3}{2n}\right)\omega_n t\right].\end{aligned} \tag{16}$$

At first glance, the quantity $\langle x\rangle$ (14) is nothing special. However, in the classical limit,

$$n\to\infty,\ N\to\infty,\ N/n\to 0,\ n\hbar\to\omega\mu a/\pi(\text{i.e., }\omega_n\to\omega). \tag{17}$$

Equations (15) and (16) reduce to be,

$$I_1 = I_2 = -\sum_{l=0}^{N-1}\sum_{r=0}^{l}\frac{\cos[(2r+1)\omega t]}{(2r+1)^2}. \tag{18}$$

Then Eq. (14) becomes

$$\langle x\rangle = \frac{a}{2} - \frac{8a}{\pi^2}\frac{1}{2N+1}\sum_{l=0}^{N-1}\sum_{r=0}^{l}\frac{\cos[(2r+1)\omega t]}{(2r+1)^2}, \tag{19}$$

which, whenever finite or infinite terms are used, is exactly the same as Eq. (8). In other words, in classical limit $\langle x\rangle = x$ with x given by (2).

4. THE CLASSICAL LIMIT OF THE QUANTUM DISPERSION

The expectation value of x^2 on the RWP is

$$\begin{aligned}\langle x^2\rangle &= \frac{a^2}{3} - \frac{1}{2N+1}\frac{a^2}{2\pi^2}\sum_{m=-N}^{n}\frac{1}{(n+m)^2}\\ &\quad + \frac{2a^2}{\pi^2}\frac{1}{2N+1}\sum_{m'=-N}^{N}\sum_{m==-1}^{N}(-1)^{m'-m}\left[\frac{1}{(2n+m'+m)^2} - \frac{1}{(m'-m)^2}\right]\\ &\quad \times \exp\left[\frac{i(m'-m)(2n+m'+m)\omega_n t}{2n}\right],\end{aligned} \tag{20}$$

which is in the same limit (17) the classical quantity x^2 in the following Fejér's average form,

$$\sigma_{2N+1}(x^2) = \frac{a^2}{3} + \frac{4a^2}{\pi^2}\frac{1}{2N+1}\sum_{l=1}^{2N}\sum_{r=1}^{l}(-1)^r\frac{\cos(r\omega t)}{r^2}. \tag{21}$$

Likewise, we have for momentum p

$$\langle p\rangle = p_n\frac{2}{(2N+1)\pi}(I_1' + I_2') = \mu\frac{d}{dt}\langle x\rangle, \tag{22}$$

where

$$\begin{aligned}I_1' &= \sum_{l=0}^{N-1}\sum_{r=0}^{l}\left[\frac{1+(2N-4l+2r-1)/(2n)}{2r+1} - \frac{2r+1}{2n+2N-4l+2r-1}\right]\\ &\quad \sin\left[(2r+1)\left(1+\frac{2N-4l+2r-1}{2n}\right)\omega_n t\right],\end{aligned} \tag{23}$$

$$\begin{aligned}I_2' &= \sum_{l=0}^{N-1}\sum_{r=0}^{l}\left[\frac{1+(2N-4l+2r-3)/(2n)}{2r+1} - \frac{2r+1}{2n+2N-4l+2r-3}\right]\\ &\quad \sin\left[(2r+1)\left(1+\frac{2N-4l+2r-3}{2n}\right)\omega_n t\right],\end{aligned} \tag{24}$$

which in the classical limit is the classical quantity $p_c = \mu\, dx/dt$ with x given by (2). Moreover we have for the square of momentum $p^2 = 2\mu H$,

$$\langle p^2 \rangle = \frac{1}{2N+1}\left(\frac{\pi\hbar}{a}\right)^2 \sum_{m=-N}^{N}(n+m)^2 = \left(\frac{n\pi\hbar}{a}\right)^2\left(1+\frac{N+N^2}{3n^2}\right) \overset{in\,(17)}{=} p_c^2. \tag{25}$$

In fact, we have recently proved in general that the classical limit of expectation values of every quantity on an RWP exactly gives the Fejér's average of a Fourier series expansion of its corresponding classical quantity (Liu, 1999).

It should be noted that when N is small, the Fejér's average $\sigma_{2N+1}(f^2)$ for the square of a quantity f does not equal to the square of Fejér's average $\sigma_{2N+1}(f)$ for the same quantity f, i.e.,

$$\sigma_{2N+1}(f^2) \neq (\sigma_{2N+1}(f))^2. \tag{26}$$

When N is large enough, the difference between $\sigma_{2N+1}(f^2)$ and $(\sigma_{2N+1}(f))^2$ can sufficiently small. Then we have a classical dispersion defined by

$$(\Delta_c f)^2 \equiv \sigma_{2N+1}(f^2) - (\sigma_{2N+1}(f))^2.$$

It is evident from our investigations above, the classical dispersion $(\Delta_c f)^2$ is the classical limit of the quantum one $(\Delta_c f)^2$, i.e.,

$$(\Delta_c f)^2 \overset{in\,(17)}{=} (\Delta_c f)^2.$$

In other words, the quantum dispersion $(\Delta_c f)^2$ does have classical correspondence $(\Delta_c f)^2$. However, the classical dispersion $(\Delta_c f)^2$ comes from the incompleteness of the Fejér's average representation of the classical quantity as long as the N is small, and does not mean that there is any intrinsic uncertainty associated with a single particle. Since the incompleteness can be gradually dismissed by letting the N approach to the infinity, RWP becomes a typical quasi-classical wave packet in the limit and the expectation value of any quantity goes over to the accurate classical quantity.

5. CONCLUSION

For the quantum motion in the infinite square well represented by the RWP involving $2N+1$ successive stationary states, the quantum dispersion $(\Delta f)^2$ of any physical quantity f in the classical limit has a macroscopic value that is a well-defined mathematical quantity, defined by $\sigma_{2N+1}(f^2) - (\sigma_{2N+1}(f))^2$ with $\sigma_{2N+1}(f)$ being the Fejér's average of the first $2N+1$ partial sums of Fourier series converging to the classical quantity f.

APPENDIX A: A SHORT INTRODUCTION TO FEJÉR'S AVERAGE

Before 1900, Fourier series appeared as a stagnant subject and did not attract much attention, for the Fourier series did not appear to mathematicians as a reliable and convenient tool due to the many uncertainties on both the possibility to represent a function and the convergence of the Fourier series itself. On December 10, 1990, an unknown 20-year-old Hungarian mathematician L. Fejér proved a famous theorem (the so-called Fejér's theorem): The Fejér's average of the partial sum of the Fourier series $S_n = \sum_{k=-n}^{n} \exp(\frac{ik\pi x}{l})$ as $\sigma_n = (S_0 + S_1 + S_2 + \cdots S_{n-1})/n$ 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's average.

APPENDIX B: A DERIVATION OF EQ. (14) FROM EQ. (12)

The double sum in Eq. (12) can be redenoted by

$$\sum_{\substack{m'=-N \\ m'-m=\text{odd integer}}}^{N} \sum_{m=-N}^{N} F(m', m) \tag{27}$$

in which the function $F(m', m)$ has the following symmetry,

$$F(m', m) = F^*(m, m'). \tag{28}$$

where symbol * denote the complex conjugate. The double sum (27) can then be simplified as

$$\begin{aligned}
\sum_{\substack{m'=-N \\ m'-m=\text{odd integer}}}^{N} \sum_{m=-N}^{N} F(m', m) &= \sum_{\substack{m'=-N \\ m'-m>0}}^{N} \sum_{m=-N}^{N} F(m', m) + \sum_{\substack{m'=-N \\ m'-m<0}}^{N} \sum_{m=-N}^{N} F(m', m) \\
&= \sum_{\substack{m'=-N \\ m'-m>0}}^{N} \sum_{m=-N}^{N} (F(m', m) + F(m, m')) \\
&= \sum_{\substack{m'=-N \\ m'-m>0}}^{N} \sum_{m=-N}^{N} (F(m', m) + F^*(m', m)) \\
&= 2\mathrm{Re} \sum_{\substack{m'=-N \\ m'-m>0}}^{N} \sum_{m=-N}^{N} F(m', m).
\end{aligned} \tag{29}$$

Therefore in the double sum (27), only the terms satisfying $m' - m > 0$ need to be considered. We divide the double sum (27) into the following two parts,

$$\sum_{\substack{m'=-N \\ m'-m=\text{odd integer}}}^{N} \sum_{m=-N}^{N} F(m', m) = \sum_{l=0}^{N} \sum_{n=0}^{N} F(N-2l, N-2n)$$

$$= \sum_{l=0}^{N} \sum_{n=0}^{N-1} F(N-2l, N-2n-1)$$

$$+ \sum_{l=0}^{N-1} \sum_{n=0}^{N} F(N-2l, N-2n). \tag{30}$$

The first part $\sum_{l=0}^{N} \sum_{n=0}^{N-1} F(N-2l, N-2n-1)$ satisfying $m' - m > 0$ is

$$\sum_{l=0}^{n} F(N-2l, N-2n-1). \tag{31}$$

The second part $\sum_{l=0}^{N-1} \sum_{n=0}^{N} F(N-2l-1, N-2n)$ satisfying $m' - m > 0$ is

$$\sum_{n=1}^{N} \sum_{l=0}^{N} F(N-2l-1, N-2n) + \sum_{l=0}^{N-1} \sum_{n=0}^{N} F(N-2l-1, N-2n-2). \tag{32}$$

Finally let $n - l = r$ in above two sums (31) and (32), the double sum (27) becomes

$$\sum_{\substack{m'=-N \\ m'-m=\text{odd integer}}}^{N} \sum_{m=-N}^{N} F(m', m) = 2\mathrm{Re} \sum_{\substack{m'=-N \\ m'-m>0}}^{N} \sum_{m=-N}^{N} F(m', m) = 2\mathrm{Re}(I_1 + I_2), \tag{33}$$

where

$$I_1 = \sum_{l=0}^{N-1} \sum_{r=0}^{l} F(N-2l+2r, N-2l-1), \tag{34}$$

$$I_2 = \sum_{l=0}^{N-1} \sum_{r=0}^{l} F(N-2l+2r-1, N-2l-2). \tag{35}$$

By using the result (33), Eq. (12) gives Eq. (14).

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