Quantum and classical propagation of a Gaussian ensemble: Two examples

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The classical behaviour of a quantum ensemble is expected to be achievable only by a limiting procedure. In this communication we discuss two remarkable examples in which position and momentum probability density functions using an arbitrary Gaussian ensemble (described by a non-coherent Gaussian wave packet) develop identically both in classical and quantum mechanics. The first case is propagation in free space and the second in a harmonic oscillator potential. In both cases quantum potential and quantum force (defined in Bohm's theory) are non-zero. This may be stated to be the outcome of the present investigation.

AFTER his classic papers on wave mechanics Schrödinger[1], in 1926, showed that by suitably superposing the energy eigenfunctions of a harmonic oscillator, one can generate a Gaussian density function whose centre of mass oscillates like a classical particle and the shape of the density curve remains unaltered during motion. If we use the ensemble picture of a ψ function, then it is implied that position and momentum density functions $\rho(x, t)$ and $\rho(p, t)$ will develop identically in the two mechanics. This is the well-known coherent state of a harmonic oscillator. In 1982, Roy and Singh[2] also found an identical behaviour for coherent states. There seems to be an exact parallelism between classical and quantum motion. This appears surprising because the two formalisms are so different. Though the exact parallelism between classical and quantum mechanics has been established for a coherent wave packet, no study, to the best of our knowledge, has been made based on a non-coherent wave packet, which is much more general.

The purpose of the present investigation is to study the relationship between classical and quantum mechanics using a non-coherent Gaussian wave packet (unlike a coherent wave packet, here shape alters with time) in the ensemble formalism. Here we show that arbitrary Gaussian density functions (non-coherent wave packet) also show similar parallelism when propagating in free space or in a harmonic oscillator potential, though quantum potential and quantum force, defined in Bohm's theory[3], are non-zero in both the cases. Apparently, there seems to be no demand for this identical behaviour and the reason for such parallelism is not known at present. The two examples studied here are unique because the demonstration of the above parallelism between the two mechanics does not require any approximation.

As in the previous study on Generalized Ehrenfest Theorem (GET)[4], we interpret a ψ-function to be describing the properties of an ensemble of identically prepared particles, so that the observable quantities (distribution functions and expectation values) can be interpreted for a classical ensemble without difficulty. We believe that in discussing the problem of classical – quantum relationship, the ensemble interpretation alone offers a plausible framework.

First, we discuss the propagation of a Gaussian ensemble in free space according to quantum mechanics (QM) and then according to classical mechanics (CM).

For quantum propagation we take the initial wave function to have the form

$$\psi(x, 0) = \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} \exp\left[-\frac{(x-x_0)^2}{4\sigma^2} + \frac{ip_0}{\hbar}(x-x_0) \right], \tag{1}$$

whose Fourier transform is given by

$$\phi(p) = \sqrt{\frac{1}{\sqrt{2\pi}\sigma_p}} \exp\left[-\frac{(p-p_0)^2}{4\sigma_p^2} - \frac{i}{\hbar} p x_0 \right], \tag{2}$$

where $\sigma_p = \hbar/(2\sigma)$. To calculate the time development of the quantum ensemble, we note that

$$\psi(x, t) = \sqrt{\frac{\sigma}{\sqrt{2\pi}(\sigma^2 + \frac{i\hbar t}{2m})}} \exp\left[-\frac{(x - x_0 - \frac{p_0 t}{m})^2}{[4\sigma^2 + \frac{i2\hbar t}{m}]} \right] \times \exp\left[\frac{ip_0}{\hbar}\left(x - x_0 - \frac{p_0 t}{2m} \right) \right] \tag{3}$$

is a solution of the equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = i\hbar \frac{\partial \psi}{\partial t},$$

and at $t = 0$, it goes over to $\psi(x, 0)$, the initial state. From this $\psi(x, t)$ we calculate the following quantum density functions:

$$\rho_{1Q}(x, t) = |\psi(x, t)|^2 = \frac{1}{\sqrt{2\pi}\sigma_t} \exp\left[-\frac{(x - x_0 - \frac{p_0 t}{2m})^2}{2\sigma_t^2} \right];$$

$$\sigma_t^2 = \sigma^2 + \frac{\hbar^2 t^2}{4m^2\sigma^2}, \tag{4}$$

$$\rho_{2Q}(p, t) = |\phi(p)|^2 = \rho_{2Q}(p, 0) = \frac{1}{\sqrt{2\pi}\sigma_p} \exp\left[-\frac{(p-p_0)^2}{2\sigma_p^2} \right]. \tag{5}$$

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To calculate classical propagation we need an expression for the initial phase space of the ensemble. We take the well-known Wigner's phase space density function[5]

$$\rho(x, p, 0) = \frac{1}{\pi\hbar}\exp\left[-\left[\frac{(x-x_0)^2}{2\sigma^2}+\frac{2\sigma^2}{\hbar^2}(p-p_0)^2\right]\right], \quad (6)$$

which is obtained by using $\psi(x, 0)$ in the Wigner's function[5] defined by

$$\rho_w(x, p, t) = \frac{1}{\pi\hbar}\int\psi^*(x+y, t)\psi(x-y, t)e^{2ipy/\hbar}dy. \quad (7)$$

From this phase space density function we calculate position probability density at time t, $\rho_{1C}(x, t)$, in the following way:

$$\rho(x, p, t) = \rho(x', p', 0),$$

where x', p' are functions of x, p and t,

$$x' = x - \frac{pt}{m},$$

$$p' = p, \quad (8)$$

and

$$\rho_{1C}(x, t) = \int_{-\infty}^{\infty}\rho(x, p, t)dp$$

$$= \int_{-\infty}^{\infty}\rho(x', p', 0)dp' = \frac{1}{\sqrt{2\pi}\sigma_t}\exp\left[-\frac{(x-x_0-\frac{p_0t}{2m})^2}{2\sigma_t^2}\right]. \quad (9)$$

For momentum density we write

$$\rho_{2C}(p, t) = \int_{-\infty}^{\infty}\rho(x, p, t)dx = \rho(p, 0). \quad (10)$$

We note that the quantum and classical results agree exactly. The spreading of the density functions particularly shows exact correspondence.

From the expression for $\psi(x, t)$ given in eq. (3), we can calculate the quantum potential Q which is given by

$$Q = -\frac{\hbar^2}{2mR}\frac{\partial^2 R}{\partial x^2} = -\frac{\hbar^2}{2m}\left[\frac{4(x-x_0-\frac{p_0t}{m})^2}{D^2}-\frac{2}{D}\right], \quad (11)$$

where

$$D = \sigma^2 + \frac{\hbar^2 t^2}{4m^2\sigma^2}.$$

To determine Q, we have written $\psi(x, t)$ as $\psi(x, t) = R(x, t)\exp[iS(x, t)/\hbar]$, where $R(x, t)$ and $S(x, t)$ are real[3]. Quantum force is defined by $-\frac{\partial Q}{\partial x}$ and in this case both Q and $-\frac{\partial Q}{\partial x}$ are non-zero. Thus we see that the existence of quantum potential and quantum force does not necessarily indicate non-classical behaviour.

Now let us consider quantum propagation in a harmonic oscillator potential.

We start with the same initial state of the ensemble as in the previous example. The propagation of a Gaussian wave function in a harmonic oscillator potential has been discussed by Tsuru[6]. From his results we get the wave function $\psi(x, t)$ (eq. (3.26) therein) which satisfies the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{1}{2}m\omega^2x^2\psi = i\hbar\frac{\partial\psi}{\partial t},$$

which reduces to the initial state given by eq. (1), at $t = 0$

$$\psi(x, t) = \sqrt{\frac{1}{(\sqrt{2\pi}\sigma_t)}}\exp\left[-\frac{(x-w)^2}{4\delta}-\frac{w_1^2}{4\delta_0}+i\gamma\right], \quad (12)$$

where

$$\sigma_t^2 = \frac{(\sin^2\omega t + 4\alpha^4\sigma^4\cos^2\omega t)}{4\alpha^4\sigma^2}, \quad w = w_0 + iw_1,$$

$$w_0 = \frac{2(x_0\cos\omega t + 4\alpha^2\sigma^4k_0\sin\omega t)}{[1+4\alpha^4\sigma^4+(1-4\alpha^4\sigma^4)\cos 2\omega t]},$$

$$w_1 = \frac{4\sigma^2k_t}{[1+4\alpha^4\sigma^4+(1-4\alpha^4\sigma^4)\cos 2\omega t]},$$

$$k_t = k_0\cos\omega t - x_0\alpha^2\sin\omega t, \quad k_0 = \frac{p_0}{\hbar}, \quad \alpha^2 = \frac{m\omega}{\hbar},$$

$$\delta = \delta_0 + i\delta_1, \quad \delta_0 = \frac{2\sigma^2}{[1+4\alpha^4\sigma^4+(1-4\alpha^4\sigma^4)\cos 2\omega t]},$$

$$\delta_1 = \frac{(1-4\alpha^4\sigma^4)\sin 2\omega t}{2\alpha^2[1+4\alpha^4\sigma^4+(1-4\alpha^4\sigma^4)\cos 2\omega t]},$$

and

$$\gamma = \frac{-\alpha^2(x_0^2-4\sigma^4k_0^2)\sin 2\omega t + 8\alpha^4\sigma^4x_0k_0(\cos 2\omega t - 1)}{2[1+4\alpha^4\sigma^4+(1-4\alpha^4\sigma^4)\cos 2\omega t]}$$

$$-\frac{1}{2}\tan^{-1}\left(\frac{\tan\omega t}{2\alpha^2\sigma^2}\right).$$

The Fourier transform of $\psi(x, t)$ is given by

$$\phi(p,t)=\sqrt{\frac{2\sqrt{\delta_0}}{\sqrt{2\pi\hbar}}}\exp\left[-\left[\frac{\delta_0}{\hbar^2}(p-p_t)^2-i(\gamma+\delta_1 k^2+w_0 k)\right]\right]. \tag{13}$$

From these results we get for the position and momentum densities of the quantum ensemble

$$\rho_{1Q}(x,t)=\frac{1}{\sqrt{2\pi\sigma_t}}\exp\left[-\left[\frac{(x-x_t)^2}{2\sigma_t^2}\right]\right], \tag{14}$$

$$\rho_{2Q}(p,t)=\frac{1}{\sqrt{2\pi\sigma_p(t)}}\exp\left[-\left[\frac{(p-p_t)^2}{2(\sigma_p(t))^2}\right]\right], \tag{15}$$

where

$$x_t = x_0\cos\omega t+\frac{p_0\sin\omega t}{m\omega},$$

$$\sigma_p^2(t)=m^2\omega^2\sigma^2\sin^2\omega t+\sigma_p^2\cos^2\omega t,$$

and

$$p_t=\hbar k_t.$$

For the classical ensemble, the solution of Liouville's equation is given by

$$\rho(x, p, t) = \rho(x', p', 0),$$

where x', p' are functions of x, p and t:

$$x' = x\cos\omega t-\frac{p}{m\omega}\sin\omega t$$

$$p' = m\omega \quad \sin\omega t \quad p \qquad \omega.$$

From $\rho(x \; p \; t$ $\rho_1 \; (x \; t$ $\rho_2 \; (p \; t$ results are given below (see Appendix).

$$\rho_1 \qquad , t)=\frac{}{\sqrt{(2\pi \; \sigma_t}}\exp\left[\quad \left[\frac{(x- \quad _t \quad ^2}{2\sigma^2}\right]\right], \tag{16}$$

$$\rho_{2C}(p,t)=\frac{1}{\sqrt{(2\pi)}\sigma_p(t)}\exp\left[-\left[\frac{(p-p_t)^2}{2\sigma_p^2(t)}\right]\right], \tag{17}$$

where

$$p(t)=-m\omega x_0\sin\omega t+p_0\cos\omega t,$$

$$\sigma_p^2(t)=(m\omega\sigma\sin\omega t)^2+(\sigma_p\cos\omega t)^2,$$

x_t and σ_t are as defined earlier. As in the previous case we find the quantum and classical propagations are identical. It may be noted that for the special case $4\alpha^4\sigma^4 = 1$, $\sigma(t)$ and $\sigma_p(t)$ become constant and the ensembles propagate without any spread in the width. This is the so-called coherent state first discussed by Schrödinger[1].

The examples we have discussed show that coherent states are not the only states which show behaviour similar to those of a classical ensemble. The state for the harmonic oscillator that we have discussed, is more general than the coherent state. Here the width of the packet oscillates as it propagates. Ensembles which behave similarly in both classical and quantum mechanics are always of interest in connection with the problem of classical limit of quantum mechanics. Though classical and quantum mechanics use widely different conceptual structures, still they have some deep-rooted similarity which is manifested in the examples studied in this communication. Position and momentum probability density functions develop identically in both the mechanics. Ultimately this result may help in determining the true relationship between the two mechanics and may be helpful in developing a proper theory of the classical limit of quantum mechanics. This is the importance of the present study.

In the present case the freely propagating Gaussian packet generates an interesting problem of interpretation of quantum mechanics, as well as an interesting application in physical sciences. By placing a particle detector at a distance larger compared to the width of the packet, we can measure the mean arrival times of the particles. For the classical ensemble we can calculate this quantity from the equation of particle tracks. But in the standard interpretation of quantum mechanics, the concept of particle motion is absent and the mean arrival time cannot be computed. However, using Bohm's causal interpretation[7] of quantum mechanics, the mean arrival time can be calculated and the condition under which these results agree with the classical values can be studied. Investigation of this intriguing problem is in progress.

Appendix

Here the phase space density function is given by

$$\rho(x, p, t) = \rho(x', p', 0),$$

where x', p' are functions of x, p and t:

$$x' = x\cos\omega t-\frac{p}{m\omega}\sin\omega t$$

$$p' = m\omega x\sin\omega t+p\cos\omega t. \tag{A1}$$

Position probability density at time t is given by:

$$\rho_{1C}(x,t) = \int_{-\infty}^{\infty} \rho(x,p,t)\mathrm{d}p$$
$$= \int_{-\infty}^{\infty} \rho(x',p',0)\mathrm{d}p' = \frac{1}{\sqrt{2\pi}\sigma_t} \times \exp\left[-\left[\frac{(x - x_0\cos\omega t - \frac{p_0}{m\omega}\sin\omega t)^2}{2\sigma_t^2}\right]\right]. \quad \text{(A2)}$$

To calculate $\rho_{2C}(p,t)$, we utilize the symmetry of $\rho(x',p',0)$ given by eq. (6) (see text). To make the symmetry explicit, we redefine the quantities involved as follows:

$$x_1' = x,\ x_2' = \frac{p}{m\omega},\ \sigma_1' = \sigma,\ \sigma_2' = \frac{\sigma_p}{m\omega},$$

$$x_{01}' = x_0,\ x_{02}' = \frac{p_0}{m\omega}.$$

Using column vector notation for (x_1', x_2'), we can write

$$X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = AX',$$

where the matrix A is given by (from eq. (A1))

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{bmatrix}.$$

In the new notation, we can write (see text, eq. (6)),

$$\rho(x,p,t) = \frac{m\omega}{\pi\hbar}\exp\left[-\sum_{i=1,2}\frac{(x_i - x_{0i})^2}{2\sigma_i^2}\right]. \quad \text{(A3)}$$

The right hand side of eq. (A3) is symmetric for the interchange between suffixes 1 and 2. $\rho_{1C}(x_1,t)$, in the new notation, may be written as

$$\rho_{1C}(x_1,t) = \frac{1}{\sqrt{2\pi}\sigma_1}\exp\left[-\frac{(x_1 - x_{01})^2}{2\sigma_1^2}\right],$$

where

$$\sigma_1^2 = a_{11}\sigma_1'^2 + a_{12}\sigma_2'^2 = \sigma^2\cos^2\omega t + \frac{\sigma_p^2}{m^2\omega^2}\sin^2\omega t,$$

and

$$x_{01} = a_{11}x_{01}' + a_{12}x_{02}' = x_0\cos\omega t + \frac{p_0}{m\omega}\sin\omega t.$$

Hence from symmetry,

$$\rho_{2C}(x_2,t) = \frac{1}{\sqrt{2\pi}\sigma_2'}\exp\left[-\frac{(x_2 - x_{02})^2}{2\sigma_2^2}\right], \quad \text{(A4)}$$

where

$$x_2 = \frac{p_0}{m\omega},$$

$$x_{02} = a_{21}x_0 + a_{22}\frac{p_0}{m\omega} = -x_0\sin\omega t + \frac{p_0}{m\omega}\cos\omega t,$$

$$\sigma_2^2 = a_{21}\sigma_1'^2 + a_{22}\sigma_2'^2 = \sigma^2\sin^2\omega t + \frac{\sigma_p^2}{m^2\omega^2}\cos^2\omega t.$$

Substituting the above values of x_2, x_{02} and σ_2^2 in (eq. (A4)), we get the (eq. (17)) (see text) for $\rho_{2C}(p,t)$, where $\sigma_p(t)$ involved in $\rho_{2C}(p,t)$ and σ_2 are connected by the following relation:

$$\sigma_p^2(t) = m^2\omega^2\sigma_2^2 = m^2\omega^2\sigma^2\sin^2\omega t + \sigma_p^2\cos^2\omega t.$$

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ACKNOWLEDGEMENTS. We thank the referee for constructive comments on the paper.

Received 25 January 2002; revised accepted 3 October 2002