Quantum Mechanics and Liouville's Equation

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In non-relativistic quantum mechanics, the absolute square of Schrödinger's wave function for a particle in a potential determines the probability of finding it either at a position or momentum at a given time. In classical mechanics the corresponding problem is determined by the solution of Liouville's equation for the probability density of finding the joint position and momentum of the particle at a given time. Integrating this classical solution over either one of these two variables can then be compared with the probability in quantum mechanics. For the special case that the force is a constant, it is shown analytically that for an initial Gaussian probability distribution, the solution of Liouville's integrated over momentum is equal to Schrödinger's probability function in coordinate space, provided the coordinate and momentum initial widths of this classical solution satisfy the minimal Heisenberg uncertainty relation. Likewise, integrating Lioville's solution over position is equal to Schrödinger's probability function in momentum space.

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1 Introduction

In 1926, when Erwin Schrödinger formulated the fundamental non-relativistic equation for quantum mechanics [1], his students rhymed:

> Erwin with his *psi* can do
> Calculations quite a few
> But one thing has not been seen:
> Just what does *psi* really mean [2].

Shortly afterwards, Max Born gave a precise meaning to *psi*, Schrödinger's wave function $\psi(\vec{r}, t)$ for a particle traveling in a potential $V(\vec{r}, t)$, by proposing that $|\psi(\vec{r}, t)|^2$ is the probability density for finding it in the position interval $(\vec{r}, \vec{r} + d\vec{r})$ at time t [3, 4]. Since then, many attempts have been made to derive this interpretation from first principles, but without success, although efforts in this direction have continued up to the present time [5]. To counter early criticisms for his interpretation, Born pointed out that in classical mechanics, the unavoidable uncertainties in initial conditions imply that in practice classical mechanics is also statistical in nature [3, 4]. But recently, in an article entitled "The trouble with quantum mechanics", Steve Weinberg asked "Since Schrödinger's equation is deterministic, how do probabilities get into quantum mechanics?" [6]. The large number of responses by physicists to his article indicates that the answer to this question is still not settled [7].

In the absence of interference effects, the time evolution of the absolute square of Schrödinger's wave function is closely related to the solution of Liouville's equation for the corresponding probability function in classical mechanics. In this note, we demonstrate this correspondence for the motion of a particle moving under the action of a constant force. For the special case that the initial probability distribution is a Gaussian function, the quantum and the classical problem can both be solved analytically. Then, if the initial widths in coordinate and momentum space satisfy the minimal Heisenberg uncertainty relation, it is shown that the evolution of the quantum and classical probability distributions is identically the same.

2 Liouville equation

We consider the Liouville equation in one dimension along the direction x of a constant force. Let $P(x, v, t)$ be the probability of finding a particle at x with velocity v at time t. Then at a later time $t + dt$

$$P(x + dx, v + dv, t + dt) = P(x, v, t), \tag{1}$$

and to first order in the infinitesimals dt, dx and dv,

$$dx\frac{\partial P}{\partial x} + dv\frac{\partial P}{\partial v} + dt\frac{\partial P}{\partial t} = 0. \tag{2}$$

Setting

$$dx = vdt\ , dv = adt. \tag{3}$$

where $a = dv/dt$ is the acceleration due to an external force that can depend on x, v and t, leads to Liouville's equation

$$\frac{\partial P}{\partial t} = -v\frac{\partial P}{\partial x} - a\frac{\partial P}{\partial v}. \tag{4}$$

For an initial Gaussian dependence of P on x and v,

$$P(x, v, 0) = \frac{1}{2\pi\sigma_x\sigma_v}\exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{v^2}{2\sigma_v^2}\right), \tag{5}$$

where σ_x and σ_v are the widths in coordinate and velocity respectively.

It can be readily shown that for the case that a is a constant, the time dependent solution of Liouville's equation, Eq. 4, is

$$P(x, v, t) = \frac{1}{2\pi\sigma_x\sigma_v}\exp\left[-\frac{\left(x - vt + \frac{at^2}{2}\right)^2}{2\sigma_x^2} - \frac{(v - at)^2}{2\sigma_v^2}\right] \tag{6}$$

Proof.

$$\frac{\partial P}{\partial x} = -\frac{\left(x - vt + \frac{at^2}{2}\right)}{\sigma_x^2}P, \tag{7}$$

$$\frac{\partial P}{\partial v} = \left[\frac{\left(x - vt + \frac{at^2}{2}\right)t}{\sigma_x^2} - \frac{(v - at)}{\sigma_v^2}\right]P. \tag{8}$$

Hence

$$\begin{aligned}\frac{\partial P}{\partial t} &= \left[\frac{\left(x - vt + \frac{at^2}{2}\right)(v - at)}{\sigma_x^2} + \frac{(v - at)a}{\sigma_v^2}\right]P \\ &= -v\frac{\partial P}{\partial x} - a\frac{\partial P}{\partial v}\end{aligned} \tag{9}$$

□

To compare this result with the corresponding solution of the Schrödinger equation for a constant acceleration a, consider the probability $P'(x, t)$ for finding a particle at x at time t independent of its velocity v. Then

$$P'(x, t) = \int_{-\infty}^{+\infty} dvP(x, v, t) = \frac{1}{\sqrt{2\pi}\sigma(t)}\exp\left[-\frac{\left(x - \frac{at^2}{2}\right)^2}{2\sigma^2(t)}\right] \tag{10}$$

where $\sigma(t) = \sqrt{\sigma_x^2 + t^2\sigma_v^2}$.

For the special case that the widths σ_x and σ_v satisfy the minimal Heisenberg uncertainty relation

$$\sigma_x\sigma_v = \frac{\hbar}{2m}, \tag{11}$$

we obtain

$$\sigma(t) = \sqrt{\sigma_x^2 + \left(\frac{\hbar t}{2m\sigma_x}\right)^2}, \tag{12}$$

The corresponding time dependent Schrödinger equation for this problem is

$$\imath\hbar\frac{\partial\psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x, t)}{\partial x^2} + V(x)\psi(x, t), \tag{13}$$

for a potential $V(x) = -amx$. Let the initial state at $t = 0$ be a Gaussian wave function with the same width σ_x as in the classical problem,

$$\psi(x, 0) = \left(2\pi\sigma_x^2\right)^{-\frac{1}{4}}\exp\left(-\frac{x^2}{4\sigma_x^2}\right). \tag{14}$$

Recently, I discussed the solution of Eq. 13 with this initial condition [8], so only the results will be given here. One finds that

$$\psi(x, t) = \phi(x, t)\exp\left[\frac{\imath S(x, t)}{\hbar}\right], \tag{15}$$

where

$$\phi(x, t) = \left[2\pi\left(\sigma_x^2 + \frac{t^2\hbar^2}{4m^2\sigma_x^2}\right)\right]^{-\frac{1}{4}}\exp\left[-\frac{\left(x - \frac{at^2}{2}\right)^2}{4\sigma_x^2 + \frac{2\imath\hbar t}{m}}\right], \tag{16}$$

and

$$S(x, t) = amt\left(x - \frac{at^2}{6}\right). \tag{17}$$

Hence, according to Eq. 10

$$|\psi(x,t)|^2 = P'(x,t), \tag{18}$$

showing that in coordinate space the probability distribution in quantum mechanics is exactly the same as in classical mechanics. A similar identity is obtained for the probability distribution in momentum space.

3 Conclusion

We have demonstrated analytically that for particle motion under the action of a constant force, the spreading in coordinate space of a quantum mechanical wave packet, and a corresponding classical distribution are exactly the same. In this special case, quantum interference effects do not occur. Originally, Schrödinger interpreted $|\psi(x,t)|^2$ to be the density of a particle like the electron, and concerned with this spreading, he wrote to Lorentz:

> Would you consider it a very weighty objection against the theory if it were to turn out that the electron is incapable of existing in a completely field free space? [9, p. 59]

Even as late as 1946, he wrote to Einstein:

> I am no friend of the probability theory, I have hated it from the first moment when our dear friend Max Born gave it birth. For it could be seen how easy and simple it made everything, in principle, everything ironed out and the true problem concealed. [10, p. 435]

Schrödinger's strong reaction to Born's probability interpretation may partly explain why it continues to be debated up to the present time.

For space dependent forces, the corresponding equations have to be solved numerically, and I have done such a calculation for the important classical and quantum problem of a central inverse square force [11, 12]. In this case the spreading of an initially well localized wave packet occurs around the center of force, and the quantum and classical distribution remain the same until the tip of the distribution catches up with its tail. Afterwards, interference effects occur in quantum mechanics that do not have a classical analog, and recurrences appear that also do not have any classical analog [13]. These recurrences have been verified experimentally for Rydberg atoms [14, 15].

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