Momentum Distributions for a Particle in a Box

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If a momentum measurement is made for a particle in a one-dimensional box in the energy eigenstate Ψ_n, what outcomes are possible? Within the box, the eigenfunction Ψ_n is a standing wave, obtained as a superposition of two traveling waves, one with momentum

$$p_n = \frac{hn}{2a}$$

and the other with momentum

$$-p_n$$

where h is Planck's constant; n is the quantum number for the energy eigenstate Ψ_n; a is the length of the box; and the particle has mass m.

Within the box, the wave function Ψ_n is an eigenfunction of the kinetic-energy operator, with eigenvalue

$$E_n = \frac{h^2 n^2}{8ma^2} = \frac{p_n^2}{2m}$$

Based on these observations, it is tempting to conclude that a momentum measurement should yield one of two values, p_n or $-p_n$, but this is not the quantum-mechanical prediction!

In this paper, we focus on the momentum distributions for systems in energy eigenstates of the particle-in-a-box Hamiltonian, a widely used quantum-mechanical model (*1–9*). We obtain simple, explicit expressions for the probabilities of observing an arbitrary momentum p for a system in state Ψ_n and demonstrate the nonclassical features of the momentum distribution. For the lowest energy eigenstate, with $n = 1$, the momentum distribution peaks at $p = 0$, rather than at the values $\pm h/2a$ predicted from E_n. With an increase in quantum number from $n = 1$ to $n = 2$, the distribution bifurcates, and the maxima for the nth level approach $\pm p_n$ as n increases, thus illustrating the transition from quantal to classical behavior.

Expression for the Momentum Wave Function

We consider a particle of mass m in a one-dimensional box of length a, described by the time-independent Schrödinger equation (*1–9*).

$$\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + \frac{8\pi^2 mE}{h^2\Psi(x)} = 0 \qquad 0 \le x \le a \tag{1}$$

for the wave function $\Psi(x)$.

The normalized energy eigenfunctions are given by (*1–9*)

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \tag{2}$$

where $n = 1, 2, 3, \ldots$, and the quantized energy levels obtained naturally from the boundary conditions

$$\Psi(0) = \Psi(a) = 0$$

are (*1–9*)

$$E = \frac{h^2 n^2}{8ma^2} \qquad \text{for } n = 1, 2, 3, \ldots \tag{3}$$

From a classical standpoint, the particle is expected to move back and forth in the box at constant speed, with momentum values $p_n = \pm\sqrt{2mE_n}$. In contrast, quantum mechanically, the energy eigenstate $\Psi_n(x)$ is not an eigenstate of the momentum operator because

$$\begin{aligned} p\sqrt{\frac{2}{a}}\sin\left(\frac{npx}{a}\right) &= -i\left(\frac{h}{2\pi}\right)\frac{\mathrm{d}}{\mathrm{d}x}\left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right) \\ &= -i\left(\frac{h}{2\pi}\right)\left(\frac{n\pi}{a}\right)\sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{a}\right) \\ &\ne p_0\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \end{aligned} \tag{4}$$

This means that the outcome of a momentum measurement for the particle cannot be predicted with certainty.

Because

$$\Psi_n(x)\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) = -\frac{i}{\sqrt{2a}}\left(e^{(in\pi x/a)} - e^{-(in\pi x/a)}\right) \qquad 0 \le x \le a \tag{5}$$

and the time-dependent wave-function $\Psi_n(x, t)$ satisfies

$$\Psi_n(x, t) = e^{-(iE_n t/\hbar)}\Psi_n(x)$$

it follows that the wave function inside the box is a superposition of traveling waves moving in opposite directions (*4*). Each of the two components of $\Psi_n(x)$ on the right-hand side of eq 5 is an eigenfunction of the momentum operator. The eigenvalues are $\pm p_n = \pm hn/2a$.

Obtaining a Momentum Wave Function

Does the quantum uncertainty correspond simply to a classical uncertainty about the direction of motion of the particle? We can answer this question by determining the probability distribution for the particle in state Ψ_n in the momentum space. Just as the probability density to find the particle located within the infinitesimal range dx about x is

$$\rho_n(x) = |\Psi_n(x)|^2 \tag{6}$$

the probability density to find the momentum within the infinitesimal range dp about p is

$$\rho_n(p) = |\Phi_n(p)|^2 \tag{7}$$

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where $\Phi_n(p)$ is the momentum wave function for the state Ψ_n. The momentum wave function $\Phi_n(p)$ is found by Fourier transformation of $\Psi_n(x)$ (*1, 2, 10*).

$$\Phi_n(p) = \left(\frac{1}{\sqrt{h}}\right)\int_{-\infty}^{\infty} \Psi_n(x)\, e^{-(2\pi i p x/h)}\mathrm{d}x \tag{8}$$

Therefore, for the particle in a box, in the state $\Psi_n(x)$,

$$\Phi_n(p) = \frac{1}{\sqrt{h}}\int_0^a \left(\sqrt{\frac{2}{a}}\right)\sin\left(\frac{n\pi x}{a}\right)e^{-(2\pi i p x/h)}\mathrm{d}x$$

$$= \frac{-i}{\sqrt{2ah}}\int_0^a \left(e^{(in\pi x/a)} - e^{-(in\pi x/a)}\right)e^{-(2\pi i p x/h)}\mathrm{d}x$$

$$= \left(\sqrt{\frac{h}{2\pi^2 a}}\right)\left(\frac{p_n}{p_n^2 - p^2}\right)\left(1 - (-1)^n e^{-(2\pi i p a/h)}\right)$$

$$= \begin{cases} \dfrac{2i\left(\sqrt{\dfrac{h}{2\pi^2 a}}\right)(p_n)\sin\left(\dfrac{pa\pi}{h}\right)e^{-(i\pi p a/h)}}{p_n^2 - p^2} & (n \text{ even}) \\[2ex] \dfrac{2\left(\sqrt{\dfrac{h}{2\pi^2 a}}\right)(p_n)\cos\left(\dfrac{pa\pi}{h}\right)e^{-(i\pi p a/h)}}{p_n^2 - p^2} & (n \text{ odd}) \end{cases} \tag{9}$$

where

$$p_n = \frac{nh}{2a} \qquad n = 1, 2, 3, \ldots$$

Equation 9 gives an explicit, simple expression for the momentum wave function, from which it is easily seen that the wave functions are amplitude-modulated and n-dependent.

Determining the Probability Distribution

The most important observation from eq 9 is that $\Phi_n(p)$ is nonzero for p values other than $\pm p_n$! The quantum uncertainty is an uncertainty in the value of the momentum, as well as its sign. This is very different from the classical behavior. It is also different from expectations based on the observation that $\Psi_n(x)$ in eq 5 is a superposition of two momentum eigenfunctions (*4, 6*). The difference reflects a "quantum confinement" effect. Equation 5 holds only within the box. To satisfy the boundary conditions, $\Psi_n(x) = 0$, elsewhere. If $\Psi(x)$ is specified by

$$\Psi(x) = \begin{cases} e^{\pm(in\pi x/a)} & \text{for } 0 \le x \le a \\ 0 & \text{for } x < 0 \text{ or } x < 0 \end{cases} \tag{10}$$

then $\Psi(x)$ is not an eigenfunction of the momentum operator. Only if $\Psi(x) = e^{\pm(in\pi x/a)}$ holds without spatial restriction is a momentum eigenfunction obtained.

The corresponding probability densities to observe the momentum in the infinitesimal range dp about p are

$$\rho_{2k}(p) = \frac{\left(\dfrac{2h}{a\pi^2}\right)(p_{2k}^2)\sin^2\left(\dfrac{p\pi a}{h}\right)}{\left(p_{2k}^2 - p^2\right)^2} \qquad (n \text{ even}, n = 2k)$$

$$\rho_{2k-1}(p) = \frac{\left(\dfrac{2h}{a\pi^2}\right)(p_{2k-1}^2)\cos^2\left(\dfrac{p\pi a}{h}\right)}{\left(p_{2k-1}^2 - p^2\right)^2} \qquad (n \text{ odd}, n = 2k - 1) \tag{11}$$

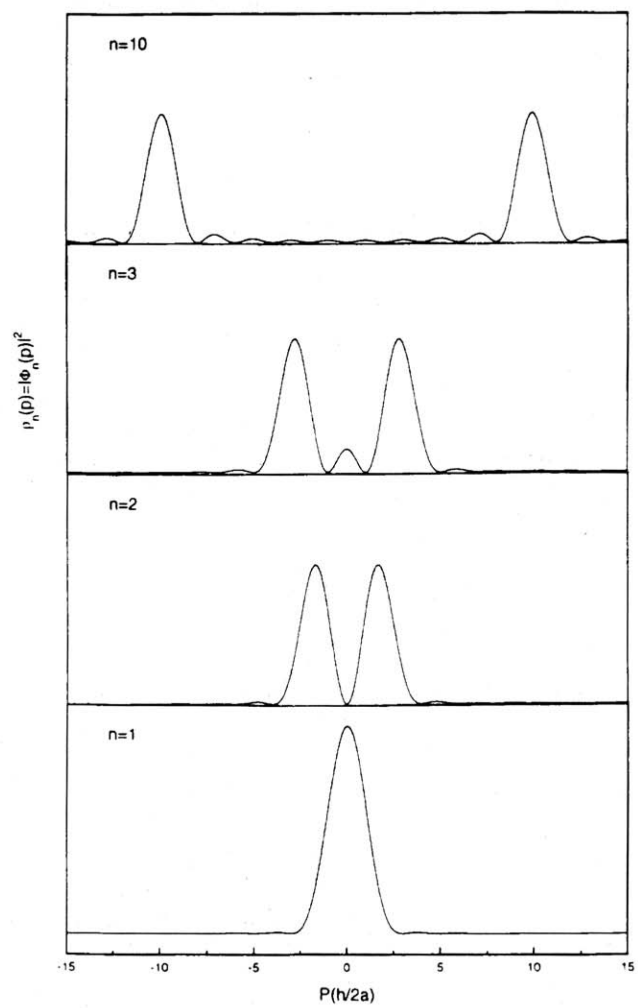
where $k = 1, 2, 3, \ldots$

The figure shows the momentum probability densities for the particle in the first several energy eigenstates. The figure and eq 11 show clearly that there is a nonzero probability density to obtain many values other than $\pm nh/2a$ from a given momentum measurement.

A discussion of the momentum probability distribution can be found in the text *Quantum Mechanics* by C. Cohen–Tannoudji, B. Diu, and F. Laloë (*1*); they provide a physical interpretation in terms of "diffraction functions". However, they do not simplify to the explicit forms of our eqs 9 and 11, and we have not found these in any other texts.

From eq 11, one can find the maxima and minima of the momentum distribution. From d$\rho(p)$/dp = 0, the conditions for the maxima are

$$\cot\left(\frac{pa\pi}{h}\right) = \frac{-2\left(\dfrac{ph}{a\pi}\right)}{p_{2k}^2 - p^2} \qquad (n \text{ even}, p \neq \pm p_{2k})$$



Momemtum distribution of a particle for various values of *n*.

$$\tan\left(\frac{pa\pi}{h}\right)=\frac{2\left(\dfrac{ph}{a\pi}\right)}{p_{2k-1}^2-p^2}\qquad (n\text{ odd}, p\neq \pm p_{2k-1})\tag{12}$$

These equations can be solved numerically (see remark 4, below). The minima of the momentum distributions occur when $\rho(p) = 0$, that is, when

$$\sin\left(\frac{pa\pi}{h}\right)=0\qquad (n\text{ even}, p\neq \pm p_n)$$

or

$$\cos\left(\frac{pa\pi}{h}\right)=0\qquad (n\text{ odd}, p\neq \pm p_n)\tag{13}$$

The separation between typical minima in the momentum distribution is obviously n-independent and equals h/a.

Remarks

1. The momentum distribution of a particle in a box gives a definite probability for observing values of p other than those corresponding to the eigen energies of the particle. Interestingly, in analogy with the nodes in the position distribution of the particle (points in space where the particle has zero probability density to be found), the momentum distributions also have zeroes at special values of the momentum. In even n states ($n = 2k$), the particle cannot have the momentum values of $p = lh/a$, where $l \neq k$, whereas in odd n states ($n = 2k - 1$), momentum values of $p = (2l - 1)h/2a$ (with $l \neq k$) cannot be observed. We can regard the momentum wave function as a standing wave set up in the momentum space, but it is amplitude-modulated.
2. The momentum of the particle in an eigenstate averages to zero due to the symmetry of momentum distribution; $\rho(p)$ is an even function of p. Thus,

$$\langle p\rangle_n=\int_{-\infty}^{\infty}p\rho_n(p)\mathrm{d}p=\int_{-\infty}^{\infty}\Psi_n(x)\left(\frac{-ih}{2\pi \mathrm{d}}\mathrm{d}x\right)\Psi_n(x)\mathrm{d}x=0\tag{14}$$

The probability densities at zero momentum are

$$\rho_{2k}(0)=0$$

$$\rho_{2k-1}(0)=\frac{8a}{(2k-1)^2h\pi^2}\tag{15}$$

In even n states, one cannot observe the particle with zero momentum (the probability is zero), whereas in odd n states, one does observe zero momentum of the particle with a certain probability. Surprisingly, in the state $\Psi_1(x)$, with $n = 1$, the most probable momentum is zero, rather than $\pm\, p_1 = h/2a$. When n becomes larger (for odd n), the probability of finding the particle with zero momentum decreases.

3. The uncertainty product $\Delta p\Delta x$ is bounded below, according to the Heisenberg uncertainty principle. Its value is n-dependent for particle-in-a-box energy eigenstates, as shown next. The average value of the position for the particle is

$$\langle x\rangle_n=\int_{-\infty}^{\infty}\Psi_n(x)x\Psi_n(x)\mathrm{d}x=(2/a)\int_0^a x\sin^2\left(\frac{n\pi x}{a}\right)\mathrm{d}x=a/2\tag{16}$$

as expected. The average value of x^2 is

$$\langle x^2\rangle_n=\int_{-\infty}^{\infty}\Psi_n(x)x^2\Psi_n(x)\mathrm{d}x$$

$$=(2/a)\int_0^a x^2\sin^2\left(\frac{n\pi x}{a}\right)\mathrm{d}x=\left(\frac{a}{2}n\pi\right)^2\left(\frac{4n^2\pi^2}{3}-2\right).\tag{17}$$

Thus the root-mean-square deviation of the position for the particle is

$$\Delta x=\sqrt{\langle x^2\rangle_n-\langle x\rangle_n^2}=\left(\frac{a}{2n\pi}\right)\sqrt{\left(\frac{n^2\pi^2}{3}-2\right)}\tag{18}$$

The mean value of p^2 is given by

$$\langle p^2\rangle_n=\int_{-\infty}^{\infty}p^2\rho_n(p)\mathrm{d}p=\int_{-\infty}^{\infty}\Psi_n(x)\left(\frac{-ih}{2\pi}\frac{\mathrm{d}}{\mathrm{d}x}\right)^2\Psi_n(x)\mathrm{d}x=\left(\frac{nh}{2a}\right)^2\tag{19}$$

and the root-mean-square deviation of the momentum is

$$\Delta p=\sqrt{\langle p^2\rangle_n-\langle p\rangle_n^2}=\frac{nh}{2a}\tag{20}$$

Combining eqs 18 and 20, one obtains

$$\Delta p\Delta x=\left(\frac{nh}{2a}\right)\left(\frac{a}{2n\pi}\right)\sqrt{\left(\frac{n^2\pi^2}{3}-2\right)}\geq h/4\pi\tag{21}$$

This exceeds the requirements of the uncertainty principle. The uncertainty product grows as n increases! At first glance, this might appear to conflict with expectations that the behavior grows increasingly classical as n increases. However, an interesting result emerges from a calculation of the uncertainty product $\Delta p\Delta x$ for a purely classical particle subject to the following assumptions.

- The particle has equal probability to be observed anywhere in the box.
- The momentum of the particle is either $nh/2a$ or $-nh/2a$, with equal probability.
- The energy is constant at the value $n^2h^2/(8ma^2)$.

For the classical particle, the position and momentum averages satisfy

$$\langle x\rangle_n = a/2,\ \langle x^2\rangle_n = a^2/3,\ \langle p\rangle_n = 0, \text{ and } \langle p^2\rangle_n = n^2h^2/(4a^2).$$

This yields $\Delta p\Delta x = nh/4\sqrt{3}$, which is precisely the large n limiting behavior of eq 21. The classical uncertainty product is independent of the size of the box.

4. The probability density at $p = \pm p_n$ is a constant (n-independent).

$$\lim_{p\to p_n}\rho(p)=\frac{a}{2h}\tag{22}$$

Most Probable Momentum

The most probable momentum is not $\pm p_n$ when the particle is in state $\Psi_n(x)$. Instead, by numerical calculations (eq 12) we find the following values for the most probable momentum p_m in different states.

n	p_m ($\pm h/2a$)
1	0.000
2	1.675
3	2.790
4	3.845
5	4.950
...	
10	9.985

The figure shows that the momentum distribution for the particle bifurcates from a single peak (in the $n = 1$ state) to two separate peaks near $p = \pm p_n$ (for all states $n \geq 2$). Only when n becomes large does the probability density $\rho(p)$ reach its maximum at $p_m \cong \pm p_n$. Then the quantum and classical descriptions are similar, in accord with the Bohr correspondence principle.

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