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The particle in a box is not simple

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Naive use of the position representation wave functions for a particle in either a finite or infinite square well predicts properties of the momentum distribution in disagreement with those calculated in the momentum representation. The discrepancy is removed by explicit consideration of the effects of the discontinuity in the potential at the walls on position space calculations.

I. INTRODUCTION

The particle in a one-dimensional box is universally presented to students as one of their first quantum-mechanical problems both for its mathematical simplicity and for the fact it incorporates most of the unique features of a quantum-mechanical system. If one transforms the position wave functions to momentum space and considers the expectation values, $\langle p^s \rangle$, for powers of the linear momentum $\mathbf{p}$, one soon notes the simplicity is deceptive as the two representations at first glance give discordant results. Similar discrepancies are found for the finite square-well problem. We explore here the source and resolution of the disparity in the two systems.

II. THE PROBLEM

For the particle in a one-dimensional box of length a the x axis is divided into three regions with potentials

$$\begin{aligned} V &= \infty, \quad x < -a/2 \quad \text{(region I)}, \\ V &= 0, \quad -a/2 < x < a/2 \quad \text{(region II)}, \\ V &= \infty, \quad a/2 < x \quad \text{(region III)}, \end{aligned} \tag{1}$$

and wave functions

$$\psi_{\rm I}(x) = \psi_{\rm III}(x) = 0,$$

$$\psi_{\rm II}(x)_n = (2/a)^{1/2} \cos(bx) \quad (n \text{ odd}), \tag{2}$$

$$\psi_{\rm II}(x)_n = (2/a)^{1/2} \sin(bx) \quad (n \text{ even}),$$

$$b = (2mE_n/\hbar^2)^{1/2}, \qquad E_n = n^2\pi^2\hbar^2/2ma^2. \tag{3}$$

Using $\psi_{\rm II}$ and the integration range $-a/2 \le x \le a/2$ it is easy to show that for even s

$$\langle p^s \rangle_n = \langle p^2 \rangle_n{}^{s/2} = (2mE_n)^{s/2}, \tag{4}$$

which implies a finite value for $\langle p^s \rangle$ for all even s and a momentum distribution consisting of δ functions at $p = \pm(2mE_n)^{1/2}$ for all values of the box width. The latter follows from recognizing that the probability of finding the particle with a value of p in the range p to $p + dp$ must be positive definite and that in the integral for $\langle p^s \rangle$ the factor p^s acts as a weighting function which varies with p. If the distribution were continuous, Eq. (4) would not obtain as it implies a constant (in absolute magnitude) weighting.

Taking the Fourier transform of $\psi(x)$ as in Eq. (5)

$$\phi_n(p) = (2\pi\hbar)^{-1/2} \int_{-a/2}^{a/2} \exp\left(\frac{-ipx}{\hbar}\right) \psi_{\rm II}(x)_n \, dx, \tag{5}$$

one obtains for the momentum functions normalized to unity[1]

$$\phi_n(t) = \frac{N_n \sin t}{1 - (2t/n\pi)^2} \quad (n \text{ even}),$$

$$\phi_n(t) = \frac{N_n \cos t}{1 - (2t/n\pi)^2} \quad (n \text{ odd}), \tag{6}$$

$$t = pa/2\hbar,$$

$$N_n = (4a/n^2\pi^3\hbar)^{1/2} (-1)^{(n+1)/2}. \tag{7}$$

For given n the distribution has major peaks centered near $p = \pm(2mE_n)^{1/2}$ which collapse to δ functions as the box becomes very large.[2] The distribution function $I_n(p)$ is not two-valued and, as it is everywhere positive and decays as p^{-4} for large p, moments with even $s \ge 4$ are infinite.[3]

Since the two representations are equivalent, these discrepancies force a closer look at the calculation of $\langle p^s \rangle$ in position space.

A similar need arises in the case of a finite well where the potential is

$$\begin{aligned} V(x) &= V_0, \quad x < -a/2 \quad \text{(region I)}, \\ V(x) &= 0, \quad -a/2 < x < a/2 \quad \text{(region II)}, \\ V(x) &= V_0, \quad a/2 < x \quad \text{(region III)}. \end{aligned} \tag{8}$$

The even-parity position wave functions for regions I and II are[4]

$$\psi_{\rm I}(x) = A \cos(\beta a/2) \exp[\alpha(x + a/2)],$$

$$\psi_{\rm II}(x) = A \cos(\beta x), \tag{9}$$

with A a normalization constant and the constants α and β as given in Appendix A where the momentum wave functions obtained as the Fourier transforms of the even- and odd-position parity functions are presented. Of interest is that for large p, $I(p)$ decays as p^{-6} such that in momentum space $\langle p^s \rangle$ is infinite for even $s \ge 6$ while in position space it remains finite if one does just the three integrations implied by Eq. (8).

Considering the particle in a box and the finite well systems together it is clear the problem involves the discontinuity in V with the change from a finite to an infinite potential jump only shifting the discrepancy from $s = 6$ to $s = 4$.

III. SOLUTION

The source of the problem appears in a qualitative consideration of a box with rounded corners and very steeply rising V for which V and all its derivatives are continuous. The wave function for this rounded box will have continuous derivatives and approach the true squared box function asymptotically outside a small region about $x = \pm a/2$. In Fig. 1 we show the first few derivatives for such a function near the left-hand corner of the box. The function is discussed briefly in Appendix B. The rapid sharp oscillations in Fig. 1 imply that since $\langle p^s \rangle \propto \langle d^s/dx^s \rangle$ one cannot ignore, out of hand, the wall region as was done in calculating $\langle p^s \rangle_n$ in the limiting case of a squared box in Eq. (5).

For an infinite square well $d\psi(x)/dx$ is discontinuous at each wall. It then follows[5] that $d^2\psi(x)/dx^2$ is a δ function, $\kappa\delta(x)$, and $d^4\psi(x)/dx^4$ is $\kappa d^2\delta(x)/dx^2$ at $x = \pm a/2$. Properly then in position space,

$$\langle p^s \rangle = (2mE_n)^{s/2} + 2 \int_{-a/2-\epsilon}^{-a/2+\epsilon} \psi(x) \frac{d^s}{dx^s} \psi(x)\, dx. \tag{10}$$

where ϵ is a vanishingly small positive number. Letting

$$t = a/2 + x,$$

the integral in Eq. (10) can be rewritten as

$$\int_{-a/2-\epsilon}^{-a/2+\epsilon} \psi(x) \frac{d^s}{dx^s} \psi(x)\, dx = \kappa \int_0^\epsilon [\psi_{\mathrm{II}}(t) - \psi_{\mathrm{I}}(-t)] \times \frac{d^{s-2}}{dt^{s-2}} \delta(t)\, dt. \tag{11}$$

As $\psi_{\mathrm{I}}(t) = 0$ for $t < 0$ and $\psi_{\mathrm{II}}(t) \propto \sin(bt) = bt$, for small $t > 0$, the integrals of concern for $\langle p^2 \rangle$ and $\langle p^4 \rangle$, respectively, are

$$\int_0^\epsilon t\delta(t)dt = 0, \tag{12}$$

$$\int_0^\epsilon t \frac{d^2\delta(t)}{dt^2}\, dt = 2 \int_0^\epsilon t^{-1}\delta(t)\, dt = \infty. \tag{13}$$

The relation in Eq. (13) may be found by integration by parts or by direct differentiation and reuse of the relation[5]

$$x\delta'(x) = -\delta(x) \tag{14}$$

to obtain

$$x\delta''(x) = -2\delta'(x) = \delta(x)/x \tag{15}$$

and for later reference

$$x\delta'''(x) = -6\delta(x)/x^2. \tag{16}$$

Thus the wall effects do not change the value for $\langle p^2 \rangle$ but completely determine $\langle p^s \rangle$ for even $s \geq 4$ and eliminate the discrepancy between the position and momentum representations.

For a finite square well $d^2\psi(x)/dx^2$ is the first discontinuous derivative such that here $d^3\psi(x)/dx^3 = \kappa'\delta(x)$. Expansion of $\psi_{\mathrm{I}}(x)$ and $\psi_{\mathrm{II}}(x)$ from Eq. (9) about $x = -a/2$ gives for small t

$$\psi_{\mathrm{II}}(t) - \psi_{\mathrm{I}}(-t) \propto t^2 + O(t^3).$$

For $\langle p^4 \rangle$ and $\langle p^6 \rangle$ one has, respectively, the integrals

$$\int_0^\epsilon t^2 \frac{d\delta(t)}{dt}\, dt = -\int_0^\epsilon t\delta(t)\, dt = 0, \tag{17}$$

$$\int_0^\epsilon t^2 \frac{d^3\delta(t)}{dt^3}\, dt = -6 \int_0^\epsilon t^{-1}\delta(t)\, dt = \infty, \tag{18}$$

such that consideration of the discontinuity effect again results in accord between the two representations.

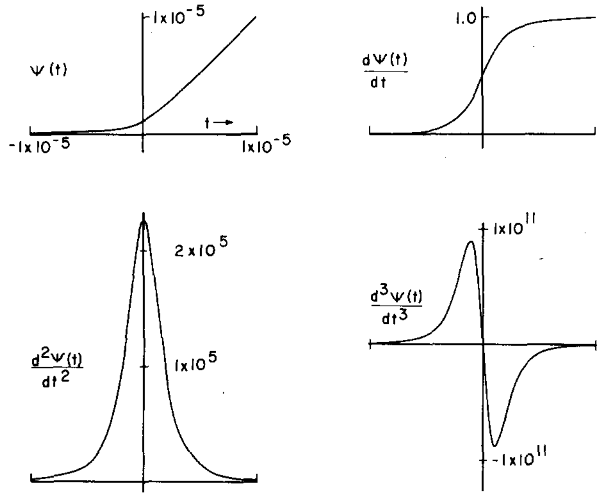

Fig. 1. Model position wave function and its first three derivatives at the left-hand wall of a particle in a box with rounded corners.

IV. CONCLUSION

We have shown that the quantum-mechanical problem of a particle in a box is not as simple as it seems at first sight because of the discontinuity in the potential V. Here, as in other systems, transformation to the momentum representation provides information which is less readily apparent in the position representation. The result for the finite square well is a general one. A discontinuity in V requires a discontinuity in $d^2\psi(x)/dx^2$ from the Schroedinger equation which in turn implies that $\psi_a(t) - \psi_b(-t) \propto t^2$ if the two wave functions in the adjoining regions are expanded in powers of t about the point of discontinuity in V. Thus, for any system with a finite discontinuity in V, $\langle p^6 \rangle = \infty$.

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APPENDIX A

For the finite well of depth V_0 and width a, the momentum wave functions found from the odd-parity position wave functions[4] as the Fourier transform are

$$\phi(z) = A_0[\beta \sin(d) \cos(za/2) - z \cos(d) \sin(za/2)] \times [(\alpha^2 + \beta^2)/(\alpha^2 + z^2)(\beta^2 - z^2)], \tag{A.1}$$

with

$$z = p/\hbar, \qquad \alpha = [2m(V_0 - E)/\hbar^2]^{1/2},$$
$$d = \beta a/2, \qquad \beta = (2mE/\hbar^2)^{1/2}, \tag{A.2}$$
$$\tan(d) = (V_0/E - 1)^{1/2},$$

$$A_0 = 2^{3/2}(2\pi\hbar)^{-1/2} \{[\cos(2d) + 1]/\alpha + \sin(2d)/\beta + a\}^{-1/2}. \tag{A.3}$$

Those for the even-parity functions are

$$\phi(z) = A_e[-\beta \cos(d) \sin(za/2) + z \sin(d) \cos(ca/2)] \times [(\alpha^2 + \beta^2)/(\alpha^2 + z^2)(\beta^2 - z^2)], \tag{A.4}$$

$$A_e = 2^{3/2}(2\pi\hbar)^{-1/2}\{[1-\cos(2d)]/\alpha - \sin(2d)/\beta + a\}^{-1/2}. \quad \text{(A.5)}$$

APPENDIX B

Taking the origin for a particle in a box at the left-hand wall and letting the length $a = 2$ and $t = bx$, the position wave functions are

$$\psi_{\rm I}(t)_n = 0 \qquad \text{(region I and III)},$$

$$\psi_{\rm II}(t)_n = \sin(t) \qquad \text{(region II)}. \quad \text{(B.1)}$$

To investigate the wall effects for a steeply rising potential with continuous derivatives we seek a function which reduces to $\psi_{\rm I}$ and $\psi_{\rm II}$ in the limit, has continuous derivatives, and closely approximates or approaches asymptotically $\psi_{\rm I}$ and $\psi_{\rm II}$ outside a small region about $t = 0$ although not necessarily for large t. The hyperbolic type function

$$y = 0.5\{\sin(t) + [\sin^2(t) + 2c^2/\tan(\pi/8)]^{1/2}\} \quad \text{(B.2)}$$

fulfills these conditions. This function and its first three derivatives are plotted in Fig. 1 for $c = 1.0 \times 10^{-6}$ in the range $-1.0 \times 10^{-5} \leq t \leq 1.0 \times 10^{-5}$. For this value of c the function, y, and its first three derivatives are within 0.07% of the true values at $|t| = 0.01$.

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