Addendum

Addendum to ‘Divergence of \(\langle p^6 \rangle\) in discontinuous potential wells’ (2018 Eur. J. Phys. 39 055402)

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Abstract

In an earlier article (Eur. J. Phys. 39 055402), potential wells with discontinuous jump have been found to have the expectation value \(\langle p^s \rangle\) to be divergent for all bound states. Here in this addendum, we prove and demonstrate that for continuous but non-differentiable wells it diverges for even states and converges for odd states; here, \(p\) denotes momentum. We present three exactly solvable models.

Keywords: Schrödinger equation, bound states, momentum space eigenfunctions, expectation values of \(p^2s\), divergence in \(\langle p^s \rangle\)

(Some figures may appear in colour only in the online journal)

Earlier, the divergence of expectation value of even powers of momentum \(p^2s\), \(s = 2, 3, 5 \ldots\) has been argued and demonstrated \([1, 2]\) even for simple textbook \([3]\) models like infinitely deep well (IDW) and square well potentials. More recently, we proved and demonstrated the divergence of \(\langle p^s \rangle\) for half-potential wells with jump discontinuity \([4]\). Here in this addendum we consider potential wells which are continuous but non-differentiable at \(x = 0\). In them, we report that \(\langle p^6 \rangle\) diverges for even parity states but it converges for the odd ones.

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Expectation value of $p^6$ for three potentials in figure 1: the expectation value of $p^6$ is given in terms of various derivatives of the potential $V$ [4]

$$\langle p^6 \rangle = \int_{-\infty}^{\infty} F_2[\psi, \psi', V, V', V'', V^{(iv)}] dx$$

$$-\langle \psi | E - V(x) | \psi \rangle. \quad (1)$$

In the above equation (1) the part $\langle \psi(x) | V^{(iv)}(x) | \psi(x) \rangle$ is the main source of divergence in $\langle p^6 \rangle$. For $V_1(x)$ we have

$$\langle V^{(iv)}(x) \rangle \rightarrow 2V_0 \int_{-\epsilon}^{\epsilon} \delta''(x) \psi^2(x) dx$$

$$\rightarrow -4V_0 \int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x^2} \psi^2(x) dx, \quad (2)$$

which is finite for an odd state ($\psi_o(x) \approx Bx$) and infinite for an even state ($\psi_e(x) \approx A$). For $V_2(x)$, $V^{(iv)}(x) \rightarrow \frac{4V_0}{a} \exp[-2|x/a| \delta''(x)]$. So for $V_2(x)$, we have

$$\langle V^{(iv)}(x) \rangle \rightarrow \frac{8V_0}{a} \int_{-\epsilon}^{\epsilon} \exp[-2|x/a| \delta(x)] \frac{\delta(x)}{x^2} \psi^2(x) dx, \quad (3)$$

which diverges for an even parity state ($\psi(x) \approx A$) and converges for the odd one ($\psi(x) \approx Bx$). Similar results follow for $V_3(x)$. The expectation of higher even powers of $p$, e.g. $\langle p^8 \rangle$, will consist of $\delta''(x)$ and hence it will diverge.

In the following, we study the momentum distributions $p^2 I(p)$, $p^4 I(p)$ and $p^6 I(p)$ for three exactly solvable models for the ground state and the first excited state by finding $\phi(p)$ from their position space eigenfunction $\psi(x)$ using the Fourier transform of $\psi(x)$, as $\phi(p) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$. The momentum distribution $I(p)$ is obtained as $|\phi(p)|^2$.

1. **Symmetric triangular well**: This potential is given as

$$V(x) = V_0 \frac{|x|}{a}, \quad V_0 > 0. \quad (4)$$

The Schrödinger equation for this potential when $x \geq 0$ can be transformed to the Airy differential equation [7] as
This second order equation has two linearly independent solutions called Airy functions $A_i(y)$ and $B_i(y)$. It is $A_i(y)$ that vanishes as $x \to \infty$, so we admit the solution of (5) as

$$A_i'(y_0) = 0, \quad \psi(x) = C A_i(y(x)), \quad y_0 = -\frac{2mE}{\hbar^2 g^2}.$$  \hfill (6)

For the odd parity states we demand $\psi(0) = 0$, so the eigenvalue condition and the eigenfunctions are

$$A_i(y_0) = 0, \quad \psi(x) = C \text{sgn}(x) A_i(y(x)),$$  \hfill (7)

We take $V_0 = 5$ and $a = 1$ in arbitrary units, the well has two bound states at $E = 2.9789$ and $E = 6.8366$ as per equations (6) and (7). The three momentum distributions are plotted for the first even and the first odd state in figures (a) and (b), respectively. $p^2\psi(p)$ and $p^2|\psi(p)|^2$ show fast convergence to zero in both parts (a) and (b) but $p^2\psi(p)$ has long tail in (a) displaying a divergence for $p^6$, whereas the odd parity states presents short range characteristic of the distribution $p^6|\psi(p)|^2$.

2. Symmetric (convergent) exponential well: This potential is given as

$$V(x) = -V_0 \exp(-2|x|/a), \quad V_0 > 0$$  \hfill (8)

The Schrödinger equation for this potential can be transformed to the Bessel equation [5, 7] as

$$\frac{d^2\psi}{dw^2} + w \frac{d\psi}{dw} + \left(k^2 w^2 + w^2\right)\psi = 0,$$  \hfill (9)

$$w = qa e^{-|x|/a}, \quad k = \frac{\sqrt{2m(-E)}}{\hbar}, \quad E < 0,$$  \hfill (9)

$$q = \frac{\sqrt{2mV_0}}{\hbar}.\hfill (9)$$

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Figure 2. Various momentum distributions $p^j\psi(p)$, $j = 1, 2, 3$ for the triangular potential well (4): (a) for first even parity state, (b) for the first odd parity state. Distributions for $j = 1, 2$ are convergent, however for $j = 3$ in (a) the distribution shows a long tail for even parity state.
whose two linearly independent solutions are $J_{ka}(w)$ and $J_{-ka}(w)$. Noting that when $w$ is very small $J_{ka}(w) \approx \frac{\sin(w)}{\Gamma(1 + ka)}$ so when $x > 0$, $J_{ka}(w) \sim e^{-kw}$ represents a bound solution. So we choose $\psi(x) = C J_{ka}(qae^{-|x|/a})$. For even parity states, we demand $\psi'(0) = 0$ to get quantization condition and the corresponding eigenfunctions as

$$J'_{ka}(qa) = 0, \quad \psi(x) = C J_{ka}(qae^{-|x|/a}). \quad (10)$$

For the odd parity states, we demand $\psi(0) = 0$ and get the quantization condition and the corresponding eigenfunctions as

$$J_{ka}(qa) = 0, \quad \psi(x) = C \text{sgn}(x) J_{ka}(qae^{-|x|/a}). \quad (11)$$

For $V_0 = 15$, $a = 1$ equation (10) yields the ground state eigenvalue as $E = -7.346$ 0 and equation (11) yields the eigenvalue of the first excited state as $E = -1.062$ 2. For the first two states, we plot various distributions as in figure 2. One can visualize the long tail in $p^6\langle p^6 \rangle$ in figure 3(a) that would give rise to divergence in $\langle p^6 \rangle$ for the even parity state.

3. Symmetric (divergent) exponential well: This potential is written as

$$V(x) = V_0[e^{2|x|/a} - 1], \quad (12)$$

for which the Schrödinger equation when $x \geq 0$ can be transformed to the cylindrical Bessel equation as [6, 7]

$$z^2 \frac{d^2 \psi}{dz^2} + z \frac{d\psi}{dz} + (-\kappa^2a^2 - z^2)\psi = 0,$$

$$z = qae^{x|/a}, \quad \kappa = \sqrt{2m(E + V_0)}/\hbar, \quad q = \sqrt{2mV_0}/\hbar. \quad (13)$$

Out of two linearly independent solutions of (13) as modified Bessel function: $I_{ka}(z)$ and $K_{ka}(z)$. Here, we choose $K_{ka}(z)$ as the solution of (13) since it vanishes for $|x| \sim \infty$. For even parity states we demand $\psi'(0) = 0$, then the quantization condition and eigenfunctions are given as

$$K'_{ka}(qa) = 0, \quad \psi(x) = C K_{ka}(qae^{x|/a}). \quad (14)$$

For odd parity state we demand $\psi'(0) = 0$, we get the eigenvalue equation and eigenfunctions as
For $V_0 = 5$ and $a = 1$, we get first two bound states in the potential at $E = 6.4646$ and $E = 17.5365$. The three distributions are plotted in figure 4, where the solid line in figure 4(a) yet again indicates a much longer tail justifying the divergence of $\langle p^6 \rangle$ for the even parity state.

We would like to mention that if $\langle p^6 \rangle$ is divergent, hence $\langle p^{2j} \rangle$, $j = 4, 5, 6...$ also diverge. Also, $\langle p^{2j+1} \rangle$ for $j = 0, 1, 2, ...$ vanish due to the antisymmetry of the integrands. We believe that this addendum adds significantly to the interesting investigations \[1, 2, 4\], wherein even and odd parity states show a new disparate behaviour respectively in the divergence and the convergence of $\langle p^6 \rangle$.

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**Figure 4.** The same as in figure 2, for the divergent exponential potential well (12). Note the much longer tail in (a) in the solid curve, indicating the divergence of $\langle p^6 \rangle$ for the even parity state.

\[
K_{\text{isol}}(qa) = 0, \quad \psi(x) = C \text{ sgn}(x)K_{\text{isol}}(qa\sqrt{x}/a),
\]

(15)
Divergence of $\langle p^6 \rangle$ in discontinuous potential wells

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Abstract

The surprising divergence of the expectation value $\langle p^n \rangle$ for the square well potential is known. Here, we prove and demonstrate the divergence of $\langle p^6 \rangle$ in potential wells which have a finite jump discontinuity. Apart from the square well, two-piece half-potential wells are such examples. These half-potential wells can be expressed as $V(x) = -U(x) \Theta(x)$, where $\Theta(x)$ is the Heaviside step function. $U(x)$ are continuous and differentiable functions with a minimum at $x = 0$ and which may or may not vanish as $x \to \infty$.

Keywords: Schrödinger equation, discontinuous potential wells, momentum distributions, expectation values of even powers of momentum

(Some figures may appear in colour only in the online journal)

In quantum mechanics [1–3] students are told to find the expectation value $\langle \psi(x)|F|\psi(x) \rangle$ of an operator $F$ using the eigenfunction of a bound state that is a continuous and normalizable solution of the Schrödinger equation,

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0. \quad (1)$$

Recently, it has been pointed out that $\psi(x)$ needs to vanish faster than $|x|^{-3/2}$ [4] in order to have a finite value for $\langle x^2 \rangle$ and the uncertainty in position $\Delta x$. Otherwise, the state will be a

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bound but (infinitely) extended state. Interestingly, the potential \( V(x) \) with a ground state where the asymptotic fall-off is slower than this is found to have only one bound state.

Students are also advised to work in momentum representation \([1–3]\) where the wave function \( \psi(x) \) is given as

\[
\psi(x) = \frac{1}{(2\pi\hbar)^{-1/2}} \int_{-\infty}^{\infty} \psi(x)e^{-i\pi/p^2}dx,
\]

the Fourier transform of \( \psi(x); \mathcal{F}[\psi(x)] \). The two representations are physically equivalent. One can find \( \langle x^2 \rangle \) as \( \langle \psi(x)|x^2|\psi(x)\rangle \) or \( \langle \phi(p)|-\hbar^2(\partial^2/\partial x^2)|\phi(p)\rangle \). Similarly, \( \langle p^2 \rangle \) can be found as \( \langle \psi(x)|-\hbar^2(\partial^2/\partial x^2)|\psi(x)\rangle \) or \( \langle \phi(p)|p^2|\phi(p)\rangle \). We can again demand that in order to have \( \langle \phi(p)|p^2|\phi(p)\rangle \) and \( \Delta p \) as finite, \( \phi(p) \) needs to vanish faster than \( |p|^{-3/2} \). The question arises as to what property of \( V(x) \) ensures a finite value for \( \langle p^2 \rangle \) in a potential well.

Most often the mathematical forms of \( \psi(x) \) and \( \phi(p) \) are different, so much so that for finding something, one option is either easier to do or more transparent than the other one. Also, these two options present different mathematical situations. For instance, for an infinite square well (ISW), the \( p \)-integral in finding \( \langle p^2 \rangle \) is improper \([5]\) whereas the \( x \)-integrals are proper and simple.\(^1\) For ISW, \( \langle p^4 \rangle \) in the position representation gives a finite value: it actually diverges in momentum space. A similar experience is found \([6]\) in the finite square well (FSW), where it is \( \langle p^6 \rangle \) that presents an interesting discrepancy between the two representations.

This discrepancy was first pointed out in a largely unnoticed paper \([7]\) where for FSW \( \langle \phi(p)^2 \rangle \) was derived to show a surprising asymptotic fall-off as \( p^{-6} \), however the details of \( \phi \) (\( p \)) were incorrect and these have been corrected recently \([6]\). The consequent divergence of \( \langle p^6 \rangle \) in FSW in position space was revealed in terms of the Dirac delta discontinuities in the second and higher order derivatives of \( \psi(x) \) at the end points \( x = \pm a \). Unfortunately, this proof \([7]\) turns out to be tautological even for FSW.

Here, in this paper, we wish to prove and demonstrate the general divergence of \( \langle p^6 \rangle \) when a potential well has a finite jump discontinuity. Apart from the square well, two-piece half-potential wells (figure 1) are like

\(^1\) The well-known integral \( \int_{0}^{\infty} \frac{x}{x^2 + 1}dx = \pi/2 \) is improper but convergent as its integrand exists as a finite limit when \( x \to 0 \). But \( \int_{0}^{\infty} \frac{\ln x}{x}dx \) is an improper integrand which diverges. See e.g., \([5]\).
$V(x) = -U(x) \Theta(x), \quad \Theta(x < 0) = 0, \quad \Theta(x \geq 0) = 1,$  

where $U(x)$ are continuous and differentiable functions with a non-zero minimum at the junction ($x = 0$). $U(x)$ may or may not vanish as $x \to \infty$, see figure 1. We also call them half-potential wells because for $x > 0$ they are half parts of the well-known parabolic $U(x) = -V_0(1 - x^2/\alpha^2)$ [1], triangular $U(x) = -V_0(1 - |x|/\alpha)$ [2], Eckart $U(x) = -V_0\text{sech}^2(x/\alpha)$ [2, 3] and exponential $U(x) = -V_0(2 - \exp(-2|x|/\alpha))$ [8] wells.

A definite integral $\int_a^b f(x)\,dx$ is real and finite if it is continuous at each and every point of the domain $[a, b]$, $f(x)$ may also be piecewise continuous for this integral to exist. Otherwise, the integrals are improper which may be convergent (finite) or divergent (infinite) [5]. One can evaluate the expectation value of $p^2$ for the $n^{th}$ bound state as

$$\langle \psi_n | p^2 | \psi_n \rangle = 2m \int_{-\infty}^{\infty} \psi_n(x)[E_n - V(x)] \psi_n(x)\,dx,$$  

which is easily finite. Let us fix $2m = 1 = \hbar^2$ for the sequel. The eigenstate $\psi_n(x)$ is both continuous and differentiable in $(-\infty, \infty)$, for continuous $V(x)$ the above integral is finite. $V(x) = -2\delta(x)$ is an interesting digression wherein $\langle p^2 \rangle$ is finite owing to the interesting property that $\int_{-\infty}^{\infty} f(x)\delta(x)\,dx = f(0)$.

Next, we suggest $\langle p^4 \rangle$ be evaluated as

$$-\int_{-\infty}^{\infty} \psi(x) \frac{d^2}{dx^2}[E - V(x)]\psi(x)\,dx,$$  

which can be rewritten in an inspiring form as

$$\langle p^4 \rangle = \int_{-\infty}^{\infty} F[\psi, \psi', V', V'']\,dx + \langle \psi | (E - V(x))^2 | \psi \rangle.$$  

Ordinarily, the first integral in the above simplifies to $[V'(x)\psi^2(x)]_{-\infty}^{\infty}$. When $V(x)$ is continuous and differentiable, it vanishes since $\psi(x)$ are bound states that converge to zero, asymptotically. Alternatively, inside the first integral in (6), there occur terms like $V'(x)\psi(x)\psi'(x) + V''(x)\psi^2(x)$. For the Dirac delta well $V(x) = -2\delta(x)$, using the interesting derivatives [9] $V'(x) = 2\delta'(x)/x$ and $V'' = -4\delta(x)/x^2$; $\psi_0(x) = e^{-|x|}$, the second term causes strong divergence in $\langle p^4 \rangle$ near $x = 0$ as

$$\int_{-\epsilon}^{\epsilon} V''(x)\psi^2(x)\,dx = -4 \int_{-\epsilon}^{\epsilon} e^{-2|x|}\delta(x)\,dx \to \infty.$$  

Had there been odd eigenstate(s), this integral would have been convergent and finite. This explains the divergence of $\langle p^4 \rangle$ in position space which is obvious in momentum space as $\phi(p) = \sqrt{2/\pi} (1 + p^2)^{-1}$ [10]. Next, we verify that the expectation value of force $(-V'(x))$, namely

$$\langle \psi | V'(x) | \psi \rangle \to 2\int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x} \psi^2(x)\,dx \to 2 \int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x} (1 - 2|x|)\,dx$$  

vanishes as there is an odd integrand between symmetric limits. The vanishing of integrals in equation (8), may not be without arguments. Here, we underline that otherwise the Ehrenfest theorem will be defied by the Dirac delta well potential which is the most popular among potential wells.

By virtue of the fact that eigenfunctions of bound states are continuous and differentiable at any point in the domain of the potential, one can plot a tangent on $\psi(x)$ that behaves locally as $n\delta(x) = -\delta'(x)$ see [9]. Further successive differentiations yield: $x^n\delta^{(n)}(x) = (-1)^n n! \delta'(x)$.
\[ \psi(x) \approx \alpha + \beta(x - x_0), \forall x_0 \in (-\infty, \infty) \]  

(9)

in the close vicinity of any point \( x = x_0 \). In particular, for half-potential wells discussed here, due to asymmetry of the potential, even around \( x = 0, \alpha \neq 0 \). Strangely, in [7] (see above equation (17)), \( \psi(x) \) near the point of discontinuity of FSW has been assumed to be \( \psi(x) \approx \gamma(x - x_0)^2 \) which cannot be true, since a more general approximation could be \( \psi(x) \approx \alpha + \beta(x - x_0) + \gamma(x - x_0)^2 \), where in any case the linear term will dominate by orders. This makes this proof of divergence of \( \langle p^4 \rangle \) in FSW tautological.

First, we would like to give a correct proof of convergence of \( \langle p^4 \rangle \) and the divergence of \( \langle p^6 \rangle \) in the square well potential [7],

\[ V(x) = -V_0[\Theta(x) - \Theta(x - a)]. \]  

(10)

Let us consider the integrals of expectation value (6) in the infinitesimal domain \((-\epsilon, \epsilon)\) around \( x = 0 \) for (10). Here we have \( V' = -V_0[\delta(x) - \delta(x - a)] \), \( V'' = -V_0[\delta'(x) - \delta'(x - a)] \), \( V''' = -V_0[\delta''(x) - \delta''(x - a)] \), \( Viv = -V_0[\delta^iv(x) - \delta^iv(x - a)] \). As seen above in (7), \( \langle \psi^iv[Viv]\psi(x) \rangle \) is the main source of divergence in \( \langle p^4 \rangle \). So, for the square well we can write

\[
\langle \psi[V'[\psi] \rangle = -V_0 \int_{-\infty}^{\infty} [\delta'(x) - \delta'(x - a)] \psi^2(x) dx \\
\rightarrow V_0 \left( \alpha^2 \int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x} dx + \alpha_1^2 \int_{-\epsilon}^{\epsilon} \frac{\delta(t)}{t^2} dt \right). 
\]  

(11)

where \( \alpha \) and \( \alpha_1 \) are due to the local behavior of \( \psi(x) \) as per equation (9) at points \( x = 0 \) and \( x = a \), respectively. These are \( y \)-axis cuts of tangents on \( \psi(x) \) at these points which are essentially unequal (see the appendix). As in equation (8), these two integrals vanish and hence \( \langle p^4 \rangle \) is convergent. In \( \langle p^6 \rangle \) the source of divergence is the term \( \langle V'iv\psi(x) \rangle \), which in the infinitesimal domain around \( x = 0 \) and \( x = a \) can be written as

\[
\langle \psi[V''[\psi] \rangle = -V_0 \int_{-\infty}^{\infty} [\delta''(x) - \delta''(x - a)] \psi^2(x) dx \\
\rightarrow 12V_0 \left( \alpha\beta \int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x^2} dx + \alpha_1\beta_1 \int_{-\epsilon}^{\epsilon} \frac{\delta(t)}{t^2} dt \right). 
\]  

(12)

The parameters \( \beta \) and \( \beta_1 \) are slopes of tangents on \( \psi(x) \) at points \( x = 0 \) and \( x = a \), respectively. These two parameters may be equal or may be equal but of opposite signs (see the appendix), consequently we end up with \( \alpha\beta = \alpha_1\beta_1 \). This leads to the divergence in equation (12) as in equation (7). Hence in square well, \( \langle p^6 \rangle \) diverges. Next, the expectation value of force for equation (10) is

\[ \langle \psi_\alpha(x)[V'(x)]\psi_\alpha(x) \rangle = V_0[\psi_\alpha^2(0) - \psi_\alpha^2(a)]= 0, \]  

(13)

which can be verified by using the eigenfunctions of square well potential.

Further, owing to interesting derivatives, namely \( \Theta'(x) = \delta(x) \) and \( \delta'(x) = -\delta(x)/x \) [9], for the potentials (3) the term \( \langle \psi(x)[V'(x)]\psi(x) \rangle \) in (6) in the infinitesimally small domain \((-\epsilon, \epsilon)\) appears as

\[ -\int_{-\epsilon}^{\epsilon} U(x) \frac{\delta(x)}{x} (\alpha + \beta x)^2 dx \rightarrow V_0 \alpha^2 \int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x} dx, \]  

(14)

which can be taken to vanish as in equation (8). Therefore, \( \langle p^4 \rangle \) for the type of potentials (3) discussed here is convergent.
For the expectation value of $\langle p^6 \rangle$, we get

$$\langle p^6 \rangle = \int_{-\infty}^{\infty} F_2[\psi, \psi', V, V', V''', V'''']dx. \quad (15)$$

In the above equation the part $\langle \psi(x)|V'''(x)|\psi(x)\rangle$ is the main source of divergence in $\langle p^6 \rangle$.

The potentials (3) which are piecewise continuous with finite jump discontinuity at $x = 0$, the successive derivatives of $V(x)$ are: $V'(x) = U'(x)\Theta(x) + U(x)\delta(x)$, $V''(x) = U''(x)\Theta(x) + 2U'(x)\delta(x) + U(x)\delta'(x)$, $V'''(x) = U'''(x)\Theta(x) + 3U''(x)\delta(x) + 3U'(x)\delta'(x) + U(x)\delta''(x)$ and $V''''(x) = U''''(x)\Theta(x) + 4U'''(x)\delta(x) + 6U''(x)\delta'(x) + 4U'(x)\delta''(x) + U(x)\delta'''(x)$.

Noting the interesting derivatives [9] as $\Theta(x) = \delta(x)$, $x\delta'(x) = -\delta(x)$, $x\delta''(x) = 2\delta(x)/x$, $x\delta'''(x) = -6\delta(x)/x^2$, we find that in $\langle p^6 \rangle$ (equation (10)) the term $\langle \psi(x)|V'''(x)|\psi(x)\rangle$ can cause divergence in the infinitesimal domain $(-\epsilon, \epsilon)$ as

$$\langle p^6 \rangle = \int_{-\infty}^{\infty} U(x)\delta''(x) \psi^2(x) dx \rightarrow 12\alpha_\beta>V_0 \int_{-\epsilon}^{\epsilon} \frac{\delta(x)}{x^2} dx,$$  

which diverges.

We would like to re-emphasize that in our proofs given above our assumption for the eigenstates (9) and vanishing of the integral $\int_{-\infty}^{\infty} [\delta(x)/x] dx$, play the most crucial role.

In the following, we present four analytically solvable models of half-potential wells (equation (3)) wherein a much longer tail of $p^6 I(p)$ would justify the acclaimed (equation (12)) divergence of $\langle p^6 \rangle$. $I(p)$ denotes the momentum distribution calculated as $I(p) = |\psi(p)|^2$, where $\psi(p)$ is the Fourier transform (2) of $\psi(x)$ that will be obtained in the sequel. In the fifth and sixth solvable models, which are continuous but nondifferentiable wells, we show that $\langle p^6 \rangle$ is convergent.

1. **Half-parabolic well**: This potential is written as

$$V(x) = -V_0 \left[ 1 - \frac{x^2}{a^2} \right] \Theta(x), \quad (17)$$

For $x \geq 0$, the Schrödinger equations (1) for (17) can be transformed to a parabolic cylindrical differential equation [1, 11] as

$$\frac{d^2\psi}{dz^2} + \left[ \nu + \frac{1}{2} - \frac{z^2}{4} \right] \psi = 0, \quad z = \gamma x, \quad \nu = \frac{E + V_0}{\omega} - \frac{1}{2}, \quad (18)$$

where $\omega = \sqrt{\frac{2m\hbar^2}{\alpha^2}}, \quad \gamma = \frac{\alpha}{\sqrt{\frac{8mV_0}{\hbar^2}}}. \quad$ One of the two linearly independent solutions $D_\nu(\pm z)$ (called parabolic cylinder functions) of this equation is $D_\nu(z)$ which vanishes at $z = \infty$ and can be taken to be the correct solution for $x \geq 0$ as $\psi(x \geq 0) = BD_\nu(z)$. The solution of equation (1) for $x < 0$ is $\psi(x < 0) = Ae^{\pm \nu x}$. By matching these two pieces and their derivative at $x = 0$, we get an eigenvalue equation as

$$\gamma D_\nu'(0) = k D_\nu(0), \quad k = \sqrt{\frac{2mE}{\hbar^2}}. \quad (19)$$

The energy eigenfunctions are given as

$$\psi(x < 0) = C D_\nu(0) e^{\nu x}, \quad \psi(x \geq 0) = C D_\nu(\gamma x). \quad (20)$$

We propose to fix $2m = 1 = \hbar^2, a = 2, V_0 = 15$ in arbitrary units for all the wells to be considered in the sequel. Solving equation (19), we find bound states at $E = -10.6370, -3.9894$. In figure 2, we plot the distributions $p^2 I(p)$ (dotted line), $p^4 I(p)$ (dashed line) and $p^6 I(p)$ (solid line) for the ground state. Notice the higher and longer tail in the solid curve than that of the dashed curve, indicating that $\langle p^6 \rangle$ would actually diverge.
2. Half-triangular well: This potential is given as

\[ V(x \geq 0) = -V_0 \left[ 1 - \frac{x}{a} \right], \quad V(x > 0) = 0. \] (21)

The Schrödinger equation (1) for this potential when \( x \geq 0 \) can be transformed to the Airy differential equation as

\[ \frac{d^2 \psi}{dy^2} - y\psi = 0, \quad y(x) = \frac{2m}{g^2 h^2} \left[ \frac{V_0 x}{a} - E - V_0 \right], \quad g = \sqrt{\frac{2mV_0}{\hbar^2 a}}. \] (22)

This second order equation has two linearly independent solutions called Airy functions, \( Ai(y) \) and \( Bi(y) \). It is \( Ai(y) \) that vanishes as \( y \to \infty \), so we admit the solution of (22) as \( \psi(x \geq 0) = BAi(y) \) and for \( x < 0 \), we have \( \psi(x < 0) = Ae^{kt} \). Matching these two solutions and their derivative at \( x = 0 \), we obtain the energy quantization condition as

\[ gAi'(y_0) = kAi(y_0), \quad y_0 = -\frac{2m E + V_0}{\hbar^2 g^2}. \] (23)

For these discrete energies the eigenfunctions are given as

\[ \psi(x < 0) = CAi(y_0)e^{kt}, \quad \psi(x \geq 0) = CAi(y(x)). \] (24)

We take \( V_0 = 15 \) and \( a = 2 \) in arbitrary units; the well has two bound states at \( E = -8.1408 \) and \( -1.8025 \). For the ground state, we plot various distributions as in figure 3. We confirm the high and long tail in \( p^2I(p) \) that would give rise to divergence in \( \langle p^6 \rangle \).

3. Half-Eckart potential: This potential is expressed as

\[ V(x \geq 0) = -V_0 \text{sech}^2(x/a), \quad V(x < 0) = 0. \] (25)

The Schrödinger equation (1) for this potential when \( x \geq 0 \) can be transformed to the Gauss hypergeometric equation as \([2, 3, 11]\)
The solution of (26) which vanishes for \( x \sim \infty \) is given as

\[
\psi(x \geq 0) = C(1 - z^2)^{1/2} \, {}_2F_1[ka - s, ka + s + 1, ka + 1, \frac{1}{2}(1 - z)].
\]  

(27)

For \( x < 0 \), we have \( \psi(x < 0) = C_0 F_1[ka - s, ka + s + 1, ka + 1; 1/2]e^{kt} \). By matching these two solutions and their derivative at \( x = 0 \), we get the eigenvalue equation in terms of hypergeometric function \( {}_2F_1[a, b, c; 1/2] \) [8] which are known in terms of Gamma functions \( \Gamma(t) \) [11]. Utilizing such results, we obtain the eigenvalue equation as

\[
ka + 2 \Gamma[(1 + ka - s)/2] \Gamma[(2 + ka + s)/2] = 0.
\]

(28)

For \( V_0 = 15 \) and \( a = 2 \), we get four bound states in the potential at \( E = -10.9628, -5.8470, -2.2641, -0.3400 \). Distributions: \( p^j I_j, j = 1, 2, 3 \) for ground state are shown in figure 4.

4. Half-exponential well: This potential is written as

\[
V(x \geq 0) = -V_0[2 - e^{2x/a}], \quad V(x < 0) = 0
\]

(29)

for which the Schrödinger equation (1) when \( x \geq 0 \) can be transformed to the cylindrical Bessel equation as \([8, 11]\)

\[
\frac{1}{z} \frac{d^2\psi}{dz^2} + \frac{1}{z} \frac{d\psi}{dz} + \left(-\kappa^2a^2 - z^2\right)\psi = 0, \quad z = qae^{-x/a},
\]

\[
\kappa = \sqrt{2m(E + 2V_0)/\hbar}, \quad q = \sqrt{2mV_0}/\hbar.
\]

(30)

There are two linearly independent solutions of (30) as modified Bessel functions: \( I_\nu(z) \) and \( K_\nu(z) \). Here, we choose \( K_0(z) \) as the solution of (30) for \( x > 0 \) since it vanishes for \( x \sim \infty \). However, we have \( \psi(x < 0) = Ae^{kt} \). We match these two solutions and their derivative at \( x = 0 \) to get the energy eigenvalue equation
For the discrete energy roots of this equation we get the eigenfunctions for Eq. (29) as
\[ y(x) \leq K(qa) \exp(\pm x/a) \].

For \( V_0 = 15 \) and \( a = 2 \), we get one bound state in the potential at \( E = -3.9249 \). The three distributions are plotted in figure 5, where the solid line yet again presents a high and long tail, justifying the divergence of \( \langle p^6 \rangle \).

Also, for \( j \neq 0, 1, 2, \ldots \), also diverge.\( \langle p^{2j+1} \rangle \) for \( j = 0, 1, 2, \ldots \) vanish due to the antisymmetry of the integrands. Momentum distributions for other interesting one-dimensional potential wells can be seen in [12, 13].

The expectation value of force for the delta well has been shown in equation (8) to follow the Ehrenfest theorem in an interesting way. We have checked that the bound states of all the half-well potentials (equation (3)) discussed here indeed comply with the Ehrenfest theorem as.
in mathematically different ways.

In this paper, we have stated, proved and demonstrated the divergence of \( \langle p^6 \rangle \) in potential wells which have a finite jump discontinuity. Our proofs are in position space and the demonstrations in figures 2–5 are in momentum space. Our proofs are simple and transparent which also suggest corrections for the square well case [7]. We underline the fact that though both representations are physically equivalent, one is more convenient than the other for a given purpose. Four analytically solvable models, and the high and long tail of their distributions in figures 2–5, testify to our claim. Normally, the two-piece half-potential wells would be passed off like other one-piece finite-potential wells which have a finite number of bound states. The present work shows a distinction between the two. For these half-potential wells, since \( \langle p^2 \rangle \) is finite, so is the uncertainty product. So these models would continue to be of interest in normal physical applications. Additionally, now or in future, if there is a requirement for the wells which entails the divergence of \( \langle p^6 \rangle \) (sixth moment of the momentum distribution), the solvable models discussed here will be up for renewed consideration. It turns out that just one finite jump discontinuity in the potential well causes the divergence of \( \langle p^2 \rangle \) for \( j = 3, 4, 5, \ldots \). The Dirac delta well turns out to be a unique well where it is \( \langle p^2 \rangle \) which is divergent.

Appendix

For the square well potential, \( V(|x| < a) = -V_0, \quad V(|x| \geq a) = 0 \), the energy eigenfunctions can be written [14] in an interesting way as

\[
\psi(x \leq 0) = e^{\alpha x}, \quad \psi(0 < x < a) = \eta^{-1} \sin[k(x - a/2) + n\pi/2]
\]

\[
\psi(x \geq a) = (-1)^{n+1} e^{-\kappa(x-a)}.
\]

where \( \gamma = \sqrt{2mV_0 a^2/\hbar^2} \) and \( \eta = \sqrt{1 + E/V_0} \) is the root of the eigenvalue equation.

\[
\gamma \eta = (n - 1)\pi + 2 \arccos \eta, \quad n = 0, 1, 2, \ldots
\]

Notice that \( \psi(x \approx 0) = e^{\alpha x} \approx 1 + \kappa x \) but \( \psi(x \approx a) \approx (-1)^{n+1}[1 - \kappa a + \kappa x] \). Effectively, we have \( \alpha = 1 \), \( \alpha_1 = (-1)^n(1 - \kappa a) \) and \( \beta = \kappa, \beta_1 = (-1)^{n+1}\kappa \). So we have \( \alpha \beta = \alpha_1 \beta_1 \) in equation (12).

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