Bound state eigenfunctions need to vanish faster than $|x|^{-3/2}$

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Received 10 September 2015, revised 29 April 2016
Accepted for publication 16 May 2016
Published 27 May 2016

Abstract

In quantum mechanics, students are taught to practice that the eigenfunction of a physical bound state must be continuous and vanishing asymptotically so that it is normalizable in $\mathbb{R} \rightarrow \infty$. Here we caution that such states may also give rise to infinite uncertainty in the position $\Delta x = \infty$, whereas $\Delta p$ remains finite. Such states may be called loosely bound and spatially extended states, and may be avoided by an additional condition that the eigenfunction vanishes asymptotically faster than $|x|^{-3/2}$.

Keywords: Schrödinger equation, bound states, uncertainty principle

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

The bound state is an essential topic in the curriculum of introductory quantum mechanics [1, 2]. Bound state eigenfunctions $\psi_n(x)$ are solutions of the Schrödinger (1926) equation [1, 2]

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0,$$

for some potential $V(x)$ for specific allowed values of energies $E = E_n$ that obey the Dirichlet boundary condition

$$\psi_n(\pm \infty) = 0.$$  \hspace{1cm} (2)

Energies $E_n$ are called eigenvalues leading to quantization of energy. This quantization was first hypothesized by Planck in 1900 for the explanation of black body radiation, and justified much later by Bohr and Sommerfeld (in 1919) [1, 2] semi-classically for $V(x) = \frac{1}{2}m\omega^2x^2$ and other potential profiles with a single minimum, called potential wells.

As $|\psi(x)|^2$ plays the role of quantal probability, $\psi(x)$ is taught to be a continuous function on $x \in (-\infty, \infty)$ so that $\psi(x)$ is square integrable (normalizable).
The additional condition of differentiability of \( \psi(x) \) at each and every point of the domain ensures the continuity of the momentum \(-i\hbar \frac{d}{dx}\psi(x)\) unless there is a Dirac delta function in the potential [2]. When the potential contains a Dirac delta function, e.g., \( g\delta(x-a) \), the eigenfunction is allowed to become non-differentiable at \( x = a \) wherein the left and right derivatives are finite but unequal at \( x = a \).

Further, the uncertainty relation of Heisenberg (1927) \([1, 2]\)

\[
U = \Delta x \Delta p \geq \frac{\hbar}{2}, \quad \Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}, \quad \langle A \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x) A \psi(x) dx}{\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx},
\]

requires the uncertainties \( \Delta x \) and \( \Delta p \) to be finite for physically relevant cases. An interesting collection of uncertainty products for ground states of several solvable models may be seen in \([3]\). It may be mentioned that nowadays, the terms uncertainty relation and uncertainty principle are classified clearly. The term uncertainty principle is used when an inequality expresses the relationship between measurement error and disturbance. For a recent and a very interesting discussion on this, one may see \([4]\).

A definite integral \( \int_{a}^{b} f(x) dx \) is called proper if it represents the area under the curve \( y = f(x) \) from \( x = a \) to \( x = b \). This in turn requires \( f(x) \) to be continuous or piece-wise continuous in the closed interval \([a, b]\). On the other hand, an improper \([4]\) integral may not connect well to the area under the curve e.g., \( \int_{0}^{\infty} x^{-1/2} dx = 2 \). One way an integral becomes improper is when one or both of its limits are infinite. Improper integrals may or may not be convergent (finite). It is trivial yet important to see that the integral \( \int_{0}^{\infty} x^{-\beta} dx \) is convergent only if \( \beta > 1 \). This last point is crucial in determining the asymptotic behavior of \( \psi(x) \) such that \( \langle x^2 \rangle \) is finite, see below.

The finiteness of \( \Delta x \) requires \( \langle x^2 \rangle \) to be finite, thus we demand

\[
\int_{-\infty}^{\infty} x^4 |\psi(x)|^2 dx < \infty \Rightarrow |\psi(x)| < |x|^{-3/2}, \quad |x| \sim \infty.
\]

On the other hand for \( \langle p \rangle \) and \( \langle p^2 \rangle \) to be finite, \( |\psi(x)| \sim 1/x^\epsilon, \epsilon > 0 \) would suffice. Thus, condition \((5)\) would ensure the finiteness of the uncertainty product \( U \)[4]. In this paper, we point out this additional condition \((5)\) on the eigenfunction for a bound state.

One can write \((1)\) in an interesting form as

\[
V(x) - E_0 = \frac{\hbar^2}{2m} \frac{1}{|\psi_0(x)|^2} \frac{d^2|\psi_0(x)|}{dx^2}.
\]

Here we take \( 2m = 1 = \hbar \), which gives \( 2m/\hbar^2 = 1 \). It may be noted that for a particle of mass four times that of an electron, the approximate value of \( 2m/\hbar^2 \) is \( 1 (eV\ell_0^2) \) when the mass and energy are in eV and length is in \( \ell_0 \). If we put the well known ground state of the harmonic oscillator \( \psi_0(x) = e^{-x^2/2} \) in \((6)\), we get \( V(x) - E_0 = -1 + x^2 \). One may interpret that \( V(x) = x^2 \) and \( E_0 = 1 \) (or \( V(x) = x^2 - 1 \) and \( E_0 = 0 \)). This \( V(x) \) is the harmonic oscillator potential (see figure 1(a)) \( V(x) = \frac{1}{2}m\omega^2x^2 \), where \( \hbar\omega = 2eV \) and \( E_0 = 1 \) eV. The ground state \( \psi_0(x) = e^{-x^2/2} \) vanishes faster than \( |x|^{-3/2} \) because as \( x \to \infty, |x|^{3/2}e^{-x^2/2} \to 0 < 1 \). So the uncertainty product \( U_0 \) for this ground state turns out to be finite as \( U_0 = \hbar/2 \) \([1, 2]\), which equals the least bound on \( U \) \((4)\) for any physical eigenstate.

1 See p 84 in \([2]\).
Particularly in this special case of the harmonic oscillator constructing the raising and lowering operators \( [1, 2] \), one can find all eigenvalues and corresponding eigenfunctions of \( V(x) \). This is a rare feature of a potential.

But if we put \( y(x) = -e^{-x} \) in \((6)\), we get \( E_0 = -16 \) and \( E_0 = 0 \). See figure 1(b). This \( V(x) \) is a double well and \( E_0 = 0 \) is the ground state of this potential that possesses infinitely many bound states. One cannot construct the raising and lowering operators to obtain the rest of the spectrum of this double well potential. If required, the other bound states are obtained by numerically solving the Schrödinger equation for this potential.

Once again \( y(x) = -e^{-x} \) vanishes asymptotically very rapidly as \( x \to \infty \), \( |x|^{3/2}e^{-x} \to 0 < 1 \) rendering the integrals for \( \langle x \rangle \) and \( \langle x^2 \rangle \) as finite. Next, \( \langle x \rangle \) vanishes as there is an odd integrand within the symmetric limit of integration. Similarly, \( \langle p \rangle = 0 \) in general for bound states as they do not carry any momentum. We can find \( \langle x^2 \rangle \)

\[
\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 e^{-2x^4} dx}{\int_{-\infty}^{\infty} e^{-2x^4} dx} = \frac{\Gamma(3/4)}{4\sqrt{2} \Gamma(5/4)}
\]

and

\[
\langle p^2 \rangle = \langle p \rangle^2 = \langle p \psi_0(x) | p \psi_0(x) \rangle = 16 \hbar^2 \frac{\int_{-\infty}^{\infty} x^6 e^{-2x^4} dx}{\int_{-\infty}^{\infty} e^{-2x^4} dx} = \frac{\sqrt{2} \Gamma(7/4)}{\Gamma(5/4)}
\]

In equations (7) and (8), we have converted the integrals to the standard Gamma functions as \( \Gamma(z) = \int_0^\infty t^{z-1}e^{-t} dt \) [6]. Using (7) and (8) in (4), we get the uncertainty product for the ground state as

\[
U_0 = \hbar \frac{\sqrt{\Gamma(3/4)\Gamma(7/4)}}{2\Gamma(5/4)} = 0.5854 \hbar,
\]

which is more than \( \hbar/2 \) as per the uncertainty principle.

Similarly, the ground state \( \psi_0(x) = \sqrt{\frac{2}{\sqrt{\pi}}} \frac{x}{\sqrt{1+x^2}} \) vanishes a little faster than \( |x|^{-3/2} \) to have a well known value for \( U_0 = \hbar/\sqrt{2} \) (see footnote 1).

\[2\] See 2.5.4 on p 104 in [2].
Now let us take a continuous, differentiable and normalized state as
\[ \psi_0(x) = \frac{1}{\sqrt{\pi (1 + x^2)}}. \]  
(10)

which behaves as \(1/x\) as \(x \to \infty\). For this state
\[ \langle x \rangle = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{x}{1 + x^2} \, dx, \quad \langle x^2 \rangle = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{x^2}{1 + x^2} \, dx, \]  
(11)

so both of these integrals (11) are improper. Under the condition that the integration range becomes infinite while maintaining the left–right symmetry of the integration range, we get
\[ \Delta x = \infty. \]  
(12)

On the other hand the integral in
\[ \langle p \rangle = \frac{i\hbar}{\pi} \int_{-\infty}^{\infty} \frac{x}{1 + x^2} \, dx \]  
(13)
is improper but convergent because its integrand vanishes as \(1/x^3 (\beta > 1)\) asymptotically, and then it vanishes as its integrand is an odd function. Similarly \(\langle p^2 \rangle\) is improper but convergent because its integrand vanishes as \(1/x^4 (\beta > 1)\) asymptotically as shown below
\[ \langle p^2 \rangle = \langle p\psi_0|p\psi_0 \rangle = \frac{\hbar^2}{\pi} \int_{-\infty}^{\infty} \frac{x^2}{1 + x^2} \, dx = \frac{\hbar^2}{4\pi} \int_{0}^{\pi/2} [1 - \cos 4\theta] \, d\theta = \frac{\hbar^2}{8}. \]  
(14)

In the integral above, we have used the substitution \(x = \tan \theta\), finally we get a finite value of \(\Delta p\) as
\[ \Delta p = \frac{\hbar}{2\sqrt{2}}. \]  
(15)

Eventually, equations (12) and (15) render the uncertainty product as infinite.

Now let us find out from equation (6) the potential giving rise to such a ground state (10), we find
\[ V(x) = \frac{2x^2 - 1}{(1 + x^2)^2}. \]  
(16)

This potential is depicted in figure 1(c) and the state (10) is its ground state with eigenvalue \(E_0 = 0\). No state can exist below \(E = 0\) as it is a node less (ground state). For energies \(E > 0\) there are scattering states, and there may also exist a metastable (quasi bound, resonant) state. Hence the state (10) is the only bound state of this potential (16).

The examples of the ground states \(\psi_0(x)\) rendering finite uncertainty products presented here are instructive in bringing out the crucial role of faster asymptotic convergence of \(\psi_0(x)\) than \(1/x^{3/2}\). On the other hand, example (10) demonstrates our point that if an eigenstate of a bound state does not vanish faster than \(1/x^{3/2}\), despite being continuous, differentiable and normalizable, it would yield the uncertainty product \(U\) as infinite.

Similarly, for three dimensional central potentials [1, 2] in the radial Schrödinger equation, where \(r \in (0, \infty)\) and \(\psi(r) = \frac{u(r)}{r}\), \(u(r)\) needs to vanish faster than \(r^{-3/2}\) for the uncertainty \(\Delta r\) to be finite.

As such, \(\Delta x\) or the uncertainty product becoming infinite does not violate the uncertainty relation (4); this, however, may not be desirable either. Notice that this ground state (10) is a much extended state that vanishes as \(1/x\) asymptotically much slower as compared to the

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3 See pp 128–37 in [1].
states in figures 1(a) and (b). Such a state, if useful in future, may be called a loosely bound and spatially extended state.

Acknowledgement

I would like to thank Physics Trainees of 59th Batch of HRDD of BARC for their interest in the course of Quantum Mechanics.

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