

A Quantum Physics Jeopardy Problem of a One-Bound-State Double Dirac Delta Potential with a Centrifugal, Angular- Momentum-Like Tail

Spiros Konstantogiannis

spiroskonstantogiannis@gmail.com

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Abstract

Starting from a simple, one-parameter, symmetric wave function, we derive an attractive double Dirac delta potential with a centrifugal, angular-momentum-like tail, which has only one bound state, the energy of which can be set to zero.

Keywords: rational wave functions, one-bound-state potentials, double Dirac delta potential, centrifugal tail, zero-energy states, quantum physics jeopardy

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1. Introduction

In [1], Van Heuvelen and Maloney describe a new, reverse type of physics problems in which the answer is given and the question is asked. Such problems, which require from the solver to follow a working-backward approach, are called physics Jeopardy problems (the name was taken from a game show called Jeopardy).

In quantum physics Jeopardy problems, wave functions describing energy eigenstates are given and the respective potentials are asked [2].

Herein, we use a simple, one-parameter, symmetric wave function to derive an attractive, equal-coupling, double Dirac delta potential, which vanishes in the interior region (between the delta functions) and has a centrifugal, angular-momentum-like tail in the exterior region (outside the delta functions). The potential admits only one bound state, the energy of which can be chosen zero.

For a detailed study of the double Dirac delta potential, the reader may refer to [3] and to references therein, while in [4] the reader can find a detailed analysis of the Dirac delta potentials as pedagogical and physical models in quantum physics.

2. The wave function

We consider the wave function

$$\psi(\tilde{x}; s) = \frac{A}{(|\tilde{x} - \tilde{x}_1| + |\tilde{x} + \tilde{x}_1|)^s} \quad (1)$$

where $s > 3/2$ [5], $\tilde{x}_1 > 0$, A the normalization constant, and $\tilde{x} = x/x_0$, with x being the position and $x_0 > 0$ a length scale.

Since $\tilde{x}_1 \neq 0$, the expression $|\tilde{x} - \tilde{x}_1| + |\tilde{x} + \tilde{x}_1|$ is strictly positive. Then, the wave function (1) has no singularities, it is everywhere continuous and finite.

Also, we have

$$\psi(-\tilde{x}; s) = \frac{A}{(|-\tilde{x} - \tilde{x}_1| + |-\tilde{x} + \tilde{x}_1|)^s} = \frac{A}{(|-(\tilde{x} + \tilde{x}_1)| + |-(\tilde{x} - \tilde{x}_1)|)^s} \stackrel{|\cdot|}{=} \frac{A}{(|\tilde{x} + \tilde{x}_1| + |\tilde{x} - \tilde{x}_1|)^s}$$

Thus

$$\psi(-\tilde{x}; s) = \psi(\tilde{x}; s)$$

That is, $\psi(\tilde{x}; s)$ is symmetric (i.e. of even parity).

In the region $|\tilde{x}| > \tilde{x}_1$, we have

i. If $\tilde{x} < -\tilde{x}_1$, then $\tilde{x} + \tilde{x}_1 < 0$ and since $\tilde{x}_1 > 0$, $\tilde{x} - \tilde{x}_1 < \tilde{x} + \tilde{x}_1 < 0$.

Thus $|\tilde{x} - \tilde{x}_1| = -(\tilde{x} - \tilde{x}_1)$ and $|\tilde{x} + \tilde{x}_1| = -(\tilde{x} + \tilde{x}_1)$.

Then (1) becomes

$$\psi(\tilde{x}; s) = \frac{A}{(-(\tilde{x} - \tilde{x}_1) - (\tilde{x} + \tilde{x}_1))^s} = \frac{A}{(-2\tilde{x})^s} = \frac{A}{2^s (-\tilde{x})^s}$$

That is

$$\psi(\tilde{x}; s) = \frac{A}{2^s (-\tilde{x})^s} \quad (2)$$

ii. If $\tilde{x} > \tilde{x}_1$, then $\tilde{x} - \tilde{x}_1 > 0$ and since $\tilde{x}_1 > 0$, $\tilde{x} + \tilde{x}_1 > \tilde{x} - \tilde{x}_1 > 0$.

Thus $|\tilde{x} - \tilde{x}_1| = \tilde{x} - \tilde{x}_1$ and $|\tilde{x} + \tilde{x}_1| = \tilde{x} + \tilde{x}_1$.

Then (1) becomes

$$\psi(\tilde{x}; s) = \frac{A}{(\tilde{x} - \tilde{x}_1 + \tilde{x} + \tilde{x}_1)^s} = \frac{A}{(2\tilde{x})^s} = \frac{A}{2^s \tilde{x}^s}$$

That is

$$\psi(\tilde{x}; s) = \frac{A}{2^s \tilde{x}^s} \quad (3)$$

Combining (2) and (3), we obtain

$$\psi(\tilde{x}; s) = \frac{A}{2^s |\tilde{x}|^s} \quad (4)$$

for $|\tilde{x}| > \tilde{x}_1$.

In the region $|\tilde{x}| \leq \tilde{x}_1$, we have

$-\tilde{x}_1 \leq \tilde{x} \leq \tilde{x}_1$, thus $\tilde{x} - \tilde{x}_1 \leq 0$ and $\tilde{x} + \tilde{x}_1 \geq 0$.

Then $|\tilde{x} - \tilde{x}_1| = -(\tilde{x} - \tilde{x}_1)$ and $|\tilde{x} + \tilde{x}_1| = \tilde{x} + \tilde{x}_1$.

Thus (1) becomes

$$\psi(\tilde{x}; s) = \frac{A}{(-(\tilde{x} - \tilde{x}_1) + \tilde{x} + \tilde{x}_1)^s} = \frac{A}{(2\tilde{x}_1)^s}$$

That is

$$\psi(\tilde{x}; s) = \frac{A}{(2\tilde{x}_1)^s} \quad (5)$$

The wave function is constant in the region $|\tilde{x}| \leq \tilde{x}_1$.

Combining (4) and (5), we write the wave function as

$$\psi(\tilde{x}; s) = \begin{cases} \frac{A}{(2\tilde{x}_1)^s}, & |\tilde{x}| \leq \tilde{x}_1 \\ \frac{A}{2^s |\tilde{x}|^s}, & |\tilde{x}| > \tilde{x}_1 \end{cases} \quad (6)$$

Since it is continuous, $\psi(\tilde{x}; s)$ is Riemann integrable. Also, $\psi(\tilde{x}; s)$ is square integrable, as it decays as $1/|\tilde{x}|^s$, with $s > 3/2$.

The normalization constant A can be easily calculated by applying the normalization condition, i.e.

$$\int_{-\infty}^{\infty} dx |\psi(x)|^2 = 1$$

Using that $\tilde{x} = x/x_0$, we obtain $dx = x_0 d\tilde{x}$, and since $x_0 > 0$, the previous integral is written as

$$x_0 \int_{-\infty}^{\infty} d\tilde{x} |\psi(\tilde{x})|^2 = 1$$

or

$$2x_0 \int_0^{\infty} d\tilde{x} |\psi(\tilde{x})|^2 = 1 \quad (7)$$

since $\psi(\tilde{x})$ is symmetric.

Using (6), the integral in the left-hand side of (7) is written as

$$\begin{aligned}
\int_0^{\infty} d\tilde{x} |\psi(\tilde{x})|^2 &= \int_0^{\tilde{x}_1} d\tilde{x} \frac{|A|^2}{(2\tilde{x}_1)^{2s}} + \int_{\tilde{x}_1}^{\infty} d\tilde{x} \frac{|A|^2}{2^{2s} \tilde{x}^{2s}} = \frac{|A|^2}{(2\tilde{x}_1)^{2s}} \tilde{x}_1 + \frac{|A|^2}{2^{2s}} \left(-\frac{1}{2s-1} \frac{1}{\tilde{x}^{2s-1}} \Big|_{\tilde{x}_1}^{\infty} \right) = \\
&= \frac{|A|^2}{(2\tilde{x}_1)^{2s}} \tilde{x}_1 + \frac{|A|^2}{2^{2s}} \frac{1}{2s-1} \frac{1}{\tilde{x}_1^{2s-1}} = \frac{|A|^2}{2^{2s} \tilde{x}_1^{2s-1}} + \frac{1}{2s-1} \frac{|A|^2}{2^{2s} \tilde{x}_1^{2s-1}} = \left(1 + \frac{1}{2s-1} \right) \frac{|A|^2}{2^{2s} \tilde{x}_1^{2s-1}} = \\
&= \frac{2s|A|^2}{(2s-1)2^{2s} \tilde{x}_1^{2s-1}} = \frac{s|A|^2}{(2s-1)(2\tilde{x}_1)^{2s-1}}
\end{aligned}$$

That is

$$\int_0^{\infty} d\tilde{x} |\psi(\tilde{x})|^2 = \frac{s|A|^2}{(2s-1)(2\tilde{x}_1)^{2s-1}}$$

Substituting into (7) yields

$$\frac{2x_0s|A|^2}{(2s-1)(2\tilde{x}_1)^{2s-1}} = 1 \Rightarrow |A|^2 = \frac{(2s-1)(2\tilde{x}_1)^{2s-1}}{2x_0s} = \frac{(2s-1)(2\tilde{x}_1)^{2s}}{4x_0\tilde{x}_1s}$$

Thus

$$|A| = \frac{(2\tilde{x}_1)^s}{2} \sqrt{\frac{2s-1}{x_0\tilde{x}_1s}}$$

Then, up to a constant phase, the normalization constant is

$$A = \frac{(2\tilde{x}_1)^s}{2} \sqrt{\frac{2s-1}{x_0\tilde{x}_1s}} \quad (8)$$

By means of (8), (6) becomes

$$\psi(\tilde{x}; s) = \begin{cases} \frac{1}{2} \sqrt{\frac{2s-1}{x_0\tilde{x}_1s}}, & |\tilde{x}| \leq \tilde{x}_1 \\ \frac{1}{2} \sqrt{\frac{2s-1}{x_0\tilde{x}_1s}} \left(\frac{\tilde{x}_1}{|\tilde{x}|} \right)^s, & |\tilde{x}| > \tilde{x}_1 \end{cases} \quad (9)$$

Using (9), we calculate the wave function derivative, with respect to \tilde{x} .

In the region $|\tilde{x}| < \tilde{x}_1$, the wave function is constant, thus its derivative vanishes.

In the region $\tilde{x} < -\tilde{x}_1$, the wave function is, from (9),

$$\psi(\tilde{x}; s) = \frac{1}{2} \sqrt{\frac{2s-1}{x_0 \tilde{x}_1 s}} \left(\frac{\tilde{x}_1}{-\tilde{x}} \right)^s$$

Thus

$$\begin{aligned} \psi'(\tilde{x}; s) &= \frac{1}{2} \sqrt{\frac{2s-1}{x_0 \tilde{x}_1 s}} \tilde{x}_1^s \frac{(-s)(-1)}{(-\tilde{x})^{s+1}} = \frac{1}{2} \sqrt{\frac{s^2(2s-1)}{x_0 \tilde{x}_1 s}} \frac{\tilde{x}_1^s}{(-\tilde{x})^{s+1}} = \frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1}} \frac{1}{\tilde{x}_1} \left(\frac{\tilde{x}_1}{-\tilde{x}} \right)^{s+1} = \\ &= \frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}} \left(\frac{\tilde{x}_1}{-\tilde{x}} \right)^{s+1} \end{aligned}$$

In the region $\tilde{x} > \tilde{x}_1$, the wave function is, from (9),

$$\psi(\tilde{x}; s) = \frac{1}{2} \sqrt{\frac{2s-1}{x_0 \tilde{x}_1 s}} \left(\frac{\tilde{x}_1}{\tilde{x}} \right)^s$$

Then

$$\psi'(\tilde{x}; s) = \frac{1}{2} \sqrt{\frac{2s-1}{x_0 \tilde{x}_1 s}} \tilde{x}_1^s \frac{-s}{\tilde{x}^{s+1}} = -\frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}} \left(\frac{\tilde{x}_1}{\tilde{x}} \right)^{s+1}$$

Thus, the wave function derivative is

$$\psi'(\tilde{x}; s) = \begin{cases} 0, & |\tilde{x}| < \tilde{x}_1 \\ \frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}} \left(\frac{\tilde{x}_1}{-\tilde{x}} \right)^{s+1}, & \tilde{x} < -\tilde{x}_1 \\ -\frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}} \left(\frac{\tilde{x}_1}{\tilde{x}} \right)^{s+1}, & \tilde{x} > \tilde{x}_1 \end{cases} \quad (10)$$

$\psi'(\tilde{x}; s)$ is odd, as expected, since $\psi(\tilde{x}; s)$ is even.

At $\pm \tilde{x}_1$, $\psi'(\tilde{x}; s)$ is discontinuous, since from (10) we obtain

$$\psi'(-\tilde{x}_1^-; s) = \frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}}, \quad \psi'(-\tilde{x}_1^+; s) = 0$$

and

$$\psi'(\tilde{x}_1^-; s) = 0, \quad \psi'(\tilde{x}_1^+; s) = -\frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}}$$

Thus, the wave function derivative has at $-\tilde{x}_1$ and \tilde{x}_1 finite discontinuities, which are equal, since

$$\psi'(-\tilde{x}_1^+; s) - \psi'(-\tilde{x}_1^-; s) = -\frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}} \quad (11)$$

$$\psi'(\tilde{x}_1^+; s) - \psi'(\tilde{x}_1^-; s) = -\frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^3}}$$

To summarize, the wave function $\psi(\tilde{x}; s)$ is continuous, while its first derivative has equal discontinuities at $\pm\tilde{x}_1$.

3. The potential

Since $\psi(\tilde{x}; s)$ has no zeros¹, it can be the ground-state wave function of a potential consisting of a term having, at most, finite discontinuities, and of a sum of two Dirac delta functions with one of them acting at $-\tilde{x}_1$ and the other at \tilde{x}_1 (see appendix).

1. By zeros, we mean real zeros.

The first term of the potential, which has, at most, finite discontinuities, does not induce discontinuities in the wave function derivative [6, 7]. We'll refer to this term as the regular part of the potential.

A finite discontinuity in the wave function derivative is induced by a Dirac delta potential [7]. Particularly, a delta potential $\lambda\delta(x)$ induces in the wave function derivative a finite discontinuity at zero, which is given by [7]

$$\psi_+'(0) - \psi_-'(0) = \frac{2m\lambda\psi(0)}{\hbar^2} \quad (12)$$

where the prime denotes differentiation with respect to the position x .

Since $\tilde{x} = x/x_0$, we have

$$\frac{d}{dx} = \frac{1}{x_0} \frac{d}{d\tilde{x}}$$

and (12) is written as

$$\frac{1}{x_0} \left(\psi'_+(0) - \psi'_-(0) \right) = \frac{2m\lambda\psi(0)}{\hbar^2} \quad (13)$$

where now the prime denotes differentiation with respect to \tilde{x} .

Then, from (13), the finite discontinuity in $\psi'(\tilde{x}; s)$ at $-\tilde{x}_1$ is induced by a delta potential $\lambda_1 \delta(x + x_1)$ and is given by

$$\frac{1}{x_0} \left(\psi'(-\tilde{x}_1^+; s) - \psi'(-\tilde{x}_1^-; s) \right) = \frac{2m\lambda_1\psi(-\tilde{x}_1; s)}{\hbar^2}$$

Using (11) and that

$$\psi(-\tilde{x}_1; s) = \frac{1}{2} \sqrt{\frac{2s-1}{x_0\tilde{x}_1s}},$$

as given by (9), the above discontinuity condition is written as

$$\frac{1}{x_0} \left(-\frac{1}{2} \sqrt{\frac{s(2s-1)}{x_0\tilde{x}_1^3}} \right) = \frac{2m\lambda_1 \frac{1}{2} \sqrt{\frac{2s-1}{x_0\tilde{x}_1s}}}{\hbar^2}$$

Solving the last equation for the coupling λ_1 gives, after a little algebra,

$$\lambda_1 = -\frac{s\hbar^2}{2mx_0\tilde{x}_1} \quad (14)$$

The delta potential acting at $-\tilde{x}_1$ is thus attractive.

Let us do a dimensional check on (14).

Since $[\hbar] = PL$, $[x_0] = L$, and $[\tilde{x}_1] = 1$ (dimensionless), we have

$$[\lambda_1] = \frac{(PL)^2}{ML} = \frac{P^2}{M} L = EL$$

Then, since $\int_{-\infty}^{\infty} dx \delta(x) = 1$, we have $L[\delta(x)] = 1$, thus $[\delta(x)] = L^{-1}$, and then

$$[\lambda_1 \delta(x)] = E, \text{ and we are ok.}$$

The wave function is symmetric, thus $\psi(-\tilde{x}_1; s) = \psi(\tilde{x}_1; s)$, and also, the discontinuities in the wave function derivative at $\pm\tilde{x}_1$ are equal. Then, the discontinuity in the wave function derivative at \tilde{x}_1 is induced by a delta potential acting at \tilde{x}_1 , which has the same coupling as the delta potential acting at $-\tilde{x}_1$, i.e. it is induced by the delta potential $\lambda_1 \delta(x - x_1)$.

The sum of the two delta potentials is then

$$V_{\text{delta}}(x; s) = -\frac{s\hbar^2}{2mx_0\tilde{x}_1}(\delta(x+x_1) + \delta(x-x_1)) \quad (15)$$

Using that $\delta(ax) = \delta(x)/|a|$, we have, since $x_0 > 0$,

$$\delta(\tilde{x}) = \delta\left(\frac{x}{x_0}\right) = x_0\delta(x)$$

That is

$$\delta(x) = \frac{\delta(\tilde{x})}{x_0}$$

Then

$$\delta(x \pm x_1) = \frac{\delta(\tilde{x} \pm \tilde{x}_1)}{x_0}$$

where $\tilde{x}_1 = x_1/x_0$.

Then (15) is written as

$$V_{\text{delta}}(\tilde{x}; s) = -\frac{s\hbar^2}{2mx_0^2\tilde{x}_1}(\delta(\tilde{x} + \tilde{x}_1) + \delta(\tilde{x} - \tilde{x}_1)) \quad (16)$$

In order to find the regular part of the potential, we'll calculate the second derivative of the wave function.

Using (10), we have

$$\psi''(\tilde{x}; s) = \begin{cases} 0, & |\tilde{x}| < \tilde{x}_1 \\ \frac{(s+1)}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^5}} \left(\frac{\tilde{x}_1}{-\tilde{x}}\right)^{s+2}, & \tilde{x} < -\tilde{x}_1 \\ \frac{(s+1)}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^5}} \left(\frac{\tilde{x}_1}{\tilde{x}}\right)^{s+2}, & \tilde{x} > \tilde{x}_1 \end{cases}$$

or

$$\psi''(\tilde{x}; s) = \begin{cases} 0, & |\tilde{x}| < \tilde{x}_1 \\ \frac{(s+1)}{2} \sqrt{\frac{s(2s-1)}{x_0 \tilde{x}_1^5}} \left(\frac{\tilde{x}_1}{|\tilde{x}|}\right)^{s+2}, & |\tilde{x}| > \tilde{x}_1 \end{cases} \quad (17)$$

Since the wave function describes the ground state of the potential we are looking for, it satisfies the energy eigenvalue equation (in position space)², i.e.

$$\psi''(x; s) + \frac{2m}{\hbar^2} (E_0 - V(x; s)) \psi(x; s) = 0$$

with E_0 being the ground-state energy and $V(x; s)$ the potential.

2. The well-known time-independent Schrödinger equation.

Solving the energy eigenvalue equation for the potential yields

$$V(x; s) = \frac{\hbar^2}{2m} \frac{\psi''(x; s)}{\psi(x; s)} + E_0$$

Using that $\tilde{x} = x/x_0$, we obtain

$$\frac{d^2}{dx^2} = \frac{1}{x_0^2} \frac{d^2}{d\tilde{x}^2},$$

and thus, in terms of \tilde{x} , the potential is written as

$$V(\tilde{x}; s) = \frac{\hbar^2}{2m x_0^2} \frac{\psi''(\tilde{x}; s)}{\psi(\tilde{x}; s)} + E_0$$

Substituting (9) and (17) into the previous equation, we obtain, after a little algebra, that the regular part of the potential is

$$V_{reg}(\tilde{x}; s) = \begin{cases} E_0, & |\tilde{x}| < \tilde{x}_1 \\ \frac{s(s+1)\hbar^2}{2mx_0^2\tilde{x}^2} + E_0, & |\tilde{x}| > \tilde{x}_1 \end{cases} \quad (18)$$

From (18), we see that the regular part of the potential has, at $\pm\tilde{x}_1$, finite discontinuities, which are

$$V_{reg}(-\tilde{x}_1^+; s) - V_{reg}(-\tilde{x}_1^-; s) = E_0 - \left(\frac{s(s+1)\hbar^2}{2mx_0^2(-\tilde{x}_1)^2} + E_0 \right) = -\frac{s(s+1)\hbar^2}{2mx_0^2\tilde{x}_1^2}$$

$$V_{reg}(\tilde{x}_1^+; s) - V_{reg}(\tilde{x}_1^-; s) = \frac{s(s+1)\hbar^2}{2mx_0^2\tilde{x}_1^2} + E_0 - E_0 = \frac{s(s+1)\hbar^2}{2mx_0^2\tilde{x}_1^2}$$

The two discontinuities are thus opposite.

The total potential is the sum of the regular part and the delta functions, i.e.

$$V(\tilde{x}; s) = V_{reg}(\tilde{x}; s) + V_{delta}(\tilde{x}; s) \quad (19)$$

Since $V(\pm\infty; s) = V_{reg}(\pm\infty; s) = E_0$, the ground-state energy E_0 is the highest bound energy of the potential (for a detailed explanation, see, for instance, [8]).

Thus, the potential (19) has only one bound state, which is also the ground state, of energy E_0 , which is described by the wave function (9).

Choosing the infinity as reference point and setting $V(\pm\infty; s) = 0$, we obtain

$$E_0 = 0 \quad (20)$$

i.e. the ground-state energy becomes zero.

The regular part of the potential, given by (18), is then written as

$$V_{reg}(\tilde{x}; s) = \begin{cases} 0, & |\tilde{x}| < \tilde{x}_1 \\ \frac{s(s+1)\hbar^2}{2mx_0^2\tilde{x}^2}, & |\tilde{x}| > \tilde{x}_1 \end{cases} \quad (21)$$

We've thus ended up at an attractive double Dirac delta potential (of equal couplings) with an angular-momentum-like tail $s(s+1)\hbar^2/2mx_0^2\tilde{x}^2$, which, for every value of $s > 3/2$, has only one, zero-energy, bound state.

4. Appendix

For a potential consisting of a part having, at most, finite discontinuities, and of a finite sum of Dirac delta functions, if there exists a nodeless wave function $\psi_0(x)$ describing a bound energy eigenstate, then $\psi_0(x)$ is the ground-state wave function.

Proof

Let $\hat{a}(x)$ be the position-space operator

$$\hat{a}(x) = \frac{1}{p_0} \left(\hat{p}(x) + i\hbar \frac{\psi_0'(x)}{\psi_0(x)} \right) \quad (22)$$

where $\hat{p}(x) = -i\hbar d/dx$ is the momentum operator in position space and p_0 is a (positive) momentum scale.

The operator $\hat{a}(x)$ is dimensionless.

The part of the potential which has, at most, finite discontinuities does not induce discontinuities in the wave function derivative [6, 7], while each delta function induces, in the wave function derivative, a finite discontinuity, at the point where the delta function acts [7].

Since $\psi_0(x)$ is nodeless, the function $\psi_0'(x)/\psi_0(x)$ has no singularities, but it has finite discontinuities at the points where the delta functions act.

Since the number of delta functions in the potential is finite, the function $\psi_0'(x)/\psi_0(x)$ has a finite number of finite discontinuities.

Also, since $\psi_0(x)$ is a one-dimensional bound energy eigenfunction, it is real, up to a constant phase [7].

Thus, $\psi_0'(x)/\psi_0(x)$ is a real function, and then the Hermitian conjugate of the operator (22) is given by

$$\hat{a}^\dagger(x) = \frac{1}{p_0} \left(\hat{p}(x) - i\hbar \frac{\psi_0'(x)}{\psi_0(x)} \right) \quad (23)$$

Using (22) and (23), we have

$$\begin{aligned}
\hat{a}^\dagger(x)\hat{a}(x) &= \frac{1}{p_0^2} \left(\hat{p}(x) - i\hbar \frac{\psi_0'(x)}{\psi_0(x)} \right) \left(\hat{p}(x) + i\hbar \frac{\psi_0'(x)}{\psi_0(x)} \right) = \\
&= \frac{1}{p_0^2} \left(\hat{p}^2(x) + i\hbar \left[\hat{p}(x), \frac{\psi_0'(x)}{\psi_0(x)} \right] - \left(i\hbar \frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) = \\
&= \frac{1}{p_0^2} \left(\hat{p}^2(x) + i\hbar \left[\hat{p}(x), \frac{\psi_0'(x)}{\psi_0(x)} \right] + \hbar^2 \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right)
\end{aligned}$$

That is

$$\hat{a}^\dagger(x)\hat{a}(x) = \frac{1}{p_0^2} \left(\hat{p}^2(x) + i\hbar \left[\hat{p}(x), \frac{\psi_0'(x)}{\psi_0(x)} \right] + \hbar^2 \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) \quad (24)$$

If $f(x)$ is an arbitrary function, then $[\hat{p}(x), f(x)] = -i\hbar f'(x)$, provided that the derivative $f'(x)$ exists. This is easily shown by applying the previous commutator to an arbitrary wave function.

Using the previous commutator, we have

$$\left[\hat{p}(x), \frac{\psi_0'(x)}{\psi_0(x)} \right] = -i\hbar \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)' = -i\hbar \left(\frac{\psi_0''(x)}{\psi_0(x)} - \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right)$$

That is

$$\left[\hat{p}(x), \frac{\psi_0'(x)}{\psi_0(x)} \right] = -i\hbar \left(\frac{\psi_0''(x)}{\psi_0(x)} - \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) \quad (25)$$

Note

At the points where $\psi_0'(x)/\psi_0(x)$ has finite discontinuities, i.e. at the points

where the delta functions act, the derivative $\left(\psi_0'(x)/\psi_0(x) \right)'$ is a delta function.

Similarly, $\psi_0''(x)$ is a delta function at the points where the delta functions act.

Therefore, the function in the right-hand side of (25) contains delta functions.

By means of (25), (24) becomes

$$\begin{aligned}
\hat{a}^\dagger(x)\hat{a}(x) &= \frac{1}{p_0^2} \left(\hat{p}^2(x) - (i\hbar)^2 \left(\frac{\psi_0''(x)}{\psi_0(x)} - \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) + \hbar^2 \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) = \\
&= \frac{1}{p_0^2} \left(\hat{p}^2(x) + \hbar^2 \left(\frac{\psi_0''(x)}{\psi_0(x)} - \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) + \hbar^2 \left(\frac{\psi_0'(x)}{\psi_0(x)} \right)^2 \right) = \frac{1}{p_0^2} \left(\hat{p}^2(x) + \hbar^2 \frac{\psi_0''(x)}{\psi_0(x)} \right)
\end{aligned}$$

That is

$$\hat{a}^\dagger(x)\hat{a}(x) = \frac{1}{p_0^2} \left(\hat{p}^2(x) + \hbar^2 \frac{\psi_0''(x)}{\psi_0(x)} \right) \quad (26)$$

Since $\psi_0(x)$ is an energy eigenfunction, it satisfies the energy eigenvalue equation (in position space), i.e.

$$\psi_0''(x) + \frac{2m}{\hbar^2} (E_0 - V(x)) \psi_0(x) = 0$$

where E_0 is the energy of the state described by $\psi_0(x)$ and $V(x)$ is the potential.

The previous equation gives

$$\hbar^2 \frac{\psi_0''(x)}{\psi_0(x)} = 2m(V(x) - E_0)$$

Substituting the previous expression into (26) yields

$$\hat{a}^\dagger(x)\hat{a}(x) = \frac{1}{p_0^2} (\hat{p}^2(x) + 2m(V(x) - E_0)) = \frac{2m}{p_0^2} \left(\frac{\hat{p}^2(x)}{2m} + V(x) - E_0 \right)$$

Using that $\frac{\hat{p}^2(x)}{2m} + V(x)$ is the Hamiltonian $\hat{H}(x)$ (in position space), we end up to

$$\hat{a}^\dagger(x)\hat{a}(x) = \frac{2m}{p_0^2} (\hat{H}(x) - E_0) \quad (27)$$

The operator $\hat{a}^\dagger(x)\hat{a}(x)$ is Hermitian, since

$$(\hat{a}^\dagger(x)\hat{a}(x))^\dagger = \hat{a}^\dagger(x)(\hat{a}^\dagger(x))^\dagger = \hat{a}^\dagger(x)\hat{a}(x)$$

Also, using (27), we have

$$\begin{aligned} [\hat{a}^\dagger(x)\hat{a}(x), \hat{H}(x)] &= \left[\frac{2m}{p_0^2} (\hat{H}(x) - E_0), \hat{H}(x) \right] = \frac{2m}{p_0^2} [\hat{H}(x) - E_0, \hat{H}(x)] = \\ &= \frac{2m}{p_0^2} \left(\underbrace{[\hat{H}(x), \hat{H}(x)]}_0 - \underbrace{[E_0, \hat{H}(x)]}_0 \right) = 0 \end{aligned}$$

That is, the operator $\hat{a}^\dagger(x)\hat{a}(x)$ commutes with the Hamiltonian.

Next, we'll prove that $\hat{a}^\dagger(x)\hat{a}(x)$ has non-negative eigenvalues.

Proof

Let $\psi(x)$ be an eigenfunction of $\hat{a}^\dagger(x)\hat{a}(x)$ with eigenvalue λ .

Since $\hat{a}^\dagger(x)\hat{a}(x)$ commutes with the Hamiltonian $\hat{H}(x)$, $\hat{a}^\dagger(x)\hat{a}(x)$ and $\hat{H}(x)$ have a common set of eigenfunctions, and thus $\psi(x)$ is an energy eigenfunction.

$\psi(x)$ is continuous, but its derivative $\psi'(x)$ has a finite number of finite discontinuities, at the points where the delta functions of the potential act.

Let us now consider the function

$$\hat{a}(x)\psi(x) = \frac{1}{p_0} \left(\hat{p}(x) + i\hbar \frac{\psi_0'(x)}{\psi_0(x)} \right) \psi(x) \stackrel{\hat{p}(x) = -i\hbar \frac{d}{dx}}{=} -\frac{i\hbar}{p_0} \left(\psi'(x) - \frac{\psi_0'(x)\psi(x)}{\psi_0(x)} \right)$$

That is

$$\hat{a}(x)\psi(x) = -\frac{i\hbar}{p_0} \left(\psi'(x) - \frac{\psi_0'(x)\psi(x)}{\psi_0(x)} \right) \quad (28)$$

The function $\hat{a}(x)\psi(x)$ has no singularities, since $\psi_0(x)$ is nodeless, but it has a finite number of finite discontinuities.

The wave functions $\psi_0(x)$ and $\psi(x)$ as well as their derivatives $\psi_0'(x)$ and $\psi'(x)$ are everywhere finite, so that the respective probability densities and currents are everywhere finite.

Then, the Riemann integral $\int_{-\infty}^{\infty} dx |\hat{a}(x)\psi(x)|^2$ exists³.

3. If a function has a finite number of discontinuities and it is everywhere finite (i.e. if it is bounded), then it is Riemann integrable (see, for instance, [9]).

Using that $|z|^2 = z^* z$, with the asterisk denoting the complex conjugate, we have

$$\int_{-\infty}^{\infty} dx |\hat{a}(x)\psi(x)|^2 = \int_{-\infty}^{\infty} dx (\hat{a}(x)\psi(x))^* (\hat{a}(x)\psi(x)) \quad (29)$$

Also, by definition⁴

$$\begin{aligned} \int_{-\infty}^{\infty} dx \psi^*(x) \hat{a}^\dagger(x) (\hat{a}(x)\psi(x)) &= \int_{-\infty}^{\infty} dx \left((\hat{a}^\dagger(x))^\dagger \psi(x) \right)^* (\hat{a}(x)\psi(x)) \stackrel{(\hat{a}^\dagger(x))^\dagger = \hat{a}(x)}{=} \\ &= \int_{-\infty}^{\infty} dx (\hat{a}(x)\psi(x))^* (\hat{a}(x)\psi(x)) \end{aligned}$$

That is

$$\int_{-\infty}^{\infty} dx \psi^*(x) \hat{a}^\dagger(x) (\hat{a}(x)\psi(x)) = \int_{-\infty}^{\infty} dx (\hat{a}(x)\psi(x))^* (\hat{a}(x)\psi(x)) \quad (30)$$

4. In position space, the Hermitian conjugate operator $\hat{O}^\dagger(x)$ of a linear operator $\hat{O}(x)$ is defined by the relation [7, 10]

$$\int_{-\infty}^{\infty} dx \varphi_2^*(x) \hat{O}(x) \varphi_1(x) = \int_{-\infty}^{\infty} dx \left(\hat{O}^\dagger(x) \varphi_2(x) \right)^* \varphi_1(x),$$

where $\varphi_1(x), \varphi_2(x)$ are two arbitrary wave functions (in position space).

Comparing (29) and (30) yields

$$\int_{-\infty}^{\infty} dx |\hat{a}(x)\psi(x)|^2 = \int_{-\infty}^{\infty} dx \psi^*(x) \hat{a}^\dagger(x) (\hat{a}(x)\psi(x)) = \int_{-\infty}^{\infty} dx \psi^*(x) (\hat{a}^\dagger(x) \hat{a}(x)\psi(x))$$

But $\hat{a}^\dagger(x) \hat{a}(x)\psi(x) = \lambda \psi(x)$, as $\psi(x)$ is an eigenfunction of $\hat{a}^\dagger(x) \hat{a}(x)$ with eigenvalue λ .

Thus

$$\int_{-\infty}^{\infty} dx |\hat{a}(x)\psi(x)|^2 = \int_{-\infty}^{\infty} dx \psi^*(x) \lambda \psi(x) = \lambda \int_{-\infty}^{\infty} dx |\psi(x)|^2$$

That is

$$\int_{-\infty}^{\infty} dx |\hat{a}(x)\psi(x)|^2 = \lambda \int_{-\infty}^{\infty} dx |\psi(x)|^2 \quad (31)$$

In (31), both integrands are non-negative, thus both integrals are also non-negative. Moreover, since $\psi(x)$ is an eigenfunction, it is linearly independent, and thus it cannot be identically zero. Thus, the integral in the right-hand side of (31) is strictly positive and, since the integral in the left-hand side is non-negative, λ must be non-negative too.

Therefore, the eigenvalues of $\hat{a}^\dagger(x)\hat{a}(x)$ are non-negative.

Next, using (27) and that $2m/p_0^2 > 0$, we derive that the eigenvalues of $\hat{H}(x) - E_0$ are also non-negative, and thus the eigenvalues of the Hamiltonian, i.e. the energies, are greater than or equal to E_0 .

Then, since the energy E_0 exists, it is the ground-state energy, and the respective wave function $\psi_0(x)$ is the ground-state wave function.

Notes

i. We point out the significance of the existence of the Riemann integral

$$\int_{-\infty}^{\infty} dx |\hat{a}(x)\psi(x)|^2 \text{ in the proof.}$$

If the wave function $\psi_0(x)$ had nodes, the function $\hat{a}(x)\psi(x)$, as given by (28), would have singularities and the previous Riemann integral would be ill-defined.

Also, if the discontinuities in the wave function derivative $\psi_0'(x)$ would be infinite (in number or in magnitude), the previous Riemann integral would also be ill-defined.

ii. From (28), we see that $\hat{a}(x)\psi_0(x) = 0$, i.e. the operator $\hat{a}(x)$ kills the ground-state wave function.

5. References

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