On the Ground State of Potentials with, at Most, Finite Discontinuities and Simple Poles

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Abstract

For one-dimensional potentials having, at most, finite discontinuities and simple poles at which the wave functions have simple zeros, we give an algebraic – i.e. operator-based – proof that an eigenfunction having no other zeros is a minimum-energy eigenfunction, and thus it describes the ground state.

Keywords: simple poles, ground state, minimum energy, wave-function zeros

I. Preliminaries

We know that if the potential has, at most, finite discontinuities, the wave function is $C^1(R)$ [1-4].

However, the opposite does not necessarily hold, i.e. if the wave function is $C^1(R)$, the potential can be singular.

Proof

We consider the bound energy eigenfunction

$$\psi(x) = (x - x_0)\exp(f(x)) \qquad (1)$$

which has a simple zero* at x_0.

* By zero, we mean real zero.

The function $f(x)$ is a polynomial of even – and non-zero degree – with negative leading coefficient, so that $\psi(x)$ is square integrable.

$\psi(x)$ is $C^\infty(R)$, thus it is also $C^1(R)$.

Using (1), the first derivative of $\psi(x)$ is written as

$$\psi'(x) = \exp(f(x)) + f'(x)\psi(x)$$

Then, the second derivative of $\psi(x)$ is

$$\psi''(x) = f'(x)\exp(f(x)) + f''(x)\psi(x) + f'(x)\psi'(x)$$

Substituting into the last equation the expression of $\psi'(x)$ yields

$$\psi''(x) = f'(x)\exp(f(x)) + f''(x)\psi(x) + f'(x)\big(\exp(f(x)) + f'(x)\psi(x)\big) =$$
$$= \big(f''(x) + f'^2(x)\big)\psi(x) + 2f'(x)\exp(f(x))$$

Substituting $\exp(f(x))$ from (1), we obtain

$$\psi''(x) = \left(f''(x) + f'^2(x) + \frac{2f'(x)}{x - x_0}\right)\psi(x)$$

Then, the ratio $\psi''(x)/\psi(x)$ is

$$\frac{\psi''(x)}{\psi(x)} = f''(x) + f'^2(x) + \frac{2f'(x)}{x - x_0} \qquad (2)$$

Since the wave function $\psi(x)$ is an energy eigenfunction, it satisfies the energy eigenvalue equation in position space, i.e. the well-known time-independent Schrödinger equation

$$\psi''(x) + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) = 0$$

where E is the energy of the eigenstate described by $\psi(x)$ and $V(x)$ is the potential. Solving for the potential, we obtain

$$V(x) = \frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + E \qquad (3)$$

By means of (2), (3) becomes

$$V(x) = \frac{\hbar^2}{2m}\left(f''(x) + f'^2(x) + \frac{2f'(x)}{x - x_0}\right) + E$$

If $f'(x_0) \neq 0$, the potential $V(x)$ has a simple pole at x_0.

We thus showed that a simple zero in a $C^1(R)$ wave function can be related to a simple pole in the potential.

Therefore, assuming that the wave function is $C^1(R)$ does not exclude the possibility that the potential is singular.

Next, we consider an energy eigenfunction $\varphi(x)$ of some potential $V_1(x)$.

Then

$$V_1(x) = \frac{\hbar^2}{2m}\frac{\varphi''(x)}{\varphi(x)} + E_1 \qquad (4)$$

From (4), we see that, in general, the zeros of $\varphi(x)$ – if any – are singularities of the potential.

If the zeros of $\varphi(x)$ are also zeros of $\varphi''(x)$, the singularities of the potential are removable, practically the potential has no singularities.

Moreover, if the potential is $C^{\infty}(R)$, all zeros of $\varphi(x)$ are simple zeros, i.e. zeros of multiplicity 1.

Proof

If $\varphi(x)=(x-x_0)^k\,\tilde{\varphi}(x)$, with $\tilde{\varphi}(x_0)\neq 0$, then

$$\varphi'(x)=k(x-x_0)^{k-1}\,\tilde{\varphi}(x)+(x-x_0)^k\,\tilde{\varphi}'(x) \qquad (5)$$

Since the potential is continuous, $\varphi'(x)$ is continuous [1-4].

Then, from (5), $k-1\geq 0$ and we have the cases:

i) $k=1$

Then, from (5),

$$\varphi'(x_0)=\tilde{\varphi}(x_0)\neq 0$$

ii) $k>1$

Then, from (5),

$$\varphi'(x_0)=0$$

Besides, since at x_0, $\varphi(x)$ vanishes and the potential is finite, from the energy eigenvalue equation, we obtain that $\varphi''(x)$ also vanishes at x_0.

Then, using also that $\varphi'(x)$ vanishes at x_0 and that the potential is $C^{\infty}(R)$, successively differentiating the energy eigenvalue equation, we obtain that all derivatives of $\varphi(x)$ vanish at x_0, and thus $\varphi(x)$ is identically zero.

But then $\varphi(x)$ cannot be an eigenfunction, since an eigenfunction is, by definition, a linearly independent function, i.e. a non-identically-zero function.

Therefore, $k=1$, i.e. x_0 is a simple zero of $\varphi(x)$.

In what follows, we'll consider potentials having, at most, finite discontinuities and simple poles at which the wave functions have simple zeros.

From (4), we see that if x_0 is a simple zero of $\varphi(x)$ which is not a zero of $\varphi''(x)$, the potential has a simple pole at x_0, provided that $\varphi''(x)$ is finite at x_0.

Moreover, since every energy eigenfunction satisfies the same equation (4), every energy eigenfunction has a simple zero at x_0, provided that its second derivative is finite at x_0.

Thus, all energy eigenfunctions vanish at x_0, and since every wave function is written as linear combination of energy eigenfunctions, all wave functions also vanish at x_0.

II. The ground-state wave function

Let $\psi_0(x)$ be a bound energy eigenfunction of some potential $V(x)$.

We'll show that if $\psi_0(x)$ does not have other zeros, apart from the zeros at the simple poles of the potential (if any), it is the minimum-energy eigenfunction, and thus it describes the ground state.

Proof

Since $\psi_0(x)$ is a one-dimensional bound energy eigenfunction, it is real, up to a constant phase [2,3].

We'll assume that $\psi_0(x)$ is $C^1(R)$.

As shown, this does not exclude the possibility that the potential $V(x)$ has simple poles.

Since the wave functions of a potential having, at most, finite discontinuities are also $C^1(R)$, the potential $V(x)$ can have, at most, not only simple poles, but finite discontinuities too.

In position space, we consider the dimensionless differential operator

$$\hat{a}(x) = \frac{1}{p_0}\left(\hat{p}(x) + i\hbar\frac{\psi_0'(x)}{\psi_0(x)}\right) \tag{6}$$

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

Since $\psi_0(x)$ is real up to a constant phase, $\psi_0'(x)/\psi_0(x)$ is real, thus the operator $\hat{a}(x)$ has the non-zero imaginary part $i\hbar\psi_0'(x)/\psi_0(x)$, and then it is not Hermitian.
By means of (6), the action of the operator $\hat{a}(x)$ on the wave function $\psi_0(x)$ yields

$$\hat{a}(x)\psi_0(x) = \frac{1}{p_0}\left(-i\hbar\frac{d}{dx} + i\hbar\frac{\psi_0'(x)}{\psi_0(x)}\right)\psi_0(x) = \frac{i\hbar}{p_0}\left(-\psi_0'(x) + \psi_0'(x)\right) = 0$$

Thus

$$\hat{a}(x)\psi_0(x) = 0$$

That is, $\hat{a}(x)$ kills the eigenstate described by $\psi_0(x)$.

$\psi_0(x)$ either has no zeros, or all its zeros are simple and they are also simple zeros of every energy eigenfunction, and thus of every wave function too.
This holds because we assume that the poles of the potential – if any – are simple poles at which the wave function has simple zeros (see section I).
Then, if $|\psi\rangle$ is an arbitrary state, the wave function $\psi(x)$ describing, in position space, the state $|\psi\rangle$, also vanishes at the zeros of $\psi_0(x)$, and thus the wave function $\hat{a}(x)\psi(x)$ has no singularities.
As $\psi_0(x)$, $\psi(x)$ is $C^1(R)$, and then $\hat{a}(x)\psi(x)$ is continuous. Thus, the Riemann integral $\int_{-\infty}^{\infty} dx\left|\hat{a}(x)\psi(x)\right|^2$ exists, and since the integrand is a non-negative continuous function, the integral is non-negative, i.e.

$$\int_{-\infty}^{\infty} dx\left|\hat{a}(x)\psi(x)\right|^2 \geq 0 \tag{7}$$

The previous integral is the square of the norm of the state $\hat{a}|\psi\rangle$ in position space, where $\hat{a}$ is the operator $\hat{a}(x)$ in the state space, or else, $\hat{a}(x)$ is the expression of the operator $\hat{a}$ in position space [5].

Proof

For convenience, we set

$$|\phi\rangle \equiv \hat{a}|\psi\rangle \tag{8}$$

Using (8), we have

$$\left\| \hat{a}|\psi\rangle \right\|^2 = \left\| |\phi\rangle \right\|^2 = \langle\phi|\phi\rangle$$

That is

$$\left\| \hat{a}|\psi\rangle \right\|^2 = \langle\phi|\phi\rangle \tag{9}$$

Using the completeness relation of the position eigenstates, the inner product $\langle\phi|\phi\rangle$ is written as

$$\langle\phi|\phi\rangle = \left\langle \phi \left| \left(\underbrace{\int_{-\infty}^{\infty} dx|x\rangle\langle x|}_{\hat{1}} \right) \right| \phi \right\rangle = \int_{-\infty}^{\infty} dx\langle\phi|x\rangle\langle x|\phi\rangle = \int_{-\infty}^{\infty} dx\langle x|\phi\rangle^* \langle x|\phi\rangle =$$

$$= \int_{-\infty}^{\infty} dx\phi^*(x)\phi(x) = \int_{-\infty}^{\infty} dx|\phi(x)|^2$$

That is

$$\langle\phi|\phi\rangle = \int_{-\infty}^{\infty} dx|\phi(x)|^2 \tag{10}$$

where $\phi(x) = \langle x|\phi\rangle$ is the wave function of the state $|\phi\rangle$ and, in general, is not normalized.

Using (8), we have

$$\phi(x) = \langle x|\hat{a}|\psi\rangle \overset{\overbrace{\text{see ref. [5]}}}{=} \hat{a}(x)\langle x|\psi\rangle = \hat{a}(x)\psi(x)$$

That is

$$\phi(x) = \hat{a}(x)\psi(x)$$

Substituting into (10), we obtain

$$\langle\phi|\phi\rangle = \int_{-\infty}^{\infty} dx|\hat{a}(x)\psi(x)|^2$$

Substituting into (9), we obtain

$$\left\|\hat{a}\left|\psi\right\rangle\right\|^2 = \int\limits_{-\infty}^{\infty} dx \left|\hat{a}(x)\psi(x)\right|^2 \tag{11}$$

which shows that the integral $\int\limits_{-\infty}^{\infty} dx \left|\hat{a}(x)\psi(x)\right|^2$ is the square of the norm of the state $\hat{a}\left|\psi\right\rangle$.

Using (7) and (11), we derive that

$$\left\|\hat{a}\left|\psi\right\rangle\right\|^2 \geq 0 \tag{12}$$

As noted, the operator (6) is not Hermitian.

Its Hermitian conjugate is, using (6),

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

Then

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

$$= \frac{1}{p_0^2}\left(\hat{p}^2(x) + i\hbar\hat{p}(x)\frac{\psi_0'(x)}{\psi_0(x)} - i\hbar\frac{\psi_0'(x)}{\psi_0(x)}\hat{p}(x) - (i\hbar)^2\left(\frac{\psi_0'(x)}{\psi_0(x)}\right)^2\right) =$$

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

That is

$$\hat{a}^\dagger(x)\hat{a}(x) = \frac{1}{p_0^2}\left(\hat{p}^2(x) + i\hbar\left[\hat{p}(x), \frac{\psi_0'(x)}{\psi_0(x)}\right] + \hbar^2\left(\frac{\psi_0'(x)}{\psi_0(x)}\right)^2\right) \tag{13}$$

If $f(x)$ is an arbitrary $C^1(R)$ function, then

$$\left[\hat{p}(x), f(x)\right] = -i\hbar f'(x) \tag{14}$$

This can be easily shown by applying the commutator $\left[\hat{p}(x), f(x)\right]$ to an arbitrary wave function.

Using (14), we have

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

Then, (13) is written as

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

$$=\frac{1}{p_0^{\,2}}\left(\hat{p}^2(x)-(i\hbar)^2\frac{\psi_0''(x)}{\psi_0(x)}+(i\hbar)^2\left(\frac{\psi_0'(x)}{\psi_0(x)}\right)^2+\hbar^2\left(\frac{\psi_0'(x)}{\psi_0(x)}\right)^2\right)=$$

$$=\frac{1}{p_0^{\,2}}\left(\hat{p}^2(x)+\hbar^2\frac{\psi_0''(x)}{\psi_0(x)}-\hbar^2\left(\frac{\psi_0'(x)}{\psi_0(x)}\right)^2+\hbar^2\left(\frac{\psi_0'(x)}{\psi_0(x)}\right)^2\right)=$$

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

That is

$$\hat{a}^\dagger(x)\hat{a}(x)=\frac{1}{p_0^{\,2}}\left(\hat{p}^2(x)+\hbar^2\frac{\psi_0''(x)}{\psi_0(x)}\right)\tag{15}$$

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

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

where E_0 is the energy.

Solving for $\psi_0''(x)/\psi_0(x)$ yields

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

Substituting into (15) yields

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

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

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

The constant $2m/p_0{}^2$ has dimensions of inverse energy, and setting

$$\varepsilon_0 \equiv \frac{p_0{}^2}{2m} > 0$$

we end up to

$$\hat{a}^{\dagger}(x)\hat{a}(x) = \frac{1}{\varepsilon_0}\left(\hat{H}(x) - E_0\right) \tag{16}$$

The operator $\hat{a}^{\dagger}(x)\hat{a}(x)$ has non-negative eigenvalues.

Proof

We'll consider the operator $\hat{a}^{\dagger}\hat{a}$, which is the operator $\hat{a}^{\dagger}(x)\hat{a}(x)$ in the state space [5].

If $|\lambda\rangle$ is an eigenstate of $\hat{a}^{\dagger}\hat{a}$, of eigenvalue λ, we have, using the, more suitable in this case, general notation of the inner product [7],

$$\left(|\lambda\rangle, \hat{a}^{\dagger}\hat{a}|\lambda\rangle\right) = \left(\left(\hat{a}^{\dagger}\right)^{\dagger}|\lambda\rangle, \hat{a}|\lambda\rangle\right) = \left(\hat{a}|\lambda\rangle, \hat{a}|\lambda\rangle\right) = \left\|\hat{a}|\lambda\rangle\right\|^2 \geq 0$$

That is

$$\left(|\lambda\rangle, \hat{a}^{\dagger}\hat{a}|\lambda\rangle\right) \geq 0 \tag{17}$$

But

$$\hat{a}^{\dagger}\hat{a}|\lambda\rangle = \lambda|\lambda\rangle$$

Thus

$$\left(|\lambda\rangle, \hat{a}^{\dagger}\hat{a}|\lambda\rangle\right) = \left(|\lambda\rangle, \lambda|\lambda\rangle\right) = \lambda\left(|\lambda\rangle, |\lambda\rangle\right) = \lambda\left\||\lambda\rangle\right\|^2$$

That is

$$\lambda\left\||\lambda\rangle\right\|^2 = \left(|\lambda\rangle, \hat{a}^\dagger \hat{a}|\lambda\rangle\right)$$

and using (17), we obtain

$$\lambda\left\||\lambda\rangle\right\|^2 \geq 0$$

and, since $\left\||\lambda\rangle\right\|^2 \geq 0$, we end up to $\lambda \geq 0$, i.e. the eigenvalues of $\hat{a}^\dagger \hat{a}$ are non-negative.

Since $\hat{a}^\dagger(x)\hat{a}(x)$ is the expression of $\hat{a}^\dagger \hat{a}$ in position space, $\hat{a}^\dagger(x)\hat{a}(x)$ and $\hat{a}^\dagger \hat{a}$ have the same eigenvalues, thus the eigenvalues of $\hat{a}^\dagger(x)\hat{a}(x)$ are also non-negative.

Then, from (16), since $\varepsilon_0 > 0$, we derive that the eigenvalues of $\hat{H}(x) - E_0$ are also non-negative.

Thus, if E is an eigenvalue of $\hat{H}(x)$, i.e. an energy, $E \geq E_0$, i.e. E_0 is the minimum energy, and thus $\psi_0(x)$ is the minimum-energy eigenfunction, i.e. it is the ground-state wave function.

Note

If $\psi_0(x)$ has zeros at points where the potential is finite, i.e. if it has a non-zero number of typical nodes [6], then the wave function $\hat{a}(x)\psi(x)$ will have singularities, since at the typical nodes of $\psi_0(x)$, the arbitrary wave function $\psi(x)$ does not, in general, vanish.

Then, the Riemann integral $\int\limits_{-\infty}^{\infty} dx\left|\hat{a}(x)\psi(x)\right|^2$, i.e. the square of the norm of the state $\hat{a}|\psi\rangle$ in position space, is not well-defined, and the above reasoning, which results in $\psi_0(x)$ being the minimum-energy eigenfunction, is not applied.

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