EVERY ATTRACTIVE 1-DIMENSIONAL POTENTIAL HAS A BOUND STATE

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Reference: Lecture by Barton Zwiebach in MIT course 8.05.1x, week 1, Deep Dive 2 (not in the PDF notes).

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.2b.

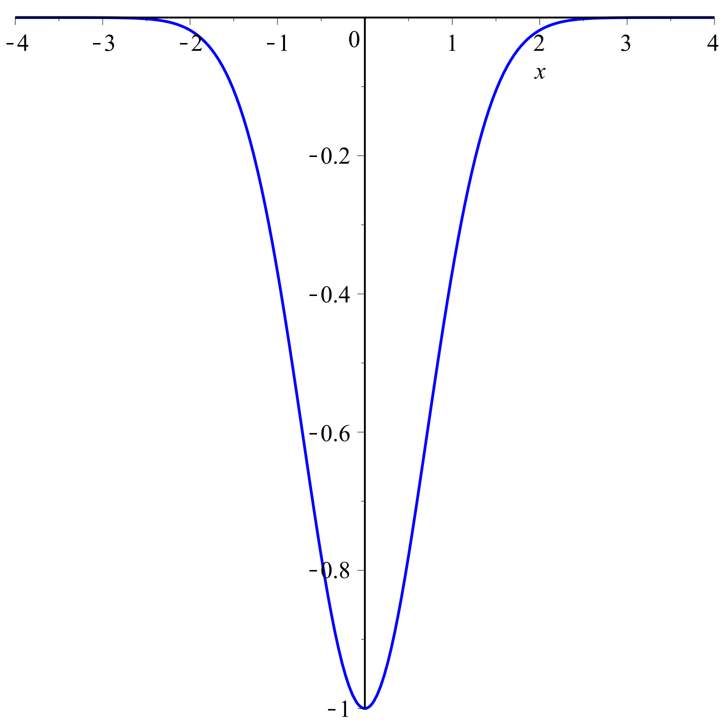
An interesting application of the variational principle in quantum mechances is the following theorem:

Theorem. ***Every 1-dimensional attractive potential has at least one bound state.***

To prove this, we need first to define what we mean by an attractive potential $V(x)$. $V(x)$ must satisfy the following conditions:

- $V(x) \to 0$ as $x \to \pm\infty$.
- $V(x) < 0$ everywhere.
- $V(x)$ is piecewise continuous. This means that it may have a finite number of jump discontinuities.

One possible form for $V(x)$ is as shown:



This is a particularly simple potential that satisfies the above conditions. We could introduce a few step functions, multiple local maxima and minima, and so on, provided we don't violate any of the 3 conditions above.

Since $V(x) < 0$ everywhere, we can write it as

$$V(x) = -|V(x)| \tag{1}$$

What we would like to prove is that for any hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)| \tag{2}$$

the ground state E_0 is a bound state, that is

$$E_0 < 0 \tag{3}$$

We can apply the variational principle, which states

If ψ is any normalized function and H is a hamiltonian, then the ground state energy E_0 of this hamiltonian has an upper bound given by

$$E_0 \leq \langle\psi|H|\psi\rangle \equiv \langle H\rangle \tag{4}$$

The use of the variational principle to prove the above theorem involves a bit of a convoluted argument, but the mathematics involved is fairly simple. Our goal is to find some wave function ψ_α (where α is some parameter that we can vary) so that

$$E_0 \leq \langle \psi_\alpha | H | \psi_\alpha \rangle = \langle H \rangle_{\psi_\alpha} < 0 \tag{5}$$

From 2 we have

$$\left\langle \hat{H} \right\rangle_{\psi_\alpha} = \int dx\ \psi_\alpha(x)\, \hat{H} \psi_\alpha(x) \tag{6}$$

$$= \langle T \rangle_{\psi_\alpha} - \langle |V(x)| \rangle_{\psi_\alpha} \tag{7}$$

where

$$\langle T \rangle_{\psi_\alpha} = -\int dx\ \psi_\alpha(x) \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_\alpha(x) \tag{8}$$

$$\langle |V(x)| \rangle_{\psi_\alpha} = \int dx\ \psi_\alpha(x) |V(x)|\, \psi_\alpha(x) \tag{9}$$

We can integrate 8 by parts once to get

$$\langle T \rangle_{\psi_\alpha} = -\int dx\ \psi_\alpha(x) \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_\alpha(x) \tag{10}$$

$$= -\frac{\hbar^2}{2m} \psi_\alpha(x) \frac{d}{dx} \psi_\alpha(x) \Big|_{-\infty}^{\infty} + \frac{\hbar^2}{2m} \int dx\ \left(\frac{d}{dx} \psi_\alpha(x) \right)^2 \tag{11}$$

$$= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx\ \left(\frac{d}{dx} \psi_\alpha(x) \right)^2 \tag{12}$$

where we invoke the usual requirement that ψ_α and its first derivative vanish at infinity.

We therefore see that since the integrand in the last line is always positive (we're assuming that ψ_α is not zero everywhere), that $\langle T \rangle_{\psi_\alpha} > 0$. Likewise, from 9, $\langle |V(x)| \rangle_{\psi_\alpha} > 0$. Thus in order that $\langle H \rangle_{\psi_\alpha} < 0$, we must have

$$\langle T \rangle_{\psi_\alpha} < \langle |V(x)| \rangle_{\psi_\alpha} \tag{13}$$

To get any further, we need to choose a test function $\psi_\alpha(x)$. We'll pick (because it works!)

$$\psi_\alpha = \left(\frac{\alpha}{\pi} \right)^{1/4} e^{-\frac{1}{2}\alpha x^2} \tag{14}$$

The factor of $\left(\frac{\alpha}{\pi}\right)^{1/4}$ is required so that ψ_α is normalized. The integral in 12 can be done using standard methods; I'll just use Maple, and we find

$$\langle T\rangle_{\psi_\alpha} = \frac{\hbar^2\alpha}{4m} \tag{15}$$

The integral 9 of course can't be done exactly if we don't know what V is, so we have just

$$\langle |V(x)|\rangle_{\psi_\alpha} = \int dx\, \psi_\alpha^2(x)\,|V(x)| \tag{16}$$

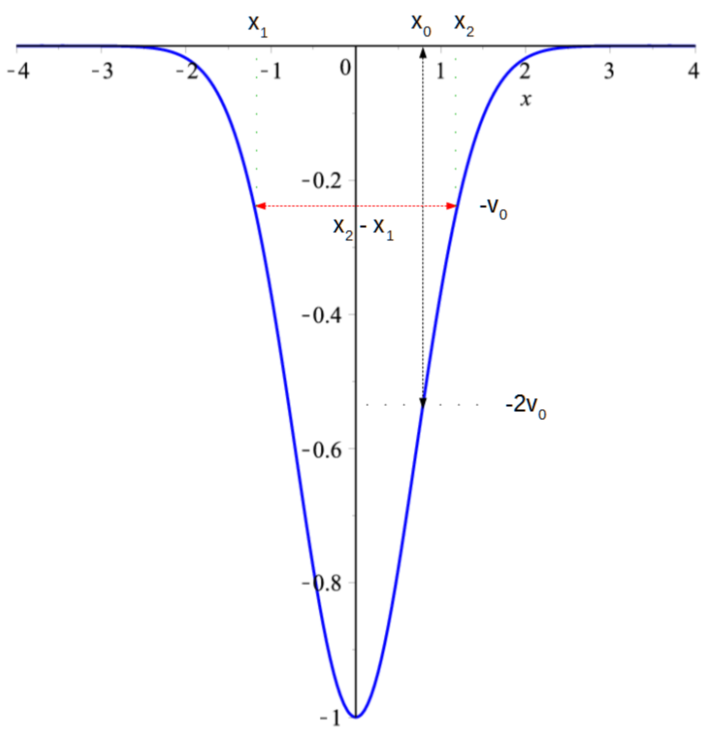
(No need for modulus signs around ψ_α since the function 14 is real.) To progress further, we need to start invoking some inequalities to get where we want to go. The argument consists of several steps, so watch carefully as we go along.

From 13 through 15 we have to show that we can satisfy the condition

$$\frac{\langle |V(x)|\rangle_{\psi_\alpha}}{\langle T\rangle_{\psi_\alpha}} = \frac{4m}{\hbar^2\sqrt{\pi}}\frac{1}{\sqrt{\alpha}}\int_{-\infty}^{\infty} e^{-\alpha x^2}\,|V(x)|\,dx > 1 \tag{17}$$

Since V is arbitrary subject to the 3 conditions above, the only thing we can legitimately fiddle with is the value of α. We can see that if we choose α small enough, we should be able to satisfy this inequality, since for small α, the $1/\sqrt{\alpha}$ term gets large, while the $e^{-\alpha x^2}$ term in the integrand is bounded between 0 and 1. We need to find some upper limit for α.

In what follows, you'll need to refer to the following diagram:



First, we choose some point x_0 at which $V(x_0)$ is continuous (that is, we ensure that x_0 isn't at one of the points where $V(x)$ has a discontinuity, or jump). The value of $V(x_0)$ is defined as $-2v_0$ where $v_0 > 0$. Because $V \to 0$ at $x \to \pm\infty$, there must be points x_1 and x_2 on either side of x_0 where V has the value $-v_0$ (actually, I'm not sure this is strictly true, because, as V is allowed a few jumps, it might jump over the point where it's equal to $-v_0$. However, as the number of jumps is required to be finite, there must be *some* points x_1 and x_2 on either side of x_0 where V attains a value that is between $-2v_0$ and 0, and I think the argument below still works if we choose those points instead.)

Now for the first inequality. We know that, because the integrand is positive

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} |V(x)|\, dx > \int_{x_1}^{x_2} e^{-\alpha x^2} |V(x)|\, dx \tag{18}$$

Second inequality: in the interval x_1 to x_2, $|V(x)| > v_0$ (see the diagram!), so we have

$$\int_{x_1}^{x_2} e^{-\alpha x^2} |V(x)|\, dx > v_0 \int_{x_1}^{x_2} e^{-\alpha x^2} dx \tag{19}$$

The last integral has no closed form solution, but we know that in the interval x_1 to x_2

$$e^{-\alpha x^2} > e^{-\alpha \max\left(x_1^2, x_2^2\right)} \tag{20}$$

Therefore

$$v_0 \int_{x_1}^{x_2} e^{-\alpha x^2} dx > v_0 \int_{x_1}^{x_2} e^{-\alpha \max\left(x_1^2, x_2^2\right)} dx \tag{21}$$

$$= v_0 \left(x_2 - x_1\right) e^{-\alpha \max\left(x_1^2, x_2^2\right)} \tag{22}$$

Now suppose we choose α to be

$$\alpha < \frac{1}{\max\left(x_1^2, x_2^2\right)} \tag{23}$$

Then

$$e^{-\alpha \max\left(x_1^2, x_2^2\right)} > e^{-1} \tag{24}$$

We can now summarize as follows:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} \left|V\left(x\right)\right| dx > v_0 \left(x_2 - x_1\right) e^{-1} \tag{25}$$

provided we choose α according to 23. Plugging this back into 17 we have

$$\frac{\left\langle \left|V\left(x\right)\right| \right\rangle_{\psi_\alpha}}{\left\langle T \right\rangle_{\psi_\alpha}} > \frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e} \frac{1}{\sqrt{\alpha}} \tag{26}$$

This expression will now be greater than 1 provided that

$$\sqrt{\alpha} < \frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e} \tag{27}$$

$$\alpha < \left[\frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e}\right]^2 \tag{28}$$

Comparing 23 and 28, we see that we can satisfy both conditions if we take

$$\alpha < \min\left\{\frac{1}{\max\left(x_1^2, x_2^2\right)}, \left[\frac{4m}{\hbar^2\sqrt{\pi}}\frac{v_0\left(x_2 - x_1\right)}{e}\right]^2\right\} \tag{29}$$

This condition depends on x_1 and x_2 but that doesn't matter, since both quantities in the RHS of 29 are positive, so there is always some positive value of α that satisfies the condition. In other words, going right back to 17 and then to 7, we can always find a value of α so that $\langle H\rangle < 0$ which means that the ground state of H must be negative, which makes it a bound state.