

Quirky Quantum Updates

The Anti-Textbook*

Updates to Quirky Quantum Concepts:

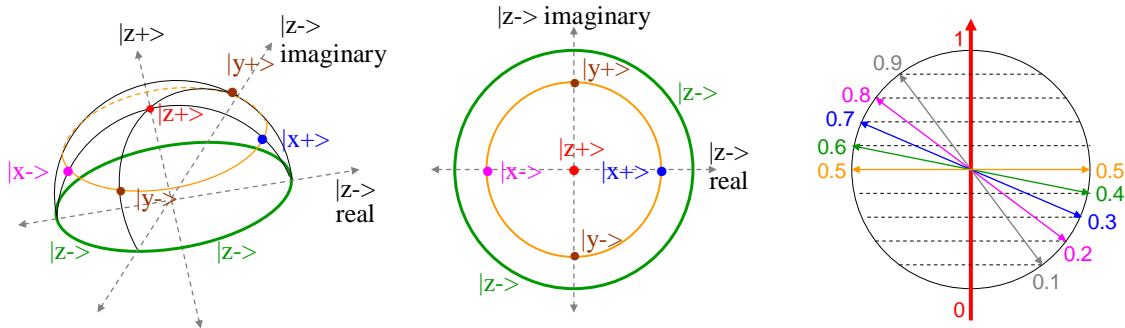
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Eric L. Michelsen



“Quantum Mechanics is a silly theory, perhaps the silliest theory to come out of the 20th century. The only reason it has any following at all is that it is completely supported by experiment.” – *Unknown physicist*

“We are all agreed that your theory is crazy. The question that divides us is whether it is crazy enough to have a chance of being correct.” – *Niels Bohr*

“Now in the further development of science, we want more than just a formula. First we have an observation, then we have numbers that we measure, then we have a law which summarizes all the numbers. But the real *glory* of science is that we can *find a way of thinking* such that the law is *evident*.” – *Richard Feynman*

* Physical, conceptual, geometric, and pictorial physics that didn't fit in your textbook.

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Physical constants: 2006 values from NIST. For more, see <http://physics.nist.gov/cuu/Constants/>.

Speed of light in vacuum	$c = 299\,792\,458\text{ m s}^{-1}$ (exact)
Gravitational constant	$G = 6.674\,28(67) \times 10^{-11}\text{ m}^3\text{ kg}^{-1}\text{ s}^{-2}$
Relative standard uncertainty	$\pm 1.0 \times 10^{-4}$
Boltzmann constant	$k = 1.380\,6504(24) \times 10^{-23}\text{ J K}^{-1}$
Stefan-Boltzmann constant	$\sigma = 5.670\,400(40) \times 10^{-8}\text{ W m}^{-2}\text{ K}^{-4}$
Relative standard uncertainty	$\pm 7.0 \times 10^{-6}$
Avogadro constant	$N_A, L = 6.022\,141\,79(30) \times 10^{23}\text{ mol}^{-1}$
Relative standard uncertainty	$\pm 5.0 \times 10^{-8}$
Molar gas constant	$R = 8.314\,472(15)\text{ J mol}^{-1}\text{ K}^{-1}$
calorie	4.184 J (exact)
Electron mass	$m_e = 9.109\,382\,15(45) \times 10^{-31}\text{ kg}$
Proton mass	$m_p = 1.672\,621\,637(83) \times 10^{-27}\text{ kg}$
Proton/electron mass ratio	$m_p/m_e = 1836.152\,672\,47(80)$
Elementary charge	$e = 1.602\,176\,487(40) \times 10^{-19}\text{ C}$
Electron g-factor	$g_e = -2.002\,319\,304\,3622(15)$
Proton g-factor	$g_p = 5.585\,694\,713(46)$
Neutron g-factor	$g_N = -3.826\,085\,45(90)$
Muon mass	$m_\mu = 1.883\,531\,30(11) \times 10^{-28}\text{ kg}$
Inverse fine structure constant	$\alpha^{-1} = 137.035\,999\,679(94)$
Planck constant	$h = 6.626\,068\,96(33) \times 10^{-34}\text{ J s}$
Planck constant over 2π	$\hbar = 1.054\,571\,628(53) \times 10^{-34}\text{ J s}$
Bohr radius	$a_0 = 0.529\,177\,208\,59(36) \times 10^{-10}\text{ m}$
Bohr magneton	$\mu_B = 927.400\,915(23) \times 10^{-26}\text{ J T}^{-1}$

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1 General Topics

Kinky Variations

The variational principle provides a fairly simple way to estimate the ground state energy of a system that we cannot solve exactly. We often hear that our choice of trial wave-function isn't very important; the variational principle works "pretty well" with most any trial wave-function [Gri ??, others]. However, we show here that making a judicious choice of trial wave-function can significantly improve the accuracy of your estimate. We compare here 6 trial wave-functions: the cosine, a symmetric exponential, two symmetric rational functions, a triangle, and a gaussian.

You may have seen a variational problem to estimate the ground state energy for a delta-function potential,

$$V(x) = -\alpha\delta(x), \quad \alpha > 0, [\alpha] = \text{J}\cdot\text{m},$$

using a cosine half-cycle as the trial wave-function (Figure 1.1a). (A delta-function can be a reasonable approximation to some tight potentials where the decay length of ψ is much longer than the width of the potential well.) The cosine wave-function is not very good, being off by a factor of ~ 2.5 in ground-state energy [Gri chap 7??]. Could we have reasonably done better? Yes.

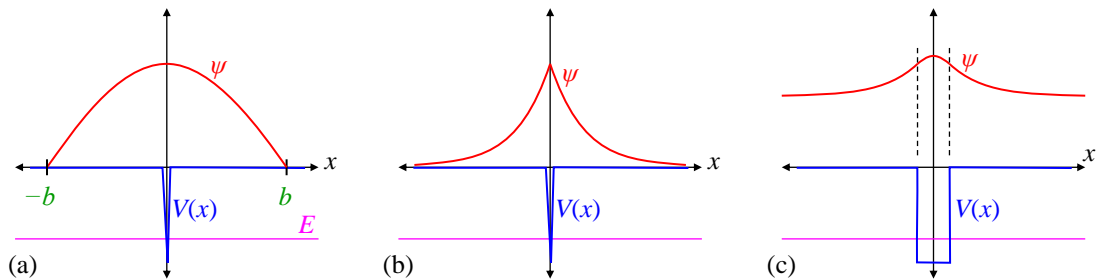


Figure 1.1 (a) A poor trial wave-function. (b) A better trial wave-function. (c) Close-up of infinitesimal behavior near the delta-function.

We compare here several trial wave-functions, with these results:

Trial Function	Error
exponential	0
$(bx + 1)^{-n}$ (two-parameter)	0
$(bx + 1)^{-2}$	6%
$(bx + 1)^{-1}$	25%
triangle	25%
gaussian	57%
cosine	150%

The exponential happens to be exact, and the best 1-parameter rational function we tried is within 6%. The smooth functions, cosine and gaussian, are off by factors of ~ 2.5 and 1.5. Finally, we minimize a two-parameter trial rational function, and find it also yields the exact answer (probably by coincidence). We conclude:

The qualitative features of the trial wave-function are important to getting an accurate estimate of the ground state energy with the variational principle.

What qualitative features might we put into our trial wave-functions? First, we expect $|\psi|^2$ to be concentrated near the attractive potential. While $\cos(\)$ has this feature, it is broad and flat near the delta-function, as is the

gaussian. A sharper concentration is likely better. Second, it is a general feature of the Schrodinger Equation (SE) that a delta function in the potential causes a discontinuity in ψ' , i.e. a “kink.” Therefore, a wave-function like Figure 1.1b is a better choice.

[We note that the entire variational principle is justified on the completeness of the eigenfunctions: any arbitrary function can be written as a superposition of eigenfunctions. This insures the ground state energy is the minimum of all possible energies. This proof works only for complete eigenfunction sets. For finite potential wells, of which the delta-function potential is a limiting case, the bound-state eigenfunctions are *not* complete. The delta-function potential has only one bound state, and the finite well has only a finite number of bound states. It's impossible to construct an arbitrary function from only a finite number of basis functions. Therefore, we have no reason to expect that the variational principle works at all for such potentials. Nonetheless, it *does* seem to work. We proceed cautiously, as we may be on shaky ground.]

Exponential Trial Wave-function

One candidate trial wave-function that looks like Figure 1.1b is:

$$\psi(x) = Ae^{-b|x|}, \quad b > 0.$$

(One can see almost immediately that this is the exact wave-function: ψ in a classically forbidden region of constant potential is always a decaying exponential. More below.) Our variational parameter is b . We now follow the usual steps for minimizing the variational energy [Gri ch. 7]:

- find the normalization factor A in terms of b ;
- compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$ as functions of b ;
- find the b that minimizes $\langle H \rangle$;
- and finally, find the minimum $\langle H \rangle$.

Normalize:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x) dx = 1 = A^2 \left[\int_{-\infty}^0 e^{+2bx} dx + \int_0^{\infty} e^{-2bx} dx \right] = A^2 \left[2 \int_0^{\infty} e^{-2bx} dx \right] = -A^2 \frac{2}{2b} \left[e^{-2bx} \right]_0^{\infty} = \frac{A^2}{b}$$

$$A^2 = b.$$

Note that b has units of m^{-1} , and $[A] = [\psi] = m^{-1/2}$, as necessary.

Compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$: The average potential energy is straightforward from the definition of the delta-function, and its integral:

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^*(x)V(x)\psi(x) dx = -\alpha A^2 \int_{-\infty}^{\infty} e^{+bx} \delta(x) e^{-bx} dx = -b\alpha, \quad \text{using } A^2 = b.$$

The kinetic energy is a little bit subtle, because we must take the 2nd derivative of ψ , which is infinite at $x = 0$ (the kink). Therefore, we split the integral into 3 parts:

$$\langle T \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) dx$$

$$= \frac{-\hbar^2}{2m} \left[A^2 \int_{-\infty}^{0^-} e^{+bx} b^2 e^{+bx} dx + \int_{0^-}^{0^+} \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) dx + A^2 \int_{0^+}^{\infty} e^{-bx} b^2 e^{-bx} dx \right].$$

The first and third integrals are simple, and equal:

$$I \equiv A^2 \int_{-\infty}^0 e^{+bx} b^2 e^{+bx} dx = b^3 \left[\frac{1}{2b} e^{2bx} \right]_{-\infty}^0 = \frac{b^2}{2}.$$

The middle integral can be evaluated from the Fundamental Theorem of Calculus, to wit: the integral of a derivative equals the difference of the original function at the endpoints:

$$\int_a^b f'(x) dx = f(b) - f(a) \Rightarrow \int_a^b \psi'' dx = \psi'(b) - \psi'(a).$$

Then the middle integral becomes:

$$\psi'(x) = \pm A b e^{\pm b x} \Rightarrow \int_{0^-}^{0^+} \psi''(x) dx = \psi'(0^+) - \psi'(0^-) = A^2 (-b e^0 - b e^0) = -2b^2.$$

Physically, we can visualize the wave-function to be as in Figure 1.1c, in the limit as the near-delta-function goes to zero width. Note that in this transition region, the KE is positive (ψ is concave toward the axis).

Combining the 3 terms:

$$\langle T \rangle = \frac{-\hbar^2}{2m} (I - 2b^2 + I) = + \frac{\hbar^2 b^2}{2m}.$$

Note that $\langle T \rangle$ is positive, as it must be on physical grounds. Mathematically, for square-integrable functions (which wave-functions must be), \hat{T} is a positive definite operator. This holds true even though the kinetic energy is negative for all of the wave-function, except at the discontinuity (where the local kinetic energy is infinite over an infinitesimal distance).

Finally:

$$\langle H \rangle = \frac{\hbar^2 b^2}{2m} - b\alpha.$$

Find the b that minimizes $\langle H \rangle$:

$$\frac{d\langle H \rangle}{db} = 0 = \frac{\hbar^2 b}{m} - \alpha, \quad b = \frac{m\alpha}{\hbar^2}. \quad (1.1)$$

Find the minimum $\langle H \rangle$:

$$\langle H \rangle_{\min} = \left[\frac{\hbar^2 b^2}{2m} - b\alpha \right]_{b=m\alpha/\hbar^2} = \frac{\hbar^2}{2m} \left(\frac{m^2 \alpha^2}{\hbar^4} \right) - \frac{m\alpha^2}{\hbar^2} = \frac{m\alpha^2}{2\hbar^2} - \frac{m\alpha^2}{\hbar^2} = -\frac{m\alpha^2}{2\hbar^2}. \quad (1.2)$$

Since we happened to guess the exact wave-function, this is the exact ground-state energy.

Another Kinky Variation: Rational Function

Our first guess for the variational wave-function turned out to be the exact wave-function. But how well would a different trial wave-function do? Let us try another “good-looking” wave-function, whose graph is qualitatively the same as before (Figure 1.1b):

$$\psi(x) = A \frac{1}{(b|x+1|)^2}, \quad b > 0.$$

It satisfies the requirement for a kink at $x = 0$, and is normalizable. Note that ‘ b ’ here is completely different from our previous ‘ b ’, though it still has units of m^{-1} . We now follow the standard four steps for the variational estimate of the ground state energy. The algebra is a little more involved than before, but straightforward. Note that our result will include dimensionless constant factors; we must compute these rigorously, because the accuracy of our result depends on them. This includes scrupulous computing and use of the normalization factor A .

Normalize: We use the even-ness of ψ , so we double the right-half integral:

$$1 = 2A^2 \int_0^\infty (bx+1)^{-4} dx = -\frac{2A^2}{3b} \left[(bx+1)^{-3} \right]_0^\infty = \frac{2A^2}{3b}, \quad A^2 = \frac{3b}{2}.$$

Compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$: The average potential energy is straightforward from the definition of the delta-function, and its integral:

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^*(x) V(x) \psi(x) dx = -\alpha A^2 \int_{-\infty}^{\infty} (1) \delta(x) (1) dx = -\frac{3b}{2} \alpha, \quad \text{using } A^2 = \frac{3b}{2}.$$

The kinetic energy is a little bit subtle, because we must take the 2nd derivative of ψ , which is infinite at $x = 0$ (the kink), so we split up the integral:

$$\langle T \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) dx = \frac{-\hbar^2}{2m} \left[\int_{0^-}^{0^+} \psi^*(x) \psi''(x) dx + 2 \int_0^{\infty} \psi^*(x) \psi''(x) dx \right].$$

The derivatives of ψ are:

$$\begin{aligned} \psi'(x > 0) &= Ab(-2)(bx+1)^{-3}, & \psi'(x < 0) &= Ab(+2)(-bx+1)^{-3} \\ \psi''(x) &= Ab^2(+6)(b|x|+1)^{-4} \end{aligned}$$

As before, we use the Fundamental Theorem of Calculus for the first integral:

$$\begin{aligned} \langle T \rangle &= \frac{-\hbar^2}{2m} \left[\int_{0^-}^{0^+} \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) dx + 2A^2 b^2 \int_0^{\infty} (bx+1)^{-2} 6(bx+1)^{-4} dx \right] && \text{Use } 2A^2 = 3b \\ &= \frac{-\hbar^2}{2m} \left\{ \psi^*(0) (\psi'(0^+) - \psi'(0^-)) + \frac{18b^2}{(-5)} \left[(bx+1)^{-5} \right]_0^{\infty} \right\} \\ &= \frac{-\hbar^2}{2m} \left\{ A^2 b (-2 - 2) - \frac{18}{5} b^2 (-1) \right\} \\ &= \frac{-\hbar^2}{2m} \left\{ -6b^2 + \frac{18}{5} b^2 \right\} = \frac{+\hbar^2}{m} \left(\frac{6}{5} \right) b^2. \end{aligned}$$

As before, we can visualize the wave-function to be as in Figure 1.1c, in the limit as the near-delta-function goes to zero width. Note that in this transition region, the KE is positive (ψ is concave toward the axis). Also, $\langle T \rangle$ is positive, as it must be on physical grounds. Mathematically, for square-integrable functions, \hat{T} is a positive definite operator. This holds true even though the kinetic energy is negative for all of the wave-function, except at the discontinuity (where kinetic energy is infinite).

Finally:

$$\langle H \rangle = \frac{\hbar^2}{m} \left(\frac{6}{5} \right) b^2 - \frac{3b}{2} \alpha.$$

Find the b that minimizes $\langle H \rangle$:

$$0 = \frac{d\langle H \rangle}{db} = \frac{12\hbar^2}{5m} b - \frac{3\alpha}{2}, \quad b = \frac{5m\alpha}{8\hbar^2}.$$

Remember, this b has nothing to do with b from our trial exponential wave-function, so the two values cannot be compared.

Find the minimum $\langle H \rangle$:

$$\begin{aligned} \langle H \rangle_{\min} &= \left[\frac{\hbar^2}{m} \left(\frac{6}{5} \right) b^2 - \frac{3b}{2} \alpha \right]_{b=5m\alpha/8\hbar^2} = \frac{\hbar^2}{m} \left(\frac{6}{5} \right) \frac{5^2 m^2 \alpha^2}{8^2 \hbar^4} - \frac{15m\alpha^2}{16\hbar^2} \\ &= \frac{15m\alpha^2}{32\hbar^2} - \frac{15m\alpha^2}{16\hbar^2} = -\frac{15}{32} \frac{m\alpha^2}{\hbar^2}. \end{aligned}$$

This is negative, and slightly higher (less negative) than the exact value. It is off the true value by only 6%. Thus we see that a qualitatively “good” trial wave-function provides much better results than a qualitatively “bad” one.

The Exact Solution

We now find the exact solution by solving the Schrodinger eigenfunction/eigenvalue equation. In a classically forbidden region where the potential is constant, ψ is always a decaying exponential:

$$\frac{-\hbar^2}{2m}\psi'' + V\psi = E\psi, \quad \psi'' - \frac{2m}{\hbar^2}(V - E)\psi = 0. \quad (1.3)$$

The solution is elementary:

$$\psi(x) = Ae^{\pm bx} \quad \text{where} \quad b = \frac{\sqrt{2m(V - E)}}{\hbar}. \quad (1.4)$$

E is the as-yet unknown eigenvalue for energy, and b is just a notational convenience to simplify the formulas. (This ψ is the form we guessed for one of our variational wave-functions, so that variational $\langle H \rangle$ must be exact.)

As always, to find the allowed (i.e., quantized) E , we must apply the auxiliary conditions. These are often boundary conditions, but with the delta-function potential, they are the matching conditions at the δ -function. The first condition is that ψ must be continuous at $x = 0$:

$$\psi(0^-) = \psi(0^+),$$

which simply means (in this case) that A for the left half of ψ must equal A for the right half. The second matching condition is that ψ' must satisfy the SE at $x = 0$. This means the discontinuity in ψ' must be “just right.” We quantify this by integrating (1.3) across the discontinuity:

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

Note that both sides scale with the normalization A , which means we can ignore A here. On the LHS we get:

$$\psi'(x) = \pm be^{\pm bx} \quad \Rightarrow \quad \psi'(0^+) - \psi'(0^-) = (-be^0 - be^0) = -2b.$$

In the RHS, only the V term contributes:

$$\frac{2m}{\hbar^2} \int_{0^-}^{0^+} V(x)\psi(x) dx = \frac{2m}{\hbar^2} \int_{0^-}^{0^+} -\alpha\delta(x)e^{bx} dx = -\frac{2m\alpha}{\hbar^2}.$$

Equating the LHS and RHS:

$$-2b = -\frac{2m\alpha}{\hbar^2} \quad \Rightarrow \quad b = \frac{m\alpha}{\hbar^2}.$$

This is the energy eigenvalue equation, written in terms of b . (Because we guessed the exact form of ψ above, this eigenvalue equation is identical to the minimum energy equation, (1.1).) To find the eigenvalue E , we simply substitute (1.4) for b , and use $V = 0$ outside the discontinuity:

$$\frac{\sqrt{2m(V - E)}}{\hbar} = \frac{m\alpha}{\hbar^2}, \quad 2m(0 - E) = \frac{m^2\alpha^2}{\hbar^2}, \quad E = -\frac{m\alpha^2}{2\hbar^2}.$$

This agrees with our lucky-guess variational estimate (1.2).

A Smooth Variation

I was challenged by a colleague to try a gaussian as a trial wave-function. Gaussians are generally “good” functions, and usually integrable in closed form. The question is: will a gaussian perform poorly like a cosine,

because the gaussian is also smooth and flat in the middle, or will a gaussian perform well, like the kinky trials, because it's, well, a gaussian. So here we go:

Normalize: $\psi(x) = A \exp(-bx^2)$. The gaussian integral is well known, $\int_{-\infty}^{\infty} \exp(-ax^2) dx = \sqrt{\frac{\pi}{a}}$:

$$1 = \int_{-\infty}^{\infty} \psi^*(x)\psi(x) dx = A^2 \int_{-\infty}^{\infty} \exp(-2bx^2) dx = A^2 \sqrt{\frac{\pi}{2b}}, \quad A^2 = \sqrt{\frac{2b}{\pi}}.$$

b has units of m^{-2} .

Compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$: The average potential energy is straightforward from the definition of the delta-function, and its integral:

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^*(x)V(x)\psi(x) dx = -\alpha A^2 \int_{-\infty}^{\infty} e^{-bx^2} \delta(x) e^{-bx^2} dx = -\alpha \sqrt{\frac{2b}{\pi}}.$$

The kinetic energy is straightforward, since all the derivatives are well-defined:

$$\begin{aligned} \psi' &= -2bx \exp(-bx^2) \\ \psi'' &= -2b \left(x \exp(-bx^2) (-2bx) + \exp(-bx^2) \right) = -2b \left[-2bx^2 \exp(-bx^2) + \exp(-bx^2) \right] \\ \langle T \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) dx \\ &= \frac{-\hbar^2}{2m} A^2 (-2b) \left[\int_{-\infty}^{\infty} e^{-bx^2} (-2b) x^2 e^{-bx^2} dx + \int_{-\infty}^{\infty} e^{-bx^2} e^{-bx^2} dx \right] \\ &= \frac{\hbar^2 b}{m} \sqrt{\frac{2b}{\pi}} \left[(-2b) \int_{-\infty}^{\infty} x^2 e^{-2bx^2} dx + \int_{-\infty}^{\infty} e^{-2bx^2} dx \right]. \end{aligned}$$

We use another standard integral, $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a^3}}$:

$$\langle T \rangle = \frac{\hbar^2 b}{m} \sqrt{\frac{2b}{\pi}} \left[(-2b) \frac{1}{2} \sqrt{\frac{\pi}{8b^3}} + \sqrt{\frac{\pi}{2b}} \right] = \frac{\hbar^2}{m} \sqrt{2} \left[-b \sqrt{\frac{1}{8}} + b \sqrt{\frac{1}{2}} \right] = \frac{\hbar^2}{2m} b.$$

This is positive, as it must be.

Find the b that minimizes $\langle H \rangle$:

$$\frac{d\langle H \rangle}{db} = 0 = \frac{\hbar^2}{2m} - \alpha \sqrt{\frac{1}{2\pi}} b^{-1/2}, \quad b^{-1/2} = \frac{\hbar^2}{2m\alpha} \sqrt{2\pi}, \quad b = \frac{2m^2 \alpha^2}{\pi \hbar^4}.$$

Find the minimum $\langle H \rangle$:

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2m} \left(\frac{2m^2 \alpha^2}{\pi \hbar^4} \right) - \alpha \sqrt{\frac{2}{\pi}} \sqrt{\frac{2}{\pi}} \frac{m\alpha}{\hbar^2} = \frac{m\alpha^2}{\pi \hbar^2} - \frac{2}{\pi} \frac{m\alpha^2}{\hbar^2} = -\frac{m\alpha^2}{\pi \hbar^2}.$$

This is off by more than a factor of 1.5 (57% error), and is substantially worse than the $(bx + 1)^2$ trial wave-function, which is only 6% off. We conclude that kinky trial wave-functions are better estimators for this potential, which requires a kink in its exact solution.

A Less Steep Rational Function

We tried a rational function that was squared in the denominator. How well would a less-steep trial wave-function do? The graph is again qualitatively the same as before (Figure 1.1b):

$$\psi(x) = A \frac{1}{b|x|+1}, \quad b > 0.$$

Our commentary is more terse this time. 'b' has units of m^{-1} . We now follow the standard four steps for the variational estimate of the ground state energy.

Normalize: We use the even-ness of ψ , so we double the right-half integral:

$$1 = 2A^2 \int_0^\infty (bx+1)^{-2} dx = -\frac{2A^2}{b} \left[(bx+1)^{-1} \right]_0^\infty = \frac{2A^2}{b}, \quad A^2 = \frac{b}{2}.$$

Compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$: The average potential energy is straightforward from the definition of the delta-function, and its integral:

$$\langle V \rangle = \int_{-\infty}^\infty \psi^*(x)V(x)\psi(x) dx = -\alpha A^2 \int_{-\infty}^\infty (1)\delta(x)(1) dx = -\frac{b}{2}\alpha, \quad \text{using } A^2 = \frac{b}{2}.$$

The kinetic energy is again a bit subtle, because we must take the 2nd derivative of ψ , which is infinite at $x = 0$ (the kink), so we split up the integral:

$$\langle T \rangle = \int_{-\infty}^\infty \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) dx = \frac{-\hbar^2}{2m} \left[\int_{0^-}^{0^+} \psi^*(x)\psi''(x) dx + 2 \int_{0^+}^\infty \psi^*(x)\psi''(x) dx \right].$$

The derivatives of ψ are:

$$\begin{aligned} \psi'(x > 0) &= Ab(-1)(bx+1)^{-2}, & \psi'(x < 0) &= Ab(+1)(-bx+1)^{-2} \\ \psi''(x) &= Ab^2(+2)(b|x|+1)^{-3} \end{aligned}$$

As before, we use the Fundamental Theorem of Calculus for the first integral:

$$\begin{aligned} \langle T \rangle &= \frac{-\hbar^2}{2m} \left[\int_{0^-}^{0^+} \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) dx + 2A^2 b^2 \int_{0^+}^\infty (bx+1)^{-1} 2(bx+1)^{-3} dx \right] && \text{Use } 2A^2 = b \\ &= \frac{-\hbar^2}{2m} \left\{ \psi^*(0) (\psi'(0^+) - \psi'(0^-)) + \frac{2b^3}{(-3)b} \left[(bx+1)^{-3} \right]_0^\infty \right\} \\ &= \frac{-\hbar^2}{2m} \left\{ A^2 b(-1-1) - \frac{2}{3} b^2 (-1) \right\} \\ &= \frac{-\hbar^2}{2m} \left\{ -b^2 + \frac{2}{3} b^2 \right\} = \frac{+\hbar^2}{6m} b^2. \end{aligned}$$

As before, we can visualize the wave-function to be as in Figure 1.1c, in the limit as the near-delta-function goes to zero width. Note that in this transition region, the KE is positive (ψ is concave toward the axis). Also, $\langle T \rangle$ is positive, as it must be on physical grounds. This holds true even though the kinetic energy is negative for all of the wave-function, except at the discontinuity (where kinetic energy is infinite for an infinitesimal distance).

Finally:

$$\langle H \rangle = \frac{\hbar^2}{6m} b^2 - \frac{b}{2} \alpha.$$

Find the b that minimizes $\langle H \rangle$:

$$\frac{d\langle H \rangle}{db} = 0 = \frac{\hbar^2}{3m}b - \frac{\alpha}{2}, \quad b = \frac{3m\alpha}{2\hbar^2}.$$

Find the minimum $\langle H \rangle$:

$$\begin{aligned} \langle H \rangle_{\min} &= \left[\frac{\hbar^2}{6m}b^2 - \frac{b}{2}\alpha \right]_{b=3m\alpha/2\hbar^2} = \frac{\hbar^2}{6m} \frac{9m^2\alpha^2}{4\hbar^4} - \frac{3m\alpha^2}{4\hbar^2} \\ &= \frac{3m\alpha^2}{8\hbar^2} - \frac{3m\alpha^2}{4\hbar^2} = -\frac{3}{8} \frac{m\alpha^2}{\hbar^2}. \end{aligned}$$

This is higher (less negative) than the exact value, by 25%. Since the exact wave-function is an exponential, which decays steeper than any rational function, we find that this less-steep function is not as good as the steeper rational function. It is still far better than the gaussian.

Triangles on Trial

How about a simple triangle function? It has a kink, but decays in a funny way:

$$\psi(x) = A \left(1 - \frac{|x|}{b} \right), \quad b > 0, \quad -b < x < b. \quad \psi(x) = 0 \text{ elsewhere.}$$

'b' has units of m. We now follow the standard four steps for the variational estimate of the ground state energy.

Normalize: We use the even-ness of ψ , so we double the right-half integral:

$$1 = 2A^2 \int_0^b (1-x/b)^2 dx = -\frac{2A^2b}{3} \left[(1-x/b)^3 \right]_0^b = \frac{2A^2b}{3}, \quad A^2 = \frac{3}{2b}.$$

Compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$: The average potential energy is straightforward from the definition of the delta-function, and its integral:

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^*(x)V(x)\psi(x) dx = -\alpha A^2 \int_{-\infty}^{\infty} (1)\delta(x)(1) dx = -\frac{3}{2b}\alpha, \quad \text{using } A^2 = \frac{3}{2b}.$$

The kinetic energy now has 3 kinks in it, at $-b$, 0 , and $+b$. The local kinetic energy at a kink is proportional to the change in slope, but the proportion is weighted ψ at the kink. We find the average KE in the usual way, by integrating. We split the integral into its three non-zero steps:

$$\begin{aligned} \langle T \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) dx \\ &= \frac{-\hbar^2}{2m} \left[\int_{-b^-}^{-b^+} \psi^*(x)\psi''(x) dx + \int_{0^-}^{0^+} \psi^*(x)\psi''(x) dx + \int_{b^-}^{b^+} \psi^*(x)\psi''(x) dx \right]. \end{aligned}$$

The first and 3rd terms are zero, because $\psi^*(-b) = \psi^*(b) = 0$. Only the middle term contributes. The derivatives of ψ are:

$$\psi'(x > 0) = \frac{A}{b}, \quad \psi'(x < 0) = -\frac{A}{b}$$

As before, we use the Fundamental Theorem of Calculus for the integral, noting that $\psi^*(0) = A$:

$$\langle T \rangle = \frac{-\hbar^2}{2m} \psi^*(0) \left(\frac{-A}{b} - \frac{A}{b} \right) = \frac{-\hbar^2}{2m} A^2 \left(\frac{-1}{b} - \frac{1}{b} \right) = \frac{3\hbar^2}{2b^2m}$$

Finally:

$$\langle H \rangle = \frac{3\hbar^2}{2b^2m} - \frac{3}{2b}\alpha.$$

Find the b that minimizes $\langle H \rangle$:

$$\frac{\partial \langle H \rangle}{\partial b} = 0 = -\frac{3\hbar^2}{m}b^{-3} + \frac{3}{2}b^{-2}\alpha, \quad \frac{3\hbar^2}{m} = \frac{3}{2}b\alpha, \quad b = \frac{2\hbar^2}{m\alpha}.$$

Confirm that b has units of meters.

Find the minimum $\langle H \rangle$:

$$\langle H \rangle_{\min} = \frac{3\hbar^2}{2m} \frac{m^2\alpha^2}{4\hbar^4} - \frac{3\alpha}{2} \frac{m\alpha}{2\hbar^2} = \frac{3m\alpha^2}{8\hbar^2} - \frac{3m\alpha^2}{4\hbar^2} = -\frac{3m\alpha^2}{8\hbar^2}.$$

This is slightly higher (less negative) than the exact value, by 25%. This agrees with the less-steep rational function, but was a little easier to compute. It is still far better than the gaussian.

How Steep Is Steep?

We've seen that the steeper rational function performed better than the less-steep one. We must certainly ask, then, what is the best steepness? To find out, we create a *two*-parameter trial wave-function, with steepness as one parameter:

$$\psi(x) = A(b|x|+1)^{-n}, \quad b, n > 0.$$

It satisfies the requirement for a kink at $x = 0$, and is normalizable (if $n > 1/2$). b has units of m^{-1} . We now follow the standard four steps for the variational estimate of the ground state energy. The algebra is a little more involved than before, but straightforward.

Normalize: We use the even-ness of ψ , so we double the right-half integral:

$$1 = 2A^2 \int_0^\infty (bx+1)^{-2n} dx = \frac{2A^2}{(-2n+1)b} \left[(bx+1)^{-2n+1} \right]_0^\infty = \frac{2A^2}{(2n-1)b}, \quad A^2 = \frac{(2n-1)b}{2}.$$

We see this agrees with our previous calculations for $n = 1$ and $n = 2$.

Compute $\langle H \rangle = \langle T \rangle + \langle V \rangle$: The average potential energy is straightforward from the definition of the delta-function, and its integral:

$$\langle V \rangle = \int_{-\infty}^\infty \psi^*(x)V(x)\psi(x) dx = -\alpha A^2 \int_{-\infty}^\infty (1)\delta(x)(1) dx = -\frac{(2n-1)b}{2}\alpha, \quad \text{using } A^2 = \frac{(2n-1)b}{2}.$$

The kinetic energy is a little bit subtle, because we must take the 2nd derivative of ψ , which is infinite at $x = 0$ (the kink), so we split up the integral:

$$\langle T \rangle = \int_{-\infty}^\infty \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) dx = \frac{-\hbar^2}{2m} \left[\int_{0^-}^{0^+} \psi^*(x)\psi''(x) dx + 2 \int_0^\infty \psi^*(x)\psi''(x) dx \right].$$

The derivatives of ψ are:

$$\begin{aligned} \psi'(x > 0) &= Ab(-n)(bx+1)^{-n-1}, & \psi'(x < 0) &= Ab(+n)(-bx+1)^{-n-1} \\ \psi''(x) &= Ab^2n(n+1)(b|x|+1)^{-n-2} \end{aligned}$$

As before, we use the Fundamental Theorem of Calculus for the first integral:

$$\begin{aligned}
\langle T \rangle &= \frac{-\hbar^2}{2m} \left[\int_0^{0^+} \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) dx + 2A^2 b^2 \int_0^\infty (bx+1)^{-n} n(n+1)(bx+1)^{-n-2} dx \right] \\
&= \frac{-\hbar^2}{2m} \left\{ \psi^*(0) (\psi'(0^+) - \psi'(0^-)) + \frac{(2n-1)n(n+1)b^2}{(-2n-1)} \left[(bx+1)^{-5} \right]_0^\infty \right\} \quad \text{Using } 2A^2 = (2n-1)b \\
&= \frac{-\hbar^2}{2m} \left\{ A^2 b(-n-n) - \frac{(2n-1)n(n+1)}{2n+1} b^2 (-1) \right\} \\
&= \frac{-\hbar^2}{2m} \left\{ -\frac{2n-1}{2} (2n)b^2 + \frac{(2n-1)n(n+1)}{2n+1} b^2 \right\} = \frac{-\hbar^2}{2m} \left[-(2n-1)n + \frac{(2n-1)n(n+1)}{2n+1} \right] b^2 \\
&= \frac{-\hbar^2}{2m} (2n-1) \left[-\frac{(2n+1)n}{2n+1} + \frac{n(n+1)}{2n+1} \right] b^2 \\
&= \frac{+\hbar^2}{2m} \frac{(2n-1)n^2}{2n+1} b^2.
\end{aligned}$$

Again, this agrees with our previous calculations for $n = 1$ and 2 . Also, $\langle T \rangle$ is positive, as it must be on physical grounds.

Finally:

$$\langle H \rangle = \frac{\hbar^2}{2m} \frac{(2n-1)n^2}{2n+1} b^2 - \frac{(2n-1)b}{2} \alpha.$$

Find the b that minimizes $\langle H \rangle$:

$$0 = \frac{d\langle H \rangle}{db} = \frac{\hbar^2}{m} \frac{(2n-1)n^2}{2n+1} b - \frac{(2n-1)\alpha}{2}, \quad b = \frac{2n+1}{2n^2} \frac{m\alpha}{\hbar^2}.$$

It agrees with past calculations. Since we have two parameters, we must also find the n that minimizes $\langle H \rangle$. Looking at the expression above for $\langle H \rangle$, we see that will be complicated. However, if we wait until we find $\langle H \rangle_{\min}$ for a given n , then b is eliminated from the formula. We can then minimize w.r.t n more easily.

Find the minimum $\langle H \rangle$:

$$\begin{aligned}
\langle H \rangle_{\min} &= \frac{\hbar^2}{2m} \left(\frac{(2n-1)n^2}{2n+1} \right) \frac{(2n+1)^2}{4n^4} \frac{m^2 \alpha^2}{\hbar^4} - \frac{(2n-1)(2n+1)m\alpha^2}{4n^2 \hbar^2} \\
&= \frac{\hbar^2}{2} \frac{(2n-1)(2n+1)}{4n^2} m\alpha^2 - \frac{(2n-1)(2n+1)m\alpha^2}{4n^2 \hbar^2} \\
&= -\hbar^2 \frac{(2n-1)(2n+1)}{8n^2} m\alpha^2.
\end{aligned}$$

We confirm again agreement with past calculations.

We can now minimize w.r.t n . The only factor that varies is the fraction above. Maximizing the fraction minimizes the energy (because of the leading negative sign). Therefore, maximize:

$$\frac{(2n-1)(2n+1)}{8n^2} = \frac{4n^2 - 1}{8n^2}.$$

By inspection, we see that larger n is better, and the limit of this fraction is $\frac{1}{2}$. This limit is the exact value for the ground state energy. You might be tempted to think this is qualitatively consistent with the fact that an

exponential drops off faster than any power, so the larger the power (faster dropoff) the better. However, the faster exponential dropoff occurs for large x ; in our variational application, all the action is focused around the origin. I think it is probably coincidence that we recover the exact value in the large n limit.