115C (QM III): The Double Well

Or, How I Learned to Stop Worrying and Love Approximations

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Contents

1 Introduction

In this sequence of exercises, we consider the quartic double-well Hamiltonian,

$$H = \frac{p^2}{2m} + V(x), \qquad V(x) = m\lambda\big(x^2 - a^2\big)^2, \tag{1.1}$$

where $m > 0$ is the mass of the particle, $a > 0$ is a constant with units of distance, and $\lambda > 0$ is a constant whose sole purpose is to make sure that V has units of energy. (Do NOT think of λ as a small parameter for use in perturbation theory!)

This Hamiltonian is a rich and interesting source of intuition on the standard approximation techniques of quantum mechanics. It is also a rare example of a system where the calculations are nontrivial enough to pose a challenge, but manageable enough to done explicitly and come away (hopefully) with insight instead of pain.

High-level summary. Let us summarize where we are headed. We begin in this section with preparatory work: we will qualitatively understand the behavior of low-energy states in this potential, bemoan the lack of an exact solution, zoom into one of the two wells and approximate it by a harmonic potential, and then write down the exact solution to this (approximate) problem. This is a zeroth-order attempt at a solution, since it only captures the behavior of the ground state in one of the wells, and is insensitive to tunneling.

We therefore turn to perturbation theory in an attempt to do better, treating the non-harmonic parts of the Hamiltonian as a "small" perturbation. After obtaining the first-order corrections to the ground state energy and wave function, we will face the harsh truth: the perturbation isn't really small, and perturbation theory fails to converge or display sensible tunneling behavior across both wells. We will then explore a variational approach to the problem, where by the use of a rather ad hoc trial wave function, we will successfully model the ground state. Finally, we will pass to a WKB analysis of the problem. We will examine tunneling and construct a proof that the energy splitting between low-lying states is nonperturbatively small. We will conclude by introducing imaginary time and its attendant reformulation of tunneling in terms of the classical motion of instantons.

(a) Qualitative Analysis

Graph the potential $V(x)$. Then, graph the approximate shape of the ground state wave function $\psi_0(x)$ and the first excited state wave function $\psi_1(x)$. Label each one.

Then, try your best to solve the potential *exactly*, i.e. to obtain the eigenstates and energies of the Hamiltonian. You will fail: the exact solutions cannot be written down in closed form using elementary functions. Such is life sometimes.

Solution. As expected, the potential $V(x)$ has a double well. It is graphed below (blue), together with the ground state (orange) and first excited state (green) wave functions. The precise shape of the wave functions should not be taken literally: their only salient features are that they have bumps localized on the wells, and that the ground state is symmetric while the first excited state is antisymmetric.

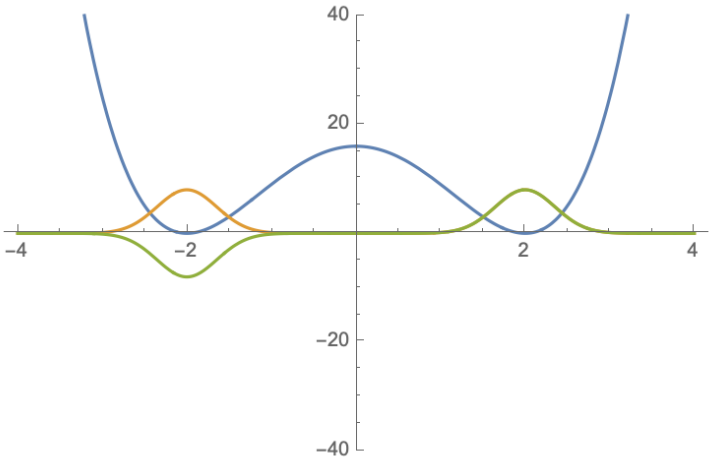

Figure 1: The double well and its low-energy states ($m = \lambda = \hbar = 1$, $a = 2$).

Looking up the double well on Wikipedia will immediately throw the reader into a firestorm of special functions, series expansions, and so on. More directly, the Schrödinger equation takes the schematic form

$$-\psi'' + (c_1 x^2 + c_2 x^4)\psi \sim E\psi. \tag{1.2}$$

This is simply a rather nasty ODE whose solutions certainly exist (and some of which look like the wave functions above), but which cannot be expressed in terms of elementary functions.

(b) Expansion about a Minimum

Expand the potential about its minimum at $x = a$. That is, calculate the Taylor series of $V(x)$ at $x = a$ to lowest nontrivial order. You should obtain a quadratic function of x; call it $V^{(2)}(x)$. Thus rewrite the full potential in the form

$$V(x) = V^{(2)}(x) + V'(x) = A(x - B)^2 + V'(x), \tag{1.3}$$

where A and B are constants that you should determine, and $V'(x)$ is the non-quadratic part of the potential, which you should also determine.

Solution. The quadratic approximation to $V(x)$ is given by taking derivatives:

$$V^{(2)}(x) = 4m\lambda a^2(x - a)^2. \tag{1.4}$$

In the notation of the problem, this gives $A = 4m\lambda a^2$ and $B = a$. As for the remaining bit of the potential, there are various ways to write it down, none of which are too enlightening:

$$\begin{aligned} V'(x) &= m\lambda(x - a)^3(x + 3a) = m\lambda(x - a)^3\big((x - a) + 4a\big) = \\ &= m\lambda x^4 - 6m\lambda a^2 x^2 + 8m\lambda a^3 x - 3m\lambda a^4. \end{aligned} \tag{1.5}$$

It may, at first sight, be disturbing that $V'(x)$ contains a quadratic term. This is to be expected, though; we expanded only around one of the two quadratic-looking minima, leaving the other one intact. So its quadratic imprint survives in V'.

(c) Zeroth-Order Solution

Consider the quadratic Hamiltonian $H^{(0)} = \frac{p^2}{2m} + V^{(2)}(x)$. By an appropriate change of coordinates from x to a new coordinate ξ, show that $H^{(0)}$ takes the same form as the Hamiltonian for a harmonic oscillator, $H_{\text{QHO}} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\xi^2$, and find the frequency ω of this oscillator in terms of the parameters a and λ. Write down the ground state wave function and the ground state energy of $H^{(0)}$.

Solution. Consider the change of coordinates given by a shift of x to the location of the minimum at a: $x \longrightarrow \xi = x - a$. Then the Hamiltonian is

$$H^{(0)} = \frac{p^2}{2m} + 4m\lambda a^2\xi^2. \tag{1.6}$$

This is the QHO Hamiltonian, with the role of $\frac{1}{2}m\omega^2$ (the usual prefactor at the quadratic term in the QHO) played by $4m\lambda a^2$. In other words, we have the identification

$$4m\lambda a^2 = \frac{1}{2}m\omega^2 \implies \omega = \sqrt{8\lambda a^2} = 2a\sqrt{2\lambda}. \tag{1.7}$$

This makes sense: the location a of the well also controls the steepness of its walls, which is precisely what the frequency ω usually measures.

The ground state wave function is given by its usual expression:

$$\psi_0^{(0)}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega\xi^2}{2\hbar}} = \left(\frac{2ma\sqrt{2\lambda}}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{ma\sqrt{2\lambda}}{\hbar}(x-a)^2\right). \tag{1.8}$$

This ground state is a Gaussian bump in the well centered at $x = a$, and is an excellent description of *half* of the true ground state of the system. But approximating $V(x)$ by $V^{(2)}$ ignores the well at $x = -a$, and the Gaussian wave function above doesn't know about it.

The ground state energy, as usual, is

$$E_0^{(0)} = \frac{\hbar\omega}{2} = \hbar a\sqrt{2\lambda}. \tag{1.9}$$

Notice that if we had expanded around $x = -a$ instead, we would have obtained a similar-looking Gaussian ground state and, importantly, the same ground state energy.

2 Perturbation Theory

In the last section we saw that the quadratic approximation of V fails to predict the correct shape of the ground state wave function. In this section, we will attempt to fix this problem by treating V' as a small perturbation on top of the unperturbed, exactly solvable Hamiltonian $H^{(0)}$. As we will soon see, this is an approximation doomed to fail. However, that will not stop us from first getting some useful results.

(a) Preparation

Recall that you found $V'(x)$ in part 1(c). Copy it down again, but this time express it in terms of ξ instead of in terms of x. Now look at the unperturbed Hamiltonian $H^{(0)}$: are there any degeneracies? If not, we are clear to use non-degenerate perturbation theory to analyze it. If so, find the "good" states in preparation for degenerate perturbation theory.

Solution. For reference, the perturbation is

$$V'(x) = m\lambda(x-a)^3\big((x-a)+4a\big) = m\lambda\xi^3(\xi+4a) = m\lambda\xi^4 + 4m\lambda a\xi^3. \tag{2.1}$$

The Hamiltonian $H^{(0)}$ is just a harmonic oscillator, so its energy levels are indexed by the integers and are nondegenerate. (This means that the eigenstates $\psi_n^{(0)}$ of $H^{(0)}$ are already "good" states.) Whew!

(b) First-Order Energy

Calculate the first-order correction to the ground state energy due to the perturbation $V'(x)$.

Solution. In nondegenerate perturbation theory, the first-order correction to the ground state energy is given by the expectation value of the perturbation:

$$E_0^{(1)} = \langle\psi_0^{(0)}|V'|\psi_0^{(0)}\rangle \tag{2.2}$$

There are several ways to go from here. Most naïvely, one could recall the explicit expressions (1.5) for $V'(x)$ and (1.8) for $\psi_0^{(0)}(x)$, and then set about to calculate a dizzying number of integrals. Things look much nicer in the ξ coordinates: here V' only has two terms, and $\psi_0^{(0)}(\xi)$ is precisely the wave function of the ground state $|0\rangle$ of the harmonic oscillator.

The calculation simplifies dramatically:

$$E_0^{(1)} = \langle 0|m\lambda\xi^4 + 4m\lambda a\xi^3|0\rangle = m\lambda\,\langle 0|\xi^4|0\rangle + 4m\lambda a\,\langle 0|\xi^3|0\rangle\,. \tag{2.3}$$

We now argue that the ξ^3 term vanishes. This can be seen by writing down the integral that defines this matrix element: the integrand is ξ^3 times a Gaussian, which is an odd function being integrated over the symmetric interval $(-\infty,\infty)$, so the integral vanishes. Equivalently, one can expand $\xi \sim a_+ + a_-$ in terms of the ladder operators. Observe that no term in the expansion of ξ^3 will have an equal number of raising and lowering operators. Thus the resulting states will always be orthogonal, and the inner product will vanish.

As for the ξ^4 term, the ladder operator method proves useful:

$$\xi = \sqrt{\frac{\hbar}{2m\omega}}(a_- + a_+) \implies E_0^{(1)} = m\lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle 0|\,(a_- + a_+)^4\,|0\rangle\,. \tag{2.4}$$

Now we need to expand the fourth power of the sum above, taking care to preserve the order of all 16 resulting terms. Fortunately, not all of these terms contribute to the result: any term with an unequal number of a_+ and a_- operators (e.g. $a_+a_-a_+^2$) will act on $|0\rangle$ by raising more times than it lowers (or vice versa), leading to a "mismatched" inner product like $\langle 0|2\rangle$.

These terms, in addition to any term where a_- acts directly on $|0\rangle$, all vanish. Only 6 terms that have two a_+ and two a_- operators, and of those, four immediately annihilate $|0\rangle$:

$$\begin{aligned}\langle 0|\,(a_- + a_+)^4\,|0\rangle &= \langle 0|\,\big(\cancel{a_+a_+a_-a_-} + \cancel{a_+a_-a_+a_-} + \cancel{a_+a_-a_-a_+} + \\ &\quad + a_-a_-a_+a_+ + a_-a_+a_-a_+ + \cancel{aa^\dagger a^\dagger a}\big)\,|0\rangle = \\ &= \langle 0|\,(a_-a_-a_+a_+ + a_-a_+a_-a_+)\,|0\rangle = 2\,\langle 0|0\rangle + 1\,\langle 0|0\rangle = 3. \end{aligned} \tag{2.5}$$

All together, then, we have

$$E_n^{(1)} = 3m\lambda\left(\frac{\hbar}{2m\omega}\right)^2 = 3m\lambda\left(\frac{\hbar}{4ma\sqrt{2\lambda}}\right)^2 = \frac{3\hbar^2}{32ma^2}. \tag{2.6}$$

To first order, then, the ground state has energy

$$E_0 \approx E_0^{(0)} + E_0^{(1)} = \hbar a\sqrt{2\lambda} + \frac{3\hbar^2}{32ma^2}. \tag{2.7}$$

This makes sense: each next term enters with a higher power of $\hbar$.

(c) First-Order Wave Function

Calculate the first-order correction to the ground state wave function due to $V'(x)$. You may leave your answer in terms of the unperturbed harmonic oscillator eigenstates $\psi_n^{(0)}$—no need to actually compute the explicit spatial wave functions.

Solution. The first-order correction to the ground state is given by

$$|\psi_0^{(1)}\rangle = \sum_{n\neq 0} \frac{\langle\psi_n^{(0)}|V'|\psi_0^{(0)}\rangle}{E_0^{(0)} - E_n^{(0)}}\,|\psi_n^{(0)}\rangle\,, \qquad V' = m\lambda\xi^4 + 4m\lambda a\xi^3. \tag{2.8}$$

The energy denominator is pretty quick to calculate:

$$E_0^{(0)} - E_n^{(0)} = \frac{\hbar\omega}{2} - \hbar\omega\left(n + \frac{1}{2}\right) = -n\hbar\omega = -2n\hbar a\sqrt{2\lambda}. \tag{2.9}$$

The main problem here is to calculate the matrix element

$$\begin{aligned} V'_{n0} &= \langle n|V'|0\rangle = \langle n|m\lambda\xi^4 + 4m\lambda a\xi^3|0\rangle = \\ &= m\lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|(a_- + a_+)^4|0\rangle + 4m\lambda a\left(\frac{\hbar}{2m\omega}\right)^{3/2} \langle n|(a_- + a_+)^3|0\rangle\,. \end{aligned} \tag{2.10}$$

(The ladder operator method is the only viable approach this time, since writing down the wave function $\psi_m^{(0)}(\xi)$ explicitly in terms of Hermite functions will get us nowhere.) This calculation is, to say the least, not entirely pleasant. The key is to verify that

$$\begin{aligned} (a_- + a_+)^4\,|0\rangle &= 3\,|0\rangle + 6\sqrt{2}\,|2\rangle + 2\sqrt{6}\,|4\rangle\,, \\ (a_- + a_+)^3\,|0\rangle &= \left(2 + \sqrt{2}\right)|1\rangle + \sqrt{6}\,|3\rangle\,. \end{aligned} \tag{2.11}$$

It remains to take the inner product of these results with all possible bras $\langle n|$ except for the ground state, since $n \neq 0$. The infinite sum above reduces to a finite number of terms:

$$\begin{aligned}|\psi_0^{(1)}\rangle &= -m\lambda\left(\frac{\hbar}{2m\omega}\right)^2 \sum_{n\neq 0} \frac{\langle n|(a_- + a_+)^4|0\rangle}{n\hbar\omega}\,|\psi_n^{(0)}\rangle - 4m\lambda a\left(\frac{\hbar}{2m\omega}\right)^{3/2} \sum_{n\neq 0} \frac{\langle n|(a_- + a_+)^3|0\rangle}{n\hbar\omega}\,|\psi_n^{(0)}\rangle = \\ &= -m\lambda\left(\frac{\hbar}{2m\omega}\right)^2 \left[\frac{6\sqrt{2}}{2\hbar\omega}\,|\psi_2^{(0)}\rangle + \frac{2\sqrt{6}}{4\hbar\omega}\,|\psi_4^{(0)}\rangle\right] - 4m\lambda a\left(\frac{\hbar}{2m\omega}\right)^{3/2} \left[\frac{2+\sqrt{2}}{\hbar\omega}\,|\psi_1^{(0)}\rangle + \frac{\sqrt{6}}{3\hbar\omega}\,|\psi_3^{(0)}\rangle\right] = \\ &= -\frac{\hbar}{64ma^3\sqrt{2\lambda}}\left[3\sqrt{2}\,|\psi_2^{(0)}\rangle + \frac{\sqrt{6}}{2}\,|\psi_4^{(0)}\rangle\right] - \left(\frac{\hbar}{64ma^3\sqrt{2\lambda}}\right)^{1/2}\left[\left(2+\sqrt{2}\right)|\psi_1^{(0)}\rangle + \frac{\sqrt{6}}{3}\,|\psi_3^{(0)}\rangle\right].\end{aligned} \tag{2.12}$$

This is a bit of a mess, but we can clean it up a bit using dimensional analysis. Observe that the quantities $m\lambda a^4$ and $\hbar\omega \propto \hbar a\sqrt{\lambda}$ both have units of energy. This means that

$$[m\lambda a^4] = [\hbar a\sqrt{\lambda}] \implies [ma^3] = \left[\frac{\hbar}{\sqrt{\lambda}}\right] \implies \left[\frac{\hbar}{ma^3\sqrt{\lambda}}\right] = [1]. \tag{2.13}$$

Thus the prefactor that appears twice in (2.12) is indeed dimensionless, and we can give it a name: let $\gamma \equiv \hbar/\left(64ma^3\sqrt{2\lambda}\right)$. Then to first order, the full wave function is

$$|\psi_0\rangle \approx |\psi_0^{(0)}\rangle + |\psi_0^{(1)}\rangle = |0\rangle - \left(2+\sqrt{2}\right)\sqrt{\gamma}\,|1\rangle - 3\sqrt{2}\,\gamma\,|2\rangle - \frac{\sqrt{6}}{3}\sqrt{\gamma}\,|3\rangle - \frac{\sqrt{6}}{2}\gamma\,|4\rangle\,. \tag{2.14}$$

(d) Second-Order Energy

Calculate the second-order correction to the ground state energy due to $V'(x)$.

Solution. The second-order correction to the ground state energy is

$$E_0^{(2)} = \sum_{n\neq 0} \frac{\left|\left\langle \psi_n^{(0)}\middle|V'\middle|\psi_0^{(0)}\right\rangle\right|^2}{E_0^{(0)} - E_n^{(0)}}, \qquad V' = m\lambda\xi^4 + 4m\lambda a\xi^3. \tag{2.15}$$

We already know that the energy denominator is $-n\hbar\omega = -2n\hbar a\sqrt{2\lambda}$, and we calculated all of the necessary matrix elements above. It remains to sum their squares:

$$\begin{aligned}E_0^{(2)} &= -(m\lambda)^2\left(\frac{\hbar}{2m\omega}\right)^4 \sum_{n\neq 0} \frac{\left|\langle n|(a_- + a_+)^4|0\rangle\right|^2}{n\hbar\omega} - (4m\lambda a)^2\left(\frac{\hbar}{2m\omega}\right)^3 \sum_{n\neq 0} \frac{\left|\langle n|(a_- + a_+)^3|0\rangle\right|^2}{n\hbar\omega} = \\ &= -(m\lambda)^2\left(\frac{\hbar}{2m\omega}\right)^4 \left[\frac{36\cdot 2}{2\hbar\omega} + \frac{4\cdot 6}{4\hbar\omega}\right] - (4m\lambda a)^2\left(\frac{\hbar}{2m\omega}\right)^3 \left[\frac{\left(2+\sqrt{2}\right)^2}{\hbar\omega} + \frac{6}{3\hbar\omega}\right] = \\ &= -\left[(m\lambda)^2\left(\frac{\hbar}{2m\omega}\right)^4 + (4m\lambda a)^2\left(\frac{\hbar}{2m\omega}\right)^3\right]\left[\frac{50+4\sqrt{2}}{\hbar\omega}\right] = \frac{\hbar^2(1+\gamma)}{32ma^2}\left(50+4\sqrt{2}\right).\end{aligned} \tag{2.16}$$

This is slightly worrying: the second-order energy correction looks larger than the first-order correction. All together, to second order we have

$$E_0 \approx E_0^{(0)} + E_0^{(1)} + E_0^{(2)} = \hbar a\sqrt{2\lambda} + \frac{\hbar^2}{32ma^2}\left[3 + (1+\gamma)\left(50 + 4\sqrt{2}\right)\right]. \tag{2.17}$$

(e) A Visual Demonstration

Using a table of the first few stationary states of the harmonic oscillator and a graphing software, plot both the unperturbed and first-order-corrected wave functions on the same graph. What happens at $x = -a$? Does this trouble you?

Solution. See the attached Mathematica notebook for the computation. We pretty much just look up and hard-code the first four stationary QHO wave functions $\psi_0^{(0)}(x), ..., \psi_4^{(4)}(x)$, being careful to substitute $2a\sqrt{2\lambda}$ for ω and $x - a$ for ξ wherever they appear.

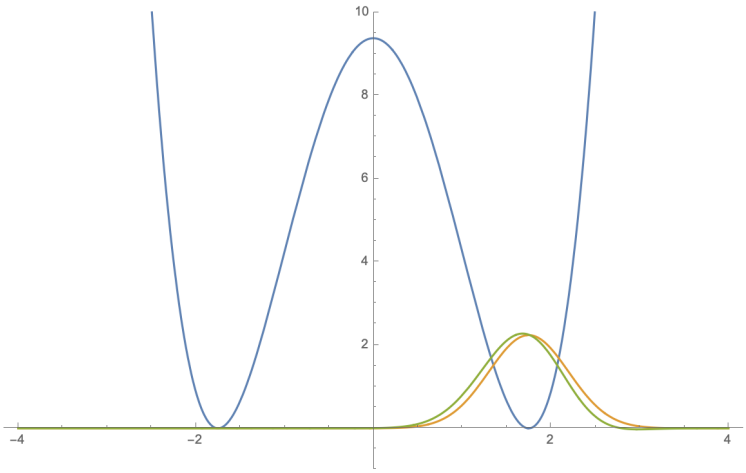

Figure 2: PT wave function, $m = \lambda = \hbar = 1$, $a = 1.75$.

The differences between $\psi_0^{(0)}$ (orange) and $\psi_0 \approx \psi_0^{(0)} + \psi_0^{(1)}$ (green) are minuscule. The corrected wave function looks like it is shifted to the left. More precisely, what happens is that the well at $x = a$ is slightly steeper than its zeroth-order harmonic approximation for $x \gtrsim a$, and slightly shallower for $x \lesssim a$. The perturbative corrections to $\psi_0^{(0)}$ respond to these effects by making the wave function decay more steeply for $x > a$ and less steeply for $x < a$. This seems somewhat promising: the true ground state has a bump in both wells, so the increased amplitude of the wave function for $x < a$ indicates that perturbation theory is at least *trying* to capture the effects of tunneling through the central barrier. Alas, no bump appears at $x = -a$, and the corrected wave function seems to pretend that the second well—which *is* certainly part of the perturbing potential—simply isn't there.

Could this forebode a failure of perturbation theory?

(f) Convergence Issues

To summarize, we are given the Hamiltonian $H = H^{(0)} + V'(\xi)$, where $H^{(0)}$ is the harmonic oscillator Hamiltonian in the coordinate ξ, and $V'(\xi)$ is viewed as a small perturbation. First-order perturbation theory for this problem seems to be tractible. However: Argue, using any means you like, that perturbation theory does not converge for this system. To be precise, this means that the all-orders *perturbative* ground state energy and wave function,

$$E_0^{(\infty)} = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + \cdots, \qquad \psi_0^{(\infty)} = \psi_0^{(0)} + \psi_0^{(1)} + \psi_0^{(2)} + \cdots, \tag{2.18}$$

are *not* equal to the true ground state energy E_0 and wave function ψ_0. You do not need to be rigorous by any means, but you do need to provide a convincing physical argument.

Solution. There are many different ways to argue here. We provide three, but these are far from the only valid reasons for the failure of the convergence of perturbation theory.

Argument 1: V' as a perturbation. The "perturbation" $V'(x)$ is *not* small! It is certainly true that when x is near a, the full potential $V(x)$ is well approximated by $V^{(2)}(x)$, and so $V'(x)$ is small there. But this approximation is only good locally, and as we move away from $x = a$ the difference $V'(x) = V(x) - V^{(2)}(x)$ grows large. In particular,

$$V'(-a) = m\lambda a^4 - 6m\lambda a^4 - 8m\lambda a^4 - 3m\lambda a^4 = -16m\lambda a^4 \tag{2.19}$$

is *huge* in the deep-well regime where a is large. So it is not really reasonable to use $V'(x)$ as a perturbation to begin with. Also, $V'(x)$ contains no explicit small parameters that distinguish its size from that of $V(x)$ or $V^{(2)}(x)$, so there is no reason to even suspect that it should be small to begin with.

Argument 2: wave functions and analyticity. The content of this argument is really only precise in the context of the WKB approximation and will be more fully fleshed out by the end of the document. For now, we keep things vague. The basic idea is that several quantities, like the WKB tunneling probability and the true energy splitting between the ground and first excited states, have expressions whose functional form includes the factor $e^{-1/\hbar}$. The function $f(x) = e^{-1/|x|}$ is well-defined and smooth for all $x \neq 0$, and has a removable singularity at $x = 0$ that can be "plugged" by defining $f(0) = 0$ to yield a globally smooth function. And yet, it is a curious fact that the Taylor series of f at $x = 0$ is *identically zero*: every single term in the Taylor series vanishes, because the function is simply too flat at the origin. It is a weird example of a smooth but non-analytic function. Physically, this means that any attempt to capture effects that look like $e^{-1/\hbar}$ in a power series is doomed to fail. We therefore say that such effects are *nonperturbative*, because they are too small to be noticed by perturbation theory.

Argument 3: "formal" "proof." Even in the absence of an explicit small parameter, we can regard this brand of perturbation theory as a series expansion in powers of $\hbar$. If you don't like this idea, we could also—for purely pedagogical purposes—modify the problem by hand and consider the perturbation $\varepsilon V'(x)$, where $\varepsilon \ll 1$ is a small parameter. (Thus in

the following, think of ε as $\hbar$.[1]) In either case, we shall see presently that $E_0^{(\infty)}$ and $\psi_0^{(\infty)}$ diverge. The key will be to remember what this means, so a brief reminder follows.

Definition 2.1 (Convergence, in physics language)**.** A power series

$$F(\varepsilon) = \sum_{k=0}^{N} a_k \varepsilon^k = a_0 + a_1\varepsilon + a_2\varepsilon^2 + \cdots + a_N\varepsilon^N \tag{2.20}$$

is said to *converge* at $\varepsilon = \varepsilon_*$ if, upon fixing $\varepsilon = \varepsilon_*$, increasing the number N of terms in the series to infinity causes it to approach a finite limit. The set of ε_* for which this is true is called the *domain of convergence* D of the series, and the largest *open* interval $(\varepsilon_0 - r, \varepsilon_0 + r)$ contained in D defines the *radius of convergence* of the series.

In the language developed above, both $E_0^{(\infty)}$ and $\psi_0^{(\infty)}$ are power series in $\varepsilon \sim \hbar$ around $\varepsilon = 0$. In particular, setting $\varepsilon = 0$ recovers $E_0^{(0)} = \hbar a\sqrt{2\lambda}$ and $\psi_0^{(0)} \sim e^{-\xi^2}$. We will show that $E_0^{(\infty)}$ has *zero* radius of convergence, which means that its power series converges for $\varepsilon_* = 0$ but for no other nearby value. Suppose, towards a contradiction, that the series *does* converge for some small, positive value ε_* of the perturbation strength. Thus the series $E_0^{(\infty)}(\varepsilon)$ is convergent at $\varepsilon = 0$, with radius of convergence at least $r = \varepsilon_*$. This implies that $E_0^{(\infty)}(-\varepsilon_*)$ must converge just as well as $E_0^{(\infty)}(\varepsilon_*)$. So far, nothing special about $E^{(\infty)}$ has been used. But attempting to compute $E_0^{(\infty)}(-\varepsilon_*)$ entails doing perturbation theory with $-\varepsilon V'$ instead of $+\varepsilon V'$, which flips the perturbing potential upside down. No matter how small $|\varepsilon_*|$ is, the inverted potential $-V'$ is unbounded below and leads to certain disaster. To wit, it causes the amplitude of the wave function to diverge when $|x| \gg a$, rendering it (and its energy) ill-defined. One sometimes describes this situation by saying that the particle will spontaneously tunnel through the inverted potential barrier into a region of negative-infinite potential. (See also the phrase "spontaneous vacuum decay.") In any case, the point is that $E_0^{(\infty)}(-\varepsilon_*)$ cannot possibly converge, so neither can $E_0^{(\infty)}(\varepsilon_*)$ for any positive value of ε_*. Thus $E_0^{(\infty)}$ has zero radius of convergence, and the same argument also works for $\psi_0^{(\infty)}$.

Addendum. This argument was first given by Dyson in the context of the renormalized perturbation theory commonly used in quantum field theory, but it applies equally well in nonrelativistic single-particle quantum mechanics.

One may be extremely confused at this point: how come we got sensible results for $E_0^{(1)}$ and $\psi_0^{(1)}$ earlier?! The answer is rather subtle and depends on the order in which limits are taken. If ε is held fixed and the number N of terms in the series is increased, the series initially approaches the correct value, reaches its best approximation at some finite $N = N_*$, and then begins to diverge from the right answer for $N > N_*$. On the other hand, if we fix N and then send $\varepsilon \longrightarrow 0$, the resulting N-term sum will approach its unperturbed ($\varepsilon = 0$) value. This holds for *any* fixed N, so even if we choose $N \gg N_*$ (where the series is a bad approximation for any finite ε), cranking down $\varepsilon \longrightarrow 0$ will make the approximation better and better. For this reason, we call such series *perturbative* or *asymptotic* series.

[1]More precisely, $\varepsilon = \hbar^{1/2}$. This is due to the annoying technical detail that V' consists of ξ^3 and ξ^4 terms, and the two terms produce energy and wave function corrections that come with half-integer and integer powers of $\hbar$, respectively. This means that the $\hbar$-expansions of E_0 and ψ_0 both look like $a_0 + a_{1/2}\hbar^{1/2} + a_1\hbar + a_{3/2}\hbar^{3/2} + \cdots$. This is a minor detail, however, and doesn't affect the argument.

3 Variational Techniques

Having understood what perturbation theory can and cannot do for us, we turn in this section to the variational principle. We will choose variational wave functions of several different forms, and examine the bounds they give on the ground state energy.

(a) One Gaussian: Minimization

Consider the trial wave function $\psi_\beta(x) = Ae^{-\beta(x-a)^2}$, where $\beta > 0$ is the variational parameter. Normalize ψ_β by finding A, and use the variational principle to determine the value of β that gives the lowest upper bound on the ground state energy of the system. Call this value β_*. Be warned: the result will not be pretty.

Solution. We begin by normalizing the wave function:

$$\begin{aligned}\langle\psi_\beta|\psi_\beta\rangle &= \int_{\mathbb{R}} \mathrm{d}x\, \psi_\beta^*(x)\psi_\beta(x) = |A|^2 \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-2(x-a)^2/\beta^2} = \\ &= |A|^2\sqrt{\frac{\pi}{2\beta}} \stackrel{!}{=} 1 \implies A = \left(\frac{2\beta}{\pi}\right)^{1/4} \implies \psi_\beta(x) = \left(\frac{2\beta}{\pi}\right)^{1/4} e^{-\beta\xi^2}. \end{aligned} \tag{3.1}$$

Next we need to use the variational principle, which states that

$$E_0 \leq \langle H\rangle_{\psi_\beta} = \langle\psi_\beta|H|\psi_\beta\rangle \equiv E_v. \tag{3.2}$$

Now there are a number of ways to calculate the matrix element. Here is one:

$$\begin{aligned} E_v &= \langle\psi_\beta|\left(\frac{p^2}{2m} + V^{(2)} + V'\right)|\psi_\beta\rangle = \\ &= \frac{1}{2m}\langle\psi_\beta|p^2|\psi_\beta\rangle + 4m\lambda a^2\langle\psi_\beta|\xi^2|\psi_\beta\rangle + 4m\lambda a\langle\psi_\beta|\xi^3|\psi_\beta\rangle + m\lambda\langle\psi_\beta|\xi^4|\psi_\beta\rangle. \end{aligned} \tag{3.3}$$

The first two terms are the kinetic energy and harmonic potential, and the second two terms are the "perturbing" terms. We dutifully calculate each one in turn:

$$\begin{aligned} \langle T\rangle_\beta &= \frac{1}{2m}\langle\psi_\beta|p^2|\psi_\beta\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\mathrm{d}x\,\psi_\beta^*(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\big(\psi_\beta(x)\big) = \frac{\hbar^2\beta}{2m}, \\ \langle V^{(2)}\rangle_\beta &= 4m\lambda a^2\langle\psi_\beta|\xi^2|\psi_\beta\rangle = 4m\lambda a^2\int_{-\infty}^{\infty}|\psi_\beta(x)|^2(x-a)^2 = \frac{m\lambda a^2}{\beta}, \\ \langle V^{(3)}\rangle_\beta &= 4m\lambda a\langle\psi_\beta|\xi^3|\psi_\beta\rangle = 4m\lambda a\int_{-\infty}^{\infty}|\psi_\beta(x)|^2(x-a)^3 = 0, \\ \langle V^{(4)}\rangle_\beta &= m\lambda\langle\psi_\beta|\xi^4|\psi_\beta\rangle = m\lambda\int_{-\infty}^{\infty}|\psi_\beta(x)|^2(x-a)^4 = \frac{3m\lambda}{16\beta^2}. \end{aligned} \tag{3.4}$$

Putting all of these together, we find a β-dependent upper bound on E_0:

$$E_0 \leq E_v(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\lambda a^2}{\beta} + \frac{3m\lambda}{16\beta^2}. \tag{3.5}$$

Now we seek the value of β that minimizes $E_v(\beta)$. To find it, we compute the derivative $\frac{\partial E_v}{\partial \beta}$, set it to zero, and solve for the minimizing value of β:

$$\left.\frac{\partial E_v}{\partial \beta}\right|_{\beta=\beta_*} = \frac{\hbar^2}{2m} - \frac{m\lambda a^2}{\beta_*^2} - \frac{3m\lambda}{8\beta_*^3} \stackrel{!}{=} 0. \tag{3.6}$$

This is a cubic equation for β_*, but luckily it can be solved exactly. There are two imaginary roots, corresponding to critical points of E_v in the unphysical region $\beta < 0$, and one real and positive root. The answer isn't pretty:

$$\begin{aligned}\beta_* &= \frac{4m^2\lambda a^2}{\hbar}\left[3m^2\lambda\left(27\hbar + \sqrt{729\hbar^2 - 1536m^2\lambda a^6}\right)\right]^{-1/3} + \\ &\quad + \frac{1}{2\hbar}\left[\frac{m^2\lambda}{9}\left(27\hbar + \sqrt{729\hbar^2 - 1536m^2\lambda a^6}\right)\right]^{1/3} = \\ &= \frac{4m^2\lambda a^2}{\hbar}(3\alpha)^{-1/3} + \frac{1}{2\hbar}\left(\frac{\alpha}{9}\right)^{1/3}, \qquad \alpha \equiv m^2\lambda\left(27\hbar + \sqrt{729\hbar^2 - 1536m^2\lambda a^6}\right).\end{aligned} \tag{3.7}$$

(b) One Gaussian: Expansion

We are interested in the regime where a is very large. Expand β_* to leading nontrivial order in a in the large-a limit, and use this approximate value of β_* to find the lowest upper bound on the ground state energy. Compare your results to perturbation theory.

Solution. It is actually possible to plug β_* directly into E_v and obtain an exact result for the lower bound on the energy. But its form is rather unenlightening. We'll make things easier on ourselves by taking a to be large, in which case the expression for α above is dominated by the a^6 term inside the square root. We therefore obtain

$$\beta_* \approx \frac{4m^2\lambda a^2}{\hbar}\left[3m^2\lambda\sqrt{-1536\lambda a^6}\right]^{-1/3} + \frac{1}{2\hbar}\left[\frac{m^2\lambda}{9}\sqrt{-1536\lambda a^6}\right]^{1/3} = \frac{ma\sqrt{2\lambda}}{\hbar}. \tag{3.8}$$

The last equality is the result of drastic and somewhat miraculous simplifications that save us at the last second from what looks like certain doom at the hands of imaginary numbers. We're in good shape: this expression looks very similar to the frequency ω we found earlier. In fact, this is exactly the value of β_* we would find if the last term in (3.5), which is the energy contribution from the ξ^4 part of the potential, wasn't there at all. So it is reasonable to suspect that we have landed back in harmonic oscillator territory, and the following calculation will confirm that suspicion.

Plugging this value of β into E_v gives the least upper bound

$$E_0 \le E_{\min} = E_v(\beta_*) \approx \frac{\hbar^2\beta_*}{2m} + \frac{m\lambda a^2}{\beta_*} + \frac{3m\lambda}{16\beta_*^2} = \hbar a\sqrt{2\lambda} + \frac{3\hbar^2}{32ma^2}, \tag{3.9}$$

which is exactly the first-order-corrected energy we found above!

(c) Two Gaussians: Minimization

By now, we are desperate to see results which mimic the behavior of the true ground state. Consider, therefore, a trial wave function with a bump in each well:

$$\psi_\beta(x) = \frac{A}{\sqrt{2}}\Big[e^{-\beta(x+a)^2} + e^{-\beta(x-a)^2}\Big]. \tag{3.10}$$

As before, normalize ψ_β by finding A, and try to determine the value of β (call it β_*) that gives the tightest upper bound on E_0. You will not be able to solve for β_* analytically in closed form. Instead, argue that it is a reasonable approximation to use the value of β_* obtained for the one-Gaussian trial wave function from above.

Solution. Here we repeat the same steps as in the two parts above. Most of the algebra was done in Mathematica, so we omit most of the intermediate steps here.

We begin by normalizing the wave function:

$$\langle\psi_\beta|\psi_\beta\rangle = |A|^2\sqrt{\frac{\pi}{2\beta}}\Big(1+e^{-2a^2\beta}\Big) \stackrel{!}{=} 1 \implies A = \left(\frac{\pi}{2\beta}\right)^{1/4}\Big(1+e^{-2a^2\beta}\Big)^{-1/2} \implies$$

$$\psi_\beta(x) = \frac{1}{\sqrt{2}}\left(\frac{\pi}{2\beta}\right)^{1/4}\Big(1+e^{-2a^2\beta}\Big)^{-1/2}\Big[e^{-\beta(x+a)^2} + e^{-\beta(x-a)^2}\Big]. \tag{3.11}$$

Next, we perform about a zillion integrals in order to compute

$$E_0 \le E_v = \langle\psi_\beta|H|\psi_\beta\rangle = \langle T\rangle_\beta + \langle V^{(2)}\rangle_\beta + \langle V^{(3)}\rangle_\beta + \langle V^{(4)}\rangle_\beta. \tag{3.12}$$

The final result contains an energy contribution from each bump of the wave function in response to each of the terms in the potential. All together, we have

$$\begin{aligned} E_v = {} & \frac{3m\lambda}{16\beta^2} + \frac{m\lambda a^2}{4\beta} + \frac{m\lambda a^4}{2} + \frac{\hbar^2\beta}{2m} - \frac{\hbar^2a^2\beta^2}{m} + \\ & + \left(\frac{3m\lambda a^2}{4\beta} - \frac{m\lambda a^4}{2} + \frac{\hbar^2a^2\beta^2}{m}\right)\tanh\big(a^2\beta\big). \end{aligned} \tag{3.13}$$

At this point, the natural thing to do is to differentiate E_v with respect to β, set the result equal to zero, and attempt to solve for β. But as threatened, $\frac{\partial E_v}{\partial\beta}\big|_{\beta=\beta_*} = 0$ has no closed-form solution for β_* in this case. Womp womp. Notice, however, that for large a, the tanh factor above rapidly approaches 1 from below. If we just replaced it by 1, then we would obtain exactly the one-Gaussian bound (3.5) on the ground state energy. So the two functions to be minimized differ by an exponentially small quantity. In particular, their minimizing values β_* are also exponentially close. But now comes the kicker: since both the one-Gaussian and two-Gaussian functions E_v are locally flat at their respective minima, using the one-Gaussian value of β_* in the two-Gaussian energy function can incur at most the *square* of an exponentially small error. This is because near the minimum, we have $E_v(\beta) \sim E_v(\beta_*) + E_v''(\beta_*)(\beta-\beta_*)^2$, and $\beta-\beta_*$ is exponentially small. This means that using the wrong value β_* cannot harm the sensitivity of E_v to exponentially small contributions.

(d) Two Gaussians: Expansion

Now use the approximate (i.e. large-a) value of β_* from part (b) to find the "best" upper bound on E_0. Compare this upper bound to the one obtained in part (b): did we do better this time? If not, why not? If so, by how much did we beat the previous bound?

Solution. The approximate value of β_* obtained for the one-Gaussian wave function was $\beta_* \approx ma\sqrt{2\lambda}/\hbar$. If we plug this value into the *exact* expression for E_v, we find

$$E_v(\beta_*) \approx -\frac{3m\lambda a^4}{2} + \frac{5\hbar a\sqrt{\lambda}}{4\sqrt{2}} + \frac{3\hbar^2}{32ma^2} + \\ + \frac{3m\lambda a^4}{2}\tanh\left(\frac{ma^3\sqrt{2\lambda}}{\hbar}\right) + \frac{3\hbar a\sqrt{\lambda}}{4\sqrt{2}}\tanh\left(\frac{ma^3\sqrt{2\lambda}}{\hbar}\right). \tag{3.14}$$

For large a, the tanh terms above rapidly approach 1 from below. Replacing them both by 1 would yield the one-Gaussian bound (3.9) on E_0. So the two results differ by an exponentially small quantity, and moreover the two-Gaussian energy is just slightly *below* the one-Gaussian energy. Let us make this a bit more quantitative:

$$\Delta E_v = E_v^{(1G)} - E_v^{(2G)} = \frac{3}{2}\left(\frac{\hbar a\sqrt{2\lambda}}{4} + m\lambda a^4\right)\left[1 - \tanh\left(\frac{ma^3\sqrt{2\lambda}}{\hbar}\right)\right] \approx \\ \approx 3\left(\frac{\hbar a\sqrt{2\lambda}}{4} + m\lambda a^4\right)\exp\left[-\frac{2ma^3\sqrt{2\lambda}}{\hbar}\right] \sim 3a^4 e^{-2\sqrt{2}a^3}. \tag{3.15}$$

Here we have used the identity $1-\tanh(x) = 2/(1+e^{2x})$ and dropped the 1 in the denominator in the large-a limit. We can see clearly that the difference between the perturbative result $E_v^{(1G)}$ and the improved variational result $E_v^{(2G)}$ is exponentially small in both the limits of large a and small $\hbar$. The $\hbar$-dependence also assumes the form $e^{-1/\hbar}$ that was threatened at the end of the perturbation theory section. Although the result has the advantage of being morally correct, it is rather ad hoc, since we had to postulate a two-Gaussian trial wave function in order to see the nonperturbative tunneling effects. Before we do things right with WKB, we turn to one last—and even more ad hoc—variational trick.

(e) First Excited State

Now consider and normalize the *antisymmetric* two-Gaussian trial wave function:

$$\psi_\beta^-(x) = \frac{A}{\sqrt{2}}\left[e^{-\beta(x+a)^2} - e^{-\beta(x-a)^2}\right]. \tag{3.16}$$

Intuitively, ψ_β^- should be an excellent proxy for the first excited state at large a. Even though the variational principle only applies to the ground state, we can throw ψ_β^- at it anyway and obtain a reasonable prediction for the energy of the first excited state. Using the same approximate value $\beta = \beta_*$ found in part (c), plug $\psi_{\beta_*}^-$ into the variational principle to obtain a "bound" on the energy of the first excited state. Compare this to your result from part (d) for E_0, and calculate the energy splitting between the two lowest states.

Solution. The calculations here are almost identical to the ones in the previous part, so we skip the algebra and report the results. We begin with normalization:

$$\langle\psi_\beta^-|\psi_\beta^-\rangle = 1 \implies A = \left(\frac{\pi}{2\beta}\right)^{1/4}\left(1-e^{-2a^2\beta}\right)^{-1/2} \implies$$
$$\psi_\beta^-(x) = \frac{1}{\sqrt{2}}\left(\frac{\pi}{2\beta}\right)^{1/4}\left(1-e^{-2a^2\beta}\right)^{-1/2}\left[e^{-\beta(x+a)^2}-e^{-\beta(x-a)^2}\right]. \tag{3.17}$$

The expectation value of H in this state is given by

$$E_v^- = \frac{3m\lambda}{16\beta^2}+\frac{m\lambda a^2}{4\beta}+\frac{m\lambda a^4}{2}+\frac{\hbar^2\beta}{2m}-\frac{\hbar^2a^2\beta^2}{m}+$$
$$+\left(\frac{3m\lambda a^2}{4\beta}-\frac{m\lambda a^4}{2}+\frac{\hbar^2a^2\beta^2}{m}\right)\coth\left(a^2\beta\right). \tag{3.18}$$

Next, we plug in $\beta_* \approx ma\sqrt{2\lambda}/\hbar$ and obtain the energy of the first excited state:

$$E_v(\beta_*) \approx -\frac{3m\lambda a^4}{2}+\frac{5\hbar a\sqrt{\lambda}}{4\sqrt{2}}+\frac{3\hbar^2}{32ma^2}+$$
$$+\frac{3m\lambda a^4}{2}\coth\left(\frac{ma^3\sqrt{2\lambda}}{\hbar}\right)+\frac{3\hbar a\sqrt{\lambda}}{4\sqrt{2}}\coth\left(\frac{ma^3\sqrt{2\lambda}}{\hbar}\right). \tag{3.19}$$

These results are identical to the ones obtained in the symmetric two-Gaussian state, except with tanh replaced by coth everywhere. This is a good sign: $\tanh(x)$ approaches 1 from below, while $\coth(x)$ approaches 1 from above, so the symmetric state has lower energy than the antisymmetric state being analyzed presently. Finally, we compute the energy splitting between the ground and first excited states:

$$\Delta E_v = E_v^- - E_v^+ = 3\left(m\lambda a^4+\frac{\hbar a\sqrt{2\lambda}}{4}\right)\operatorname{csch}\left(\frac{2ma^3\sqrt{2\lambda}}{\hbar}\right) \approx \tag{3.20}$$
$$\approx 6\left(m\lambda a^4+\frac{\hbar a\sqrt{2\lambda}}{4}\right)\exp\left[-\frac{2ma^3\sqrt{2\lambda}}{\hbar}\right] \sim 6a^4e^{-2\sqrt{2}a^3}. \tag{3.21}$$

Here we have used $\operatorname{csch}(x) = 2/(e^x-e^{-x})$ and dropped the e^{-x} in the denominator in the large-a limit. At long last, we have hacked together a "derivation" that the energy gap of the double well potential is nonperturbatively small, both in $\frac{1}{a}$ and in $\hbar$.

4 The WKB Method

We conclude our tour de force of the double well with its study through the unreasonably powerful WKB approximation. In particular, we will use the WKB method to calculate tunneling probabilities, wave functions, and energy splittings in the double well.

(a) Tunneling at Zero Energy

Consider a particle of negligible energy $E \approx 0$ stuck in the right well at $x = a$. Calculate the probability T for the particle to tunnel through the central barrier to $x = -a$. Compare your answer to the square amplitude of the Gaussian wave function, $\psi_0^{(0)}$, evaluated at $x = -a$.

Solution. The tunneling probability is expressed in terms of the *extinction coefficient* γ, which is in turn calculated from the classical momentum of the particle:

$$T = e^{-2\gamma}, \qquad \gamma = \frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}x\, |p(x)|, \qquad p(x) = \sqrt{2m(E - V(x))}. \tag{4.1}$$

We have an explicit expression for $V(x)$, and we assume $E = 0$. Therefore:

$$\begin{aligned} |p(x)| &= \left|\sqrt{2m(E - V(x))}\right| \approx \left|\sqrt{-2mV(x)}\right| = \\ &= \left|\sqrt{-2m \cdot m\lambda(x^2 - a^2)^2}\right| = m\sqrt{2\lambda}\left|x^2 - a^2\right|. \end{aligned} \tag{4.2}$$

The extinction coefficient can then be calculated exactly:

$$\gamma = \frac{m\sqrt{2\lambda}}{\hbar}\int_{-a}^{a} \mathrm{d}x\, \left|x^2 - a^2\right| = \frac{4ma^3\sqrt{2\lambda}}{3\hbar}. \tag{4.3}$$

The tunneling probability is therefore assembled:

$$T = e^{-2\gamma} = \exp\left(-\frac{8ma^3\sqrt{2\lambda}}{3\hbar}\right). \tag{4.4}$$

As expected, T decays extremely rapidly with increasing a.

Meanwhile, the probability computed from the Gaussian is

$$\begin{aligned} \psi_0^{(0)}(x) &= \left(\frac{2ma\sqrt{2\lambda}}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{ma\sqrt{2\lambda}}{\hbar}(x - a)^2\right) \implies \\ \left|\psi_0^{(0)}(-a)\right|^2 &= \sqrt{\frac{2ma\sqrt{2\lambda}}{\pi\hbar}}\exp\left(-\frac{8ma^3\sqrt{2\lambda}}{\hbar}\right). \end{aligned} \tag{4.5}$$

Evidently they have the same decay exponent! Physics works. :)

(b) The Quantization Condition

Now suppose that the energy E is small but nonzero. We will build up to a derivation of the quantization condition and the energy splitting in the double well potential. To begin, define the following related quantities:

$$\theta = \frac{1}{\hbar}\int_{x_1}^{x_2} \mathrm{d}x\, p(x), \qquad \phi = \frac{1}{\hbar}\int_{-x_1}^{x_1} \mathrm{d}x\, |p(x)|, \qquad S(x) = \int_{x}^{x_1} \mathrm{d}x'\, |p(x')|, \tag{4.6}$$

where $\pm x_1$ and $\pm x_2$ are the locations of the inner and outer turning points of the double well, respectively. Intuitively, θ and ϕ measure oscillation and extinction in their respective regions. The interpretation of $S(x)$ will remain mysterious for now.

It can be shown via the connection formulæ (but don't bother proving this) that in the region $[0, x_1]$, the WKB wave function takes the form

$$\psi_{\mathrm{WKB}}(x) = \frac{C_\pm}{\sqrt{|p(x)|}}\left[2\cos\theta e^{S(x)/\hbar} + \sin\theta e^{-S(x)/\hbar}\right], \tag{4.7}$$

It turns out to be impossible to calculate θ, ϕ, and $S(x)$ in closed form for the double well potential $V(x)$, but we can still say a few things on general grounds. Recall that the symmetry of the potential $V(x)$ forces ψ_{WKB} to be either symmetric (even) or antisymmetric (odd). In the odd case, $\psi_{\mathrm{WKB}}(0) = 0$, while in the even case, $\psi'_{\mathrm{WKB}}(x) = 0$. Impose these boundary conditions to derive the quantization condition $\tan\theta = \pm 2e^{\phi}$, where the plus sign is taken for even ψ_{WKB}, and the minus sign for odd ψ_{WKB}.

Hint: for the odd case, first prove that $\frac{\mathrm{d}|p|}{\mathrm{d}x}\big|_{x=0} = 0$.

Solution. The even case is easier: setting $\psi_{\mathrm{WKB}}(0) = 0$ yields

$$\begin{aligned}\psi_{\mathrm{WKB}}(0) = \frac{C_\pm}{\sqrt{|p(0)|}}\left[2\cos\theta e^{S(0)/\hbar} + \sin\theta e^{-S(0)/\hbar}\right] \overset{!}{=} 0 \implies \\ 2\cos\theta e^{S(0)/\hbar} = -\sin\theta e^{-S(0)/\hbar} \implies \tan\theta = -2e^{2S(0)/\hbar}.\end{aligned} \tag{4.8}$$

We're almost there! It remains to observe that since the potential is even, we have

$$S(0) = \int_0^{x_1} \mathrm{d}x'\, |p(x')| = \frac{1}{2}\int_{-x_1}^{x_1} \mathrm{d}x\, |p(x)| = \frac{\hbar}{2}\phi, \tag{4.9}$$

where the first equality follows because $p(x)$ does not change sign on $[0, x_1]$. Therefore:

$$\tan\theta = -2e^{2\phi\hbar/2\hbar} = -2e^{\phi}. \tag{4.10}$$

The even case takes a bit more work, since we need to compute the derivative of the WKB wave function. Using the chain rule and the fundamental theorem of calculus, we find

$$\begin{aligned}\psi'_{\mathrm{WKB}}(x) = \frac{C_\pm}{|p(x)|^{3/2}}\frac{\mathrm{d}|p(x)|}{\mathrm{d}x}\left[2\cos\theta e^{S(x)/\hbar} + \sin\theta e^{-S(x)/\hbar}\right] + \\ + \frac{C_\pm}{\sqrt{|p(x)|}}\left[2\cos\theta e^{S(x)/\hbar}\left(\frac{|p(x)|}{\hbar}\right) + \sin\theta e^{-S(x)/\hbar}\left(-\frac{|p(x)|}{\hbar}\right)\right].\end{aligned} \tag{4.11}$$

Now we set $x = 0$. We recall that $S(0) = \frac{\hbar}{2}\phi$, and set $p_0 = |p(0)| > 0$ for shorthand. We'll also need to show that $\mathrm{d}p/\mathrm{d}x$ vanishes at zero:

$$\frac{\mathrm{d}p}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\Big[\sqrt{2m[E - V(x)]}\Big] \propto \frac{\mathrm{d}V}{\mathrm{d}x} \implies \left.\frac{\mathrm{d}p}{\mathrm{d}x}\right|_{x=0} \propto \left.\frac{\mathrm{d}V}{\mathrm{d}x}\right|_{x=0} = 0. \tag{4.12}$$

Putting these pieces together, we find that the entire first term in $\psi'_{\mathrm{WKB}}(0)$ above vanishes:

$$\begin{aligned}\psi'_{\mathrm{WKB}}(0) = \frac{C_\pm}{\sqrt{p_0}}\Big[2\cos\theta e^{\phi}\Big(\frac{p_0}{\hbar}\Big) + \sin\theta e^{-\phi}\Big(-\frac{p_0}{\hbar}\Big)\Big] \stackrel{!}{=} 0 \implies \\ 2\cos\theta e^{\phi} = \sin\theta e^{-\phi} \implies \tan\theta = +2e^{\phi}.\end{aligned} \tag{4.13}$$

(c) Preparation I: Large-a Quantization

In the WKB limit, the two wells are deep and widely separated. Irrespective of the specific form of $V(x)$, this makes ϕ grows large. This means that $\tan\theta = \pm 2e^{\phi}$ is exponentially large, which occurs only when θ is close to a half-integer multiple of π. (This is why the formula above really was a quantization condition.) Introduce a small parameter ε and write

$$\theta = \left(n + \frac{1}{2}\right)\pi + \varepsilon. \tag{4.14}$$

The small deviation ε should be related to how large ϕ is. Upon imposing $\tan\theta = \pm 2e^{\phi}$, show that $\varepsilon \approx \mp\frac{1}{2}e^{-\phi}$ (to first order in ε), and therefore show that

$$\theta = \left(n + \frac{1}{2}\right)\pi \mp \frac{1}{2}e^{-\phi}. \tag{4.15}$$

Notice that this means that there are *two* WKB wave functions for each value of n, differing in the region $[0, x_1]$ from each other by a tiny amount parametrized by $\Delta\theta \sim e^{-\phi}$.

Solution. We begin by using an angle addition formula to isolate ε in $\tan\theta$:

$$\tan\theta = \tan\left[\left(n + \frac{1}{2}\right)\pi + \varepsilon\right] = \frac{\sin\left[\left(n + \frac{1}{2}\right)\pi + \varepsilon\right]}{\cos\left[\left(n + \frac{1}{2}\right)\pi + \varepsilon\right]} = \frac{(-1)^n\cos\varepsilon}{(-1)^{n+1}\sin\varepsilon} = -\frac{1}{\tan\varepsilon}. \tag{4.16}$$

Then, imposing the quantization condition, we have

$$\tan\theta = -\frac{1}{\tan\varepsilon} = \pm 2e^{\phi} \implies \tan\varepsilon \approx \varepsilon = \mp\frac{1}{2}e^{-\phi}. \tag{4.17}$$

This completes the proof, since we can now plug ε directly into the quantization condition:

$$\theta = \left(n + \frac{1}{2}\right)\pi + \varepsilon = \left(n + \frac{1}{2}\right)\pi \mp \frac{1}{2}e^{-\phi}. \tag{4.18}$$

(d) Preparation II: Harmonic Approximation

Find the exact locations of the four classical turning points in the double well potential $V(x)$. Call the inner ones $\pm x_1$ and the outer ones $\pm x_2$. Expand $x_{1,2}$ to leading order in large a, and check that they match the locations of the turning points in the harmonic potential $V^{(2)}(x)$. Then, calculate θ and ϕ in terms of the energy E for the harmonic potential $V^{(2)}(x)$.

Solution. The four turning points $\pm x_{1,2}$ of $V(x)$ are defined by $V(\pm x_{1,2}) = E$:

$$E = m\lambda\big(x^2 - a^2\big)^2 \implies \pm x_{1,2} = \pm\sqrt{a^2 \pm \sqrt{\frac{E}{m\lambda}}} \approx \pm\left(a \pm \frac{1}{2a}\sqrt{\frac{E}{m\lambda}}\right). \tag{4.19}$$

The outer turning points take the plus sign inside the square root, while the inner turning points take the minus sign. The overall sign tells us whether we are on the left or the right.

Meanwhile, the turning points of the harmonic potential are given by

$$E = V^{(2)}(x) = 4m\lambda a^2(x-a)^2 \implies (x-a)^2 = \frac{E}{4m\lambda a^2} \implies x_{1,2} = a \pm \frac{1}{2a}\sqrt{\frac{E}{m\lambda}}, \tag{4.20}$$

which matches the results above.

Now we attack the integration of the momentum, which is given for $V^{(2)}$ by

$$p(x) = \sqrt{2m[E - V^{(2)}(x)]} = \sqrt{2m[E - 4m\lambda a^2(x-a)^2]}. \tag{4.21}$$

The integrals defining θ and ϕ are tricky but doable; see Griffiths, problem 9.17. The θ integral can be computed exactly:

$$\theta = (\text{math}) = \frac{\pi E}{2a\sqrt{2\lambda}\hbar}. \tag{4.22}$$

The ϕ integral can also be done exactly, but the answer is not as pretty:

$$\phi = (\text{math}) = \frac{E}{a\sqrt{2\lambda}\hbar}\left[z_0\sqrt{z_0^2 - 1} - \ln\left(z_0 + \sqrt{z_0^2 - 1}\right)\right], \qquad z_0 = 2a^2\sqrt{\frac{m\lambda}{E}}. \tag{4.23}$$

In the WKB limit $E \ll V^{(2)}(x)$, this expression collapses to

$$\phi \approx \frac{E}{a\sqrt{2\lambda}\hbar}\big[z_0^2 - \ln(2z_0)\big] \approx \frac{Ez_0^2}{a\sqrt{2\lambda}\hbar} = \frac{4ma^3\sqrt{2\lambda}}{\hbar}. \qquad (!) \tag{4.24}$$

(e) The Energy Splitting

Combine your results from parts (c) and (d) to obtain a formula for the energies $E_n^{\pm}$ of the symmetric (+) and antisymmetric (−) WKB wave functions. (You do not need to show that the WKB wave functions satisfy the Schrödinger equation and therefore have well-defined energies. It is true but unenlightening to prove.) Calculate, at long last, the energy splitting $\Delta E_0 = E_0^+ - E_0^-$ between the two lowest states in the double well potential.

Solution. Let's begin by recalling and gathering our results so far:

$$\theta = \left(n + \frac{1}{2}\right)\pi \mp \frac{1}{2}e^{-\phi}, \qquad \theta = \frac{\pi E_n^{\pm}}{2a\sqrt{2\lambda}\hbar}, \qquad \phi \approx \frac{4ma^3\sqrt{2\lambda}}{\hbar}. \tag{4.25}$$

This allows us to immediately solve for the energies:

$$E_n^{\pm} = \frac{2a\sqrt{2\lambda}\hbar}{\pi}\left[\left(n + \frac{1}{2}\right)\pi \mp \frac{1}{2}e^{-\phi}\right] = 2a\sqrt{2\lambda}\hbar\left(n + \frac{1}{2}\right) \mp \frac{a\sqrt{2\lambda}\hbar}{\pi}e^{-4ma^3\sqrt{2\lambda}/\hbar}. \tag{4.26}$$

The energy splitting between any pair of symmetric and antisymmetric states, including the gap between the ground and first excited state, is

$$\Delta E_n = \frac{2a\sqrt{2\lambda}\hbar}{\pi}e^{-4ma^3\sqrt{2\lambda}/\hbar} = \frac{\hbar\omega}{\pi}e^{-m\omega a^2/\hbar}. \tag{4.27}$$

(f) Tunneling and Imaginary Time

When a particle tunnels through a potential barrier, its momentum $p = \sqrt{2m[E - V(x)]}$ becomes imaginary. Classically, this is clearly nonsense... or is it? If we think of momentum as $p = mv$, then an imaginary p implies that $v = \dot{x}$ is imaginary: we can view this as the velocity of motion that happens over an imaginary time interval.

Consider, now, the classical action for a point particle in an *arbitrary* potential $V(x)$,

$$S = \int_0^T \mathrm{d}t\, L = \int_0^T \mathrm{d}t \left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x)\right]. \tag{4.28}$$

Make the transformation $t \longrightarrow \tau = it$ with $\beta = iT$, and express the transformed (*Euclidean*) action in terms of τ. This change of coordinates is called a *Wick rotation*, and τ is called the imaginary or *Euclidean time*. You should find that

$$S \longrightarrow i\int_0^\beta \mathrm{d}\tau \left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x)\right] \equiv S_{\mathrm{E}}. \tag{4.29}$$

Obtain the Euler-Lagrange equations that follow from S'. Compare them to the usual Euler-Lagrange equations: what happened to the potential? Then explain the following cryptic claim: "Quantum tunneling is classical motion in imaginary time."

Solution. The transformation $t \longrightarrow \tau = it$ induces the following changes:

$$\mathrm{d}t \longrightarrow \mathrm{d}\tau = i\,\mathrm{d}t \iff \mathrm{d}t = -i\,\mathrm{d}\tau, \qquad \frac{\mathrm{d}}{\mathrm{d}t} \longrightarrow \frac{\mathrm{d}}{\mathrm{d}\tau} = -i\frac{\mathrm{d}}{\mathrm{d}t} \iff \frac{\mathrm{d}}{\mathrm{d}t} = i\frac{\mathrm{d}}{\mathrm{d}\tau}. \tag{4.30}$$

Substituting these changes, along with $t = T \implies iT = \beta$ into the original action yields

$$S \longrightarrow S_{\mathrm{E}} = \int_0^\beta (-i\,\mathrm{d}\tau)\left[\frac{1}{2}m\left(i\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x)\right] = i\int_0^\beta \mathrm{d}\tau\left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x)\right]. \tag{4.31}$$

As for the Euler-Lagrange equations, their derivation is completely identical to the usual case. The factor of i in front of the action does not appear in the equations of motion, and the only thing that changes is the sign of V. To wit:

$$\delta S_{\mathrm{E}} = 0 \implies \frac{\partial}{\partial\tau}\left(\frac{\partial L}{\partial(\mathrm{d}x/\mathrm{d}\tau)}\right) = \frac{\partial L}{\partial x} \implies m\frac{\mathrm{d}^2x}{\mathrm{d}\tau^2} = +\frac{\mathrm{d}V}{\mathrm{d}x}. \tag{4.32}$$

The potential evidently gets flipped upside down. This is unsurprising, since the move to imaginary time has the effect of flipping the sign of the kinetic term relative to the potential, so the Euler-Lagrange equations reflect motion in the inverted potential.

We conclude that the action for a particle that *tunnels* over a potential barrier, which is purely imaginary, can be viewed as i times the action for a particle that *rolls* in the upside-down version of the same potential. And as we saw above, such an inverted potential is obtained by putting the system in imaginary time.

(g) Instantons

Using the explicit form of the double well potential $V(x)$, solve the Euler-Lagrange equations to find the classical trajectory $x(\tau)$ of the imaginary-time system, subject to the constraints that the total energy is zero and $x(0) = x$. This solution is called an *instanton*: why? (Hint: consider large a.) Next, evaluate S_{E} on this trajectory by plugging the solution $x(\tau)$ back into S_{E} and performing the integral $\mathrm{d}\tau$ explicitly on the interval $[-\beta, \beta]$.

Finally, take the limit of large a. If the real-time action S transforms to S_{E}, what does the quantity $e^{iS/\hbar}$ transform to? Does this remind you of any of the previous results? It turns out that the phase factor $e^{iS/\hbar}$ is a crucial ingredient in the theory of Feynman path integrals. This suggests that path integrals in imaginary time have a good deal to say about the WKB approximation (indeed, at a deep level they are identical!) and about tunneling.

Solution. Our equations of motion, using overdots to denote τ-derivatives, are

$$m\ddot{x} = \frac{\mathrm{d}V}{\mathrm{d}x} = 4m\lambda x(x^2 - a^2) \implies \ddot{x} = 4\lambda x(x^2 - a^2). \tag{4.33}$$

This looks hard to solve; it is better to take advantage of the hint that the total energy is conserved and vanishes. In imaginary time, the Lagrangian is $L = T - (-V) = T + V$ (i.e. it is the energy of the *real-time* system), so the imaginary-time Hamiltonian is

$$H = T + (-V) = \frac{1}{2}m\dot{x}^2 - m\lambda\big(x^2 - a^2\big)^2 = 0. \tag{4.34}$$

This has the effect of "automatically" integrating the equation of motion partway. The resulting equation is separable and can be solved exactly:

$$\begin{aligned} \frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 = \lambda\big(x^2 - a^2\big)^2 \implies \frac{\mathrm{d}x}{\mathrm{d}\tau} = \pm\sqrt{2\lambda}\big(x^2 - a^2\big) \implies \\ -\frac{1}{a}\tanh^{-1}\left(\frac{x}{a}\right) = \pm\sqrt{2\lambda}(\tau - \tau_0) \implies x(\tau) = \pm a\tanh\Big(a\sqrt{2\lambda}\tau\Big). \end{aligned} \tag{4.35}$$

(We have set $\tau_0 = 0$ to ensure $x(0) = 0$.)

This solution is called an instanton because at large a, tanh approaches an abrupt step function. The particle sits, almost stationary, on one maximum ($x = -a$) of the inverted potential for all $t < 0$. Then, right around $t = 0$, it quickly rolls across to the other maximum ($x = a$), where it stays for all $t > 0$. The tunneling is localized in an instant, and is described by the motion of a particle (an "-on" in particle parlance), hence the name *instanton*.

It remains to plug this into the action and evaluate it. This is most easily done in Mathematica, which gives

$$V(x(\tau)) = m\lambda a^4 \operatorname{sech}^4\Big(a\sqrt{2\lambda}\,\tau\Big) = \frac{1}{2}m\left(\frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau}\right)^2 = T. \tag{4.36}$$

Therefore the Lagrangian is obtained and integrated:

$$\begin{aligned} L = T + V = 2T = 2V = 2m\lambda a^4 \operatorname{sech}^4\Big(a\sqrt{2\lambda}\,\tau\Big) \implies \\ S_{\mathrm{E}} = i\int_{-\beta}^{\beta} \mathrm{d}\tau\,(T+V) = \frac{4ma^3\sqrt{2\lambda}}{3}\tanh\Big(a\sqrt{2\lambda}\,\beta\Big)\left[1 + \frac{1}{2}\operatorname{sech}^2\Big(a\sqrt{2\lambda}\,\beta\Big)\right]i. \end{aligned} \tag{4.37}$$

Now at large a, $\operatorname{sech}(ax)$ approaches zero, and $\tanh(ax)$ approaches 1, both exponentially rapidly. Therefore in the crude large-a approximation, we have

$$S_{\mathrm{E}} \approx \frac{4ma^3\sqrt{2\lambda}}{3} \implies e^{iS/\hbar} \xrightarrow{t\to it} \exp\left[-\frac{4ma^3\sqrt{2\lambda}}{3\hbar}\right], \tag{4.38}$$

which reminds us strongly of just about every result we've obtained so far using WKB.

A beautiful story begins here: topology, path integrals, instantons, semiclassical approximations, and even quantum gravity all converge here. But this is a story for another time.

A References

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