115C (QM III): The Double Well

Or, How I Learned to Stop Worrying and Love Approximations

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April 28, 2021

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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.

(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.

(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

$$V(x) = V^{(2)}(x) + V'(x) = A(x - B)^2 + V'(x), \tag{1.2}$$

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.

(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 $H^{(0)}$.

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.

(b) First-Order Energy

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

(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.

(d) Second-Order Energy

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

(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?

(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,

$$E_0^{(\infty)} = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + \cdots, \qquad \psi_0^{(\infty)} = \psi_0^{(0)} + \psi_0^{(1)} + \psi_0^{(2)} + \cdots, \tag{2.1}$$

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.

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.

(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.

(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:

$$\psi_\beta(x) = \frac{A}{\sqrt{2}}\Big[e^{-\beta(x+a)^2} + e^{-\beta(x-a)^2}\Big]. \tag{3.1}$$

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.

(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?

(e) First Excited State

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

$$\psi_\beta^-(x) = \frac{A}{\sqrt{2}}\Big[e^{-\beta(x+a)^2} - e^{-\beta(x-a)^2}\Big]. \tag{3.2}$$

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.

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 $x = -a$.

(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:

$$\theta = \frac{1}{\hbar}\int_{x_1}^{x_2} \mathrm{d}x\, p(x), \qquad \phi = \frac{1}{\hbar}\int_{-x_1}^{x_1} \mathrm{d}x\, |p(x)|, \qquad S(x) = \int_{x}^{x_1} \mathrm{d}x'\, |p(x')|, \tag{4.1}$$

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

$$\psi_{\mathrm{WKB}}(x) = \frac{C_\pm}{\sqrt{|p(x)|}}\left[2\cos\theta e^{S(x)/\hbar} + \sin\theta e^{-S(x)/\hbar}\right], \tag{4.2}$$

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 $\frac{\mathrm{d}|p|}{\mathrm{d}x}\big|_{x=0} = 0$.

(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

$$\theta = \left(n + \frac{1}{2}\right)\pi + \varepsilon. \tag{4.3}$$

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

$$\theta = \left(n + \frac{1}{2}\right)\pi \mp \frac{1}{2}e^{-\phi}. \tag{4.4}$$

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 $\Delta\theta \sim e^{-\phi}$.

(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 $V^{(2)}(x)$.

(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.

(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 $V(x)$,

$$S = \int_0^T \mathrm{d}t\, L = \int_0^T \mathrm{d}t \left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x)\right]. \tag{4.5}$$

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

$$S \longrightarrow i \int_0^\beta \mathrm{d}\tau \left[\frac{1}{2} m \left(\frac{\mathrm{d}x}{\mathrm{d}\tau} \right)^2 + V(x) \right] \equiv S_\mathrm{E}. \tag{4.6}$$

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."

(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.