Phys 487 Discussion 8 – The Variational Principle

New subject! The **variational principle** is a technique for finding the ground state energy[1], E_{gs}, of a system when the Hamiltonian's eigenstates are not known and not easy to find. It consists of one theorem plus one technique:

- The Theorem : $\boxed{E_{gs} \le \langle \hat{H} \rangle} = \langle \psi | \hat{H} | \psi \rangle$.

  In words: the ground state energy is the lowest possible expectation value of the Hamiltonian. This is very intuitive, and becomes completely obvious once we work through the small proof.

- The Technique : Evaluate the expectation value $\langle \psi | \hat{H} | \psi \rangle$ using a trial wavefunction ψ = a function with one or more parameters that you can vary, then minimize $\langle H \rangle$ with respect to those parameters.

The result is an upper limit on the ground-state energy. It can be a very good estimate of the ground-state energy if your trial wavefunction can acquire a shape very close to the actual ground-state wavefunction. Such **variational techniques** are very common in numerical analysis.

For the integrals you must do today, feel free to use wolframalpha, but also recall that the 486 formula sheet has useful math results like Gaussian integrals.

Problem 1 : Linear Potential *Qual Problem* [2]

A particle of mass m moves in the 1D region $x > 0$ and experiences the following potential energy :

$$V(x) = \begin{cases} \infty & \text{for } x \le 0 \\ F x & \text{for } x > 0 \end{cases} \quad \text{where } F \text{ is a real, positive constant.}$$

Use a variational method to obtain an estimate for the ground state energy.

▶ **TIPS** for selecting a trial wavefunction:

- Think about the wavefunction's asymptotic behaviour, i.e. how it must behave / what values it must reach in the limits $x \to \infty$ and $x \to 0$.
- As we will discuss in class, for systems that extend to $\pm\infty$, the easiest trial wavefunctions to work with are almost always Gaussians or falling exponentials, i.e. $\exp(-\alpha x^2)$ and $\exp(\mp\alpha x)$. Either form will give you a good answer here, but one will be better than the other. And don't forget …
- The forms in the previous bullet are common choices for taking care of $x \to +\infty$ behaviour, but don't forget about the OTHER boundary condition, which in this case is not $x \to -\infty$ but $x \to 0$! You must make a small but significant modification to the previous forms before you can use them as good trial wavefunctions for this problem!

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[1] Jargon check: The **ground state energy** of a system ≡ the lowest eigenvalue of the system's Hamiltonian. Also, we will shortly learn that you can *occasionally* use the variational principle to estimate the energy of the 1st excited state as well as the ground state (e.g. problem 3).

[2] **Q1** : About the simplest trial wavefunction you can use is $\psi(x) = A\, x\, e^{-\alpha x}$, let's go with that (it's 0 at x=0 and it's square-integrable)
… The next step is to normalize your trial wavefunction … for our ψ, we get $A = 2\,\alpha^{3/2}$
… The next step is to calculate the expectation value of the Hamiltonian for the trial wavefunction … i.e. $< -\hbar^2/2m\; d^2/dx^2 + Fx >$
… For our ψ, $< H > = \alpha^2\hbar^2 / 2m + 3F / 2\alpha$
… The next step is to minimize $< H >$ … with respect to any free parameters
… Our only free parameter is α … Minimization gives $< H >_{min} = (3/2)^{5/3}\, (\hbar^2 F^2 / m)^{1/3}$, which is our estimate for E_{gs}.
Of course you will get another result if you use a different trial wavefunction. If your result is lower, you made a better guess! :-)

Problem 2 : δ Function Potential *Griffiths 7.3* [3]

Find the best bound on the ground-state energy E_{gs} for the δ-function potential $V(x) = -\alpha\delta(x)$ using as your trial wavefunction a triangular form that peaks at the origin and falls off linearly on either side to $x = \pm a/2$. (So the total width of the triangle is a … which is your adjustable parameter, and not equal to the Greek α in front of the δ-function potential, which is a given value. a and α look the same in this font, argh, but not usually when handwritten).

Problem 3 : SHO, 1st excited state *Griffiths 7.4(b)* [4]

There is a corollary to the variational principle that can be used to estimate the 1st-excited energy of *some* systems. Here is a practical version of that corollary (we will make it more general in class):

> If the system's potential energy $V(x)$ is an even function of x
> and we use trial wavefunctions $\psi(x)$ that are odd functions of x,
> then the variational principle gives us an upper bound on the energy of the 1st-excited state :

$$\boxed{E_{\text{1st excited}} \leq \langle \psi_{\text{odd}} | \hat{H}_{\text{even}} | \psi_{\text{odd}} \rangle}$$

This is not so intuitive as the main variational principle, but the proof will make it obvious too, you'll see. :)

Using this technique, find the best bound on the first excited state of the 1D harmonic oscillator that you can obtain from the following trial wavefunction :

$$\psi(x) = A\,x\,e^{-bx^2}$$

[3] **Q2** : $E_{gs} \leq -3m\alpha^2/8\hbar^2$

[4] **Q3** : $E_{1exc} \leq 3\hbar\omega/2$