Phys 487 Discussion 7 – The Variational Principle

The variational principle for finding ground state energies (and, sometimes, for 1st-excited-state energies) is so *utterly intuitive* that there is no need for a formula summary today! See if you can manage without any guidance ; otherwise, have a peek back at lecture 7A.

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

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 deciding on 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 mentioned 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 will have to make a small but significant modification to the previous forms before you can use them as good trial wavefunctions for this problem!

Problem 2 : Connecting Variational Principle & Perturbation Theory *Griffiths 7.5(a)* [2]

Use the variational principle to prove that first-order non-degenerate perturbation theory always overestimates (or more exactly, never underestimates) the ground state energy.

▶ This problem should take 5 minutes max; if you don't see the solution in that time, see footnote hints.

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[1] **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! :-)

[2] **Q2** : Call the ground state of the unperturbed Hamiltonian $|\, gs^{(0)} >$. 1st order PT estimates the ground state energy to be $E_{gs}^{(0)} + E_{gs}^{(1)}$
… $E_{gs}^{(0)}$ is just the unperturbed ground state energy, $< gs^{(0)} \,|\, H_0 \,|\, gs^{(0)} >$
… The first-order correction to the energy is $E_{gs}^{(1)} = < gs^{(0)} \,|\, H' \,|\, gs^{(0)} >$
… The full Hamiltonian, including perturbation, is $H = H_0 + H'$
… so the 1st-order PT estimate of the ground state energy is simply $< gs^{(0)} \,|\, H \,|\, gs^{(0)} >$
… which by the variational principle … is greater than or equal to … the exact ground state energy. QED.

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

Find the best bound on the first excited state of the 1D harmonic oscillator that you can obtain from the trial wavefunction

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

Problem 4 : δ Function Potential *Griffiths 7.3* [4]

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!).

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

[4] **Q4** : $E_{gs} \leq -3m\alpha^2/8\hbar^2$