PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 2 EXERCISE CLASSES (14-18 January 2019)

You are encouraged to think about (or work out) the sample questions before attending exercise class and ask the TA questions. You should attend one exercise class session per week.

SQ4: Variational method estimation of ground state energy of hydrogen atom using a gaussian trial wavefunction

SQ5: Infinite well with V-shaped bottom - trial wavefunction with two parameters and the art of choosing trial wavefunction

SQ4 *Variational Method estimation of ground state energy of a hydrogen atom by a student who only knows harmonic oscillator physics*

Background: We learned the analytic/exact solutions to the hydrogen atom last term (see class notes for a review). The energy is determined by the equation governing the radial function $R(r)$. For the ground state ($1s$ state), the angular part is $Y_{00}(\theta,\phi)$, which is just a constant. Since $\ell = 0$ for s states, the extra term $\ell(\ell+1)/2\mu r^2$ in the radial equation vanishes, where μ is the effective mass (see SQ1 and SQ2 for idea behind μ). At the end, the radial part of the $1s$ ground state wavefunction is governed by the equation

$$\hat{H}_r R(r) = \left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr})\right) - \frac{e^2}{4\pi\epsilon_0 r}\right] R(r) = E\, R(r)\ , \tag{1}$$

where $\hat{H}_r$ denotes the operator for the radial part of the problem. The range of r is $r > 0$. This can be solved analytically (Laguerre functions). Here, we pretend that we don't know the solutions.

A student learned QM and only learned the harmonic oscillator part well. Just picked up the variational method, the student proposes a trial wavefunction of the form

$$\phi(r) = A\, e^{-\lambda r^2} \quad \text{for } r > 0 \tag{2}$$

where λ will be used as the variational parameter. Here, the prefactor A is given by

$$A^2 = 8\sqrt{\frac{2\lambda^2}{\pi}} \tag{3}$$

so that $\phi(r)$ is **normalized in the form** of

$$\int_0^\infty |\phi(r)|^2\, r^2 dr = \int_0^\infty A^2 e^{-2\lambda r^2}\, r^2 dr = 1 \tag{4}$$

Note that there seems to be a missing factor of 4π in the integral, but we will also keep the same 4π missing in evaluating the energy expectation value. At the end, it makes no harm.

TA: **Evaluate** $\langle \hat{H}_r \rangle_\phi$ by working out

$$\langle \hat{H}_r \rangle_\phi = \int_0^\infty \phi^*(r) \hat{H}_r\, \phi(r)\, r^2 dr \stackrel{?}{=} \frac{3\lambda\hbar^2}{2\mu} - \frac{2e^2}{4\pi\epsilon_0}\sqrt{\frac{2\lambda}{\pi}} \tag{5}$$

It is alright to look up integral table for some integrals. Hence, **find** the value of λ_{best} that minimizes $\langle \hat{H}_r \rangle_\phi$ and the best estimate of the ground state energy. **Compare** the result with the exact value $E_{GS} = -\frac{\mu e^4}{2\hbar^2(4\pi\epsilon_0)^2}$ (obtained in QMI).

SQ5 *Variational Method applied to Infinite well with V-shaped bottom*

Background: The most useful applications of the variational method are related to using a trial wavefunction of the form $\phi_{trial} = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + \cdots$, i.e. **a linear combination of well-chosen functions**. Recall that at the beginning, the variational method is based on a theorem related to the ground state energy. So the trial wavefunction is meant to mimic the actual ground state wavefunction. A remark is that cleverly using the method can lead to useful results beyond the estimating of only the ground state energy.

[TA: Note that the general formulation of $\phi_{trial} = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + \cdots$ will be covered in Week 2. Here, don't assume students know of the general form using ϕ_{trial}.]

Consider a 1D infinite well with a V-shaped bottom. The potential energy function $U(x)$ between $0 < x < a$ is that it drops linearly from zero to $-U_0$ at $x = a/2$ (middle of the well) and then increases linearly back to 0 at $x = a$. Outside the well ($x \leq 0$ and $x \geq a$), $U(x) = \infty$.

Writing down a good trial wavefunction ϕ_{trial} is an art and a science. If ϕ_{trial} captures the key features of the actual ground state wavefunction (not known), the better will be the estimate.

Let's think like a physicist! The V-shaped $U(x)$ reminds us of the infinite well problem with a flat $U = 0$ bottom inside the well. This is the easiest QM problem and we know all the energy eigenvalues and the eigenstates. They are:

$$\phi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad \text{with} \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (n = 1, 2, 3, \ldots) \tag{6}$$

For the V-shaped problem, the ground state should *look like* ψ_1 of the flat-bottom problem. Of course, ψ_1 is not the correct ground state wavefunction. What else do we expect? It should be symmetric about the center ($x = a/2$) of the well because $U(x)$ is symmetric, and a bit higher at the middle (than ψ_1) so as to make use of the lower potential energy there. Mixing in a bit of ψ_2 (which is anti-symmetric about the center) is not a good idea, because it will ruin the symmetric feature of ψ_1 (which is a correct feature). Naturally, the next idea is to mix in a bit of ψ_3, which is symmetric about the center. This leads us to the following choice of a trial wavefunction

$$\begin{aligned} \phi_{trial}(x) &= c_1\ \psi_1(x) + c_3\ \psi_3(x) \\ &= c_1 \sqrt{\frac{2}{a}}\ \sin\left(\frac{\pi x}{a}\right) + c_3 \sqrt{\frac{2}{a}}\ \sin\left(\frac{3\pi x}{a}\right) \end{aligned} \tag{7}$$

for estimating the ground state energy. Here, we assume c_1 and c_3 to be real parameters. They will be used as the variational parameters.

TA: For ϕ_{trial}, **take** c_1 and c_3 as the variational parameters, **apply** the variational method to set up the problem, and **estimate** the ground state energy of a V-bottomed infinite well. [TA: Please do the math as plainly as possible.]

[Remarks: Here we see an example of a trial wavefunction carrying two variational parameters. It can be more. If we want to do better by including one more $\psi_n(x)$, which one will you choose? If we include more and more terms, will the accuracy of the result improve? What if we include infinitely many terms? How will the result be connected to the exact formalism of changing TISE to a huge matrix problem?]