PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 3 EXERCISE CLASSES (25-29 January 2021)

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

SQ4: Infinite well with V-shaped bottom - trial wavefunction of the form of linear combination of two functions
SQ5: Infinite well with V-shaped bottom - perturbation theory

SQ4 *Infinite well with V-shaped bottom - Variational Calculation*

Consider a one-dimensional (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 $x \geq a$), $U(x) = \infty$.

Here, TA will do a variational calculation using a trial wavefunction that linearly combines two functions after motivating it by physical sense.

TA: **Discuss qualitatively** the expected behavior of the ground state wavefunction given that $U(x)$ is symmetric about $x = a/2$. Then, by referring to the known energy eigenstates of an infinite flat-bottomed well, **discuss** the physics behind the choice of a trial wavefunction of the form

$$\begin{aligned} \phi(x) &= c_1\, \psi_1(x) + c_3\, \psi_3(x) \\ &= c_1 \sqrt{\frac{2}{a}}\, \sin\left(\frac{\pi x}{a}\right) + c_3 \sqrt{\frac{2}{a}}\, \sin\left(\frac{3\pi x}{a}\right) \end{aligned} \tag{1}$$

for estimating the ground state energy. Here, $\psi_1(x)$ and $\psi_3(x)$ are obviously the ground and second excited states of an infinite flat-bottomed well. **Why** do we **skip** $\psi_2(x)$ in the trial wavefunction? What if we have include such a term in Eq. (1)?

Taking c_1 and c_2 to be real parameters (the assumption is OK here), **apply the variational method** to estimate the ground state energy of a V-bottomed infinite well. [TA: Please do the math as plainly (thus as easier to follow) as possible.]

[Remarks: This SQ serves to illustrate that a trial wavefunction of the form of Eq. (1) leads to a matrix of the size of the linearly combined functions. If you want to do better by including one more $\psi_n(x)$, which one will you choose? Another purpose here is to stress that choosing a good trial wavefunction needs a good physical sense. Here, we make use of the knowledge of the symmetry of the ground state wavefunction (when $U(x)$ is symmetrical) and then decorate $\psi_1(x)$ by adding in a weighted portion of $\psi_3(x)$ so as to make sure that resulting trial wavefunction is symmetric about $x = a/2$. Here is an interesting twist of the variational method. What if we started with a trial wavefunction that invokes $\psi_2(x)$ and $\psi_4(x)$ only? What would the resulting best value represent?]

SQ5 *Infinite well with V-shaped bottom - Perturbation Theory*

Non-degenerate Perturbation Theory - Summary of Key Results – Given $\hat{H} = \hat{H}_0 + \hat{H}'$, but the TISE problem $\hat{H}\psi = E\psi$ does not allow analytic solutions. Fortunately, we know the solutions to the unperturbed problem $\hat{H}_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$. Thus, the whole sets of

$\{\psi_n^{(0)}\}$ and $\{E_n^{(0)}\}$ are known. Here, $\hat{H}'$ is the perturbation term. The most important result of non-degenerate perturbation theory is an approximate expression for the n-th eigenvalue of the problem

$$H\psi_n = E_n\psi_n \tag{2}$$

up to the second order given by

$$\begin{aligned} E_n &\approx E_n^{(0)} + \langle\psi_n^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle + \sum_{i\neq n} \frac{|\langle\psi_i^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_i^{(0)}} \\ &= E_n^{(0)} + \int \psi_n^{*(0)}\hat{H}'\psi_n^{(0)} d\tau + \sum_{i\neq n} \frac{|\int \psi_i^{*(0)}\hat{H}'\psi_n^{(0)} d\tau|^2}{E_n^{(0)} - E_i^{(0)}} \end{aligned} \tag{3}$$

The first-order correction to the n-th eigenstate is

$$\psi_n \approx \psi_n^{(0)} + \sum_{i\neq n} \frac{\int \psi_i^{*(0)}\hat{H}'\psi_n^{(0)} d\tau}{E_n^{(0)} - E_i^{(0)}}\ \psi_i^{(0)} \tag{4}$$

We derived these formulas in class. More important than the derivation, you should **understand the meaning of the symbols** in Eqs.(3) and (4) and **how to apply** the formulas.

Applying the results requires two levels of maturity in physics and mathematics. (a) We need to set up the problem (i.e., identify $\hat{H}_0$ and $\hat{H}'$) and then write down the integrals explicitly in Eq. (3) and Eq. (4). (b) We need to be able to do the integrals. For (a), after identifying $\hat{H}_0$, we need the exact solutions to TISE of $\hat{H}_0$. We know only a few of them, including the infinite well, harmonic oscillator (1D,2D,3D), rigid rotors, and hydrogen atom. These are covered in QM I. For (b), we need to do many integrals involving sine and cosine functions (infinite well), Hermite polynomials (harmonic oscillator), $e^{im\phi}$ and $Y_{lm}(\theta,\phi)$ (rotors), and $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$ (hydrogen atom). Some integrals are hard to do. But you shouldn't let the mathematics ruin your appreciation to the usefulness of perturbation theory.

TAs: Start Here. Consider the same infinite well with a V-shaped bottom as in SQ4.

(a) **Apply the perturbation theory** to estimate the ground state energy. [Hint: You may start with a few unperturbed states closer in energy to the unperturbed ground state, and then see if a general form of the integrals can be done. In any case, terms that are high up in energy from the unperturbed states will not contribute much. This hint also applies to part (b).] Hence, **make connection** to the variational approach in SQ4 and **compare the answers**.

(b) **Apply the perturbation theory** to estimate the ground state wavefunction. [Hint: In particular, you may work on a few most important terms. Then **discuss the result** in light of the trial wavefunction used in SQ4.] Further **discuss** (don't need to do the mathematics) that in SQ4, there are actually two answers for the energy and hence two sets of (c_1, c_2) for the two solutions. Therefore, there is another wavefunction that came out from the variational calculation. Does that wavefunction mean anything? How is it related to the perturbation theory?]

(c) To illustrate that the perturbation theory is NOT restricted to studying the ground state energy, as it is the case for the variational method, **pick another state** and **estimate its energy** by perturbation theory. [Again, it is alright to work out a few of the most important terms instead of a general expression.]