PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 3 EXERCISE CLASSES (21-25 January 2019)

What are Sample Questions (SQs)? TA will discuss the **SAMPLE QUESTIONS** in exercise classes. The Sample Questions are designed to serve several purposes. They either review what you have learnt in previous courses, supplement our discussions in lectures, or closely related to the questions in an upcoming Problem Set. You should attend one exercise class session per week. You are encouraged to think about (or work out) the sample questions before attending exercise class and ask the TA questions.

Students: The SQs are related to the time-independent perturbation theory. Read the summary first.

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, the unperturbed problem $\hat{H}_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$ is solvable and 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

$$H\psi_n = E_n\psi_n \tag{1}$$

up to the second order given by

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

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

$$\psi_n \approx \psi_n^{(0)} + \sum_{i\neq n}\frac{\int \psi_i^{*(0)}\hat{H}'\psi_n^{(0)}d\tau}{E_n^{(0)} - E_i^{(0)}}\,\psi_i^{(0)} \tag{3}$$

We derived these formulas in class. More important than the derivation, you should **understand the meaning of the symbols** in Eqs.(2) and (3) 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. (2) and Eq. (3). (b) We need 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 (refer to PHYS3021 notes). 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. There are integral tables that are helpful. But you shouldn't let the mathematics ruin your appreciation to the usefulness of perturbation theory.

The SQs here apply the perturbation results.
SQ6: 1st and 2nd order perturbation theory applied to an exactly solvable problem (harmonic oscillator)
SQ7: Shifts in hydrogen atom energies due to relativistic correction to kinetic energy - 1st order perturbation theory

SQ6 *Harmonic Oscillator – an exactly solvable problem treated by 1st and 2nd order perturbation theory*

Consider an 1D harmonic oscillator in which the potential energy function is $U(x) = \frac{1}{2}k(1+\epsilon)x^2$, where ϵ is meant to be $\epsilon \ll 1$. Referring to harmonic oscillator quantum physics, **write down** the exact eigenvalues of the problem.

Knowing the exact results, we actually don't need the perturbation theory. However, it will be interesting to see how good (or bad) perturbation theory works.

(a) The exact eigenvalues can be **expanded** into a power series in ϵ, i.e., considering $\epsilon \ll 1$. **Do it.**

(b) Now we take the unperturbed problem to be

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 \tag{4}$$

and the perturbed problem as

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}k(1+\epsilon)x^2 = \hat{H}_0 + \hat{H}' \tag{5}$$

Identify the perturbation term $\hat{H}'$ and **obtain** the 1st order perturbation in the energy for **all states**.

(c) Next consider only the **ground state**. **Find** the 2nd order perturbation to the ground state energy. Hence, **write down** the ground state energy including 0th, 1st, and 2nd order terms.

(d) **Compare** the perturbation result with the exact result in part (a) to the same order.

(e) **(Optional for TA, just for fun) How about** the 1st order correction to the ground state wavefunction?

[Remark: This is Problem 6.2 and Problem 6.4(b) in Griffiths' *Introduction to Quantum Mechanics.*]

SQ7 *Non-degenerate perturbation theory: 1st order correction to hydrogen atom energies due to relativistic correction to the kinetic energy*

Background – Schrödinger solved the hydrogen atom problem in 1926 and gave the famous $-R_\infty/n^2$ or $-13.6/n^2$ (in eV) energies as observed in hydrogen spectrum (Lyman, Balmer,... series). Despite the success, the kinetic energy term in the Hamiltonian in the Schrödinger Equation used the Newtonian form $T_{Newton} = p^2/2m$. Einstein published his papers on special relativity in 1905. Naturally, soon after Schrödinger's work, people started to consider the **relativistic corrections** to Schrödinger's solutions to the hydrogen atom. This SQ deals with one such correction. The result is important in that (i) the correction is tiny, and (ii) the small correction is characterized by the **fine structure constant squared**, or α^2.

(a) Is it really necessary to consider relativistic effects? **Think like a physicist!** Relativistic effect becomes important when a speed becomes not too small compared with the speed of light. Taking the Bohr's model of a hydrogen atom, the electron is orbiting around the nucleus. **Find** the ratio of speed v_1 of the electron in the $n = 1$ orbit (ground state in QM language) to the speed of light c. This ratio v_1/c turns out to be a very important number in physics - so important that it is given a name called the **fine structure constant**. Its value is $< 1\%$.

(b) To use perturbation theory, we need to identify $\hat{H}'$. Relativistically, the kinetic energy of a free particle can be found by the difference between the total energy and the rest energy. Thus, we start with the relativistic expression

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2 \tag{6}$$

and expand it in powers of the dimensionless parameter (p/mc) which is assumed to be small, **show** that there is a correction term to $p^2/2m$ given by

$$T \approx \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} \ . \tag{7}$$

(c) Using the kinetic energy term into the Schrödinger Equation of a hydrogen atom, we have

$$\hat{H} = \left[\frac{\hat{p}^2}{2m} + U(r)\right] - \frac{\hat{p}^4}{8m^3c^2} = \hat{H}_0 - \frac{\hat{p}^4}{8m^3c^2} \tag{8}$$

where $U(r) = -e^2/(4\pi\epsilon_0 r) = -e^2/(\kappa_0 r)$ is the Coulomb potential energy.

The unperturbed $\hat{H}_0$ problem is analytically solvable. The energy eigenvalues are the famous $E_n^{(0)} \sim -13.6/n^2$ in eV and the eigenstates $\psi^{(0)}_{n\ell m_\ell}(r,\theta,\phi)$'s are also known.

Apply 1st order perturbation theory (don't do the integrals at this point) to write down the correction to the hydrogen atom energies.

(d) Finally, **evaluate (or simply give the results of)** the integrals and hence **give an explicit expression** of the first order shift in energy due to $\hat{H}'$. It is important to **point out how small** the correction term is, in comparison to the unperturbed energy.

TA: (i) **Show** that the 1st order perturbation in energy is related to the expectation value of $\langle(\hat{H}_0 - U(r))^2\rangle$ with respect to the unperturbed hydrogen atom states. (ii) Hence, **show** that it amounts to evaluating the value of expectation values $\langle 1/r\rangle$ and $\langle 1/r^2\rangle$ for different $\psi^{(0)}_{n\ell m_\ell}(r,\theta,\phi)$. (iii) These are standard integrals of hydrogen atom physics. I looked them up from books and found that

$$\langle\frac{1}{r}\rangle_{n\ell m_\ell} = \frac{1}{n^2 a_0} \ \ , \ \ \langle\frac{1}{r^2}\rangle_{n\ell m_\ell} = \frac{1}{(\ell+\frac{1}{2})n^3a_0^2} \tag{9}$$

where the subscript (n, ℓ, m_ℓ) labels the state in which the expectation value is evaluated and $a_0 = \kappa_0\hbar^2/(me^2)$ is the Bohr radius.

Use these results to **obtain** the first order correction $E^{(1)}_{n\ell m_\ell}$. Most importantly, **show** that the magnitude of the correction is governed the **fine structure constant squared** α^2, which is about $(1/137)^2$ of the unperturbed energy $E_n^{(0)}$. This is tiny. **Tough small, spectroscopy (atomic spectrum) is sensitive enough that we need to consider such corrections.**

[For TA: It is more important to point out how those integrals emerge from the perturbation formula and what those integrals are. You need not carrying out the expectation value calculations in Eq. (9), unless you want to show off your technique.]

[Further remark: Those of you with sharp eyes may start worrying why we could apply 1st order (non-degenerate) result here, as hydrogen energy levels carry degeneracy in general, e.g. there are several $(n = 2)$ states with energy $-13.6/4$ eV. This is a tricky question that can be explained by even sharper eyes on the form of the perturbation $\hat{H}'$. For the moment, don't worry about it as the reason is a bit technical for some students. Another remark is that there will be another relativistic correction term related to the spin of the electron that we have not considered. Recall that spin is intrinsically a relativistic effect.]