PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 2 EXERCISE CLASSES (13-16 January 2020)

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 closed related to the questions in an upcoming Problem. You are encouraged to think about (or work out) the sample questions before attending exercise class and ask the TA questions.

SQ4: The relativistic correction term for hydrogen atom
SQ5: Most probable distance of finding the electron in 3d hydrogen states
SQ6: Reduced mass μ emerges when relative separation is introduced

SQ4 *The relativistic correction term for hydrogen atom*

Background – This is a follow-up of SQ2 in Week 1. Schrödinger solved the hydrogen atom problem in 1926 with $U(r) \sim -1/r$ (Coulomb) and found the famous $-13.6/n^2$ eV energies observed in hydrogen spectrum. In SQ2, we saw that these numbers are slightly off the high-precision spectroscopic data. They are 99.9% right, but a bit off. In SQ2, we tried the correction of replacing the electron mass by the reduced mass, i.e., taking into account the finite mass of the nucleus. Another possible correction is that the kinetic energy term in the Hamiltonian in the Schrödinger Equation is Newtonian $T_{Newton} = p^2/2m$. Einstein published his famous papers on special relativity in 1905. Naturally, soon after Schrödinger's work, people started to consider the relativistic corrections to the Schrödinger's solutions. This SQ deals with writing down one such correction term, i.e., $T \approx p^2/2m + (correction)$.

(a) Meeting the **fine structure constant**. Do we really need to consider relativistic effects? TA: Bohr's picture of a hydrogen atom has the the electron orbiting around the nucleus. Take the results from Bohr's model, **find** the ratio of the speed v_1 of the electron in the lowest orbit ($n = 1$ orbit or what is called the ground state in QM) to the speed of light c. The ratio v_1/c turns out to be a combination of fundamental constants that is very important in physics. This is called the fine structure constant α and it has a value of $\approx 1/137$.

(b) Some would like to interpret α differently. One is related to the hydrogen's lowest energy and the electron's rest energy. TA: Try this and see how it come out to be related to α.

(c) Next, we want to write down a correction term to $T = p^2/2m$. Starting with the relativistic expression

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2 \tag{1}$$

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

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

Important remarks: Taking into account of this relativistic correction, we need to handle the revised Hamiltonian H for a hydrogen atom of the form:

$$H = \underbrace{\frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}}_{\text{solved exactly}} \overbrace{\qquad - \frac{p^4}{8m^3c^2}}^{\text{correction to handle}} = H_0 + H' \tag{3}$$

This is a standard situation in quantum mechanics (physics in general). We have a problem that we know how to solve if we ignore some small correction term(s). To handle the problem of H, either we take H as a new problem and solve it from scratch again **or** we take the known solutions of H_0 and use them to do approximations and get at meaningful but approximated results of the H problem. The latter involves **perturbation theory**, a topic that we will discuss in our course later.

SQ5 *Most probable distance of finding the electron in 3d hydrogen states*

Background: While Born said that $|\psi_{n,\ell,m_\ell}(r,\theta,\phi)|^2$ is the probability density, i.e., $|\psi_{n,\ell,m_\ell}(r,\theta,\phi)|^2 d^3r$ is the probability of finding the electron within a volume element d^3r at the location specified by $\mathbf{r} = (r,\theta,\phi)$, it is hard to visualize it. It is simpler and more useful to ignore (or averaged away) the angular information. We then obtain the radial probability distribution function $P(r)$, with $P(r)dr$ being the probability of finding the electron at a distance r to $r+dr$ away from the origin, **regardless** of the direction (regardless of the angles). $P(r)$ is an easier function to visualize as it depends on r only. For a given $\psi_{n,\ell,m_\ell}(r,\theta,\phi)$, the corresponding $P(r) = r^2[R_{n\ell}(r)]^2$. Note that the factor r^2 increases with r, while $[R_{n\ell}(r)]^2$ drops with r at large r. Therefore, there is a peak in $P(r)$ that gives the most probable distance of finding the electron. In the Bohr model (1913), he said that the electron in the n-th orbit is at a distance n^2a_0 away.

As shown in class notes, one can readily construct the radial probability distribution function for the 1s state of a hydrogen atom as $P(r) = r^2[R_{1s}(r)]^2$ and show that the most probable distance is at the Bohr radius a_0.

TA: Look up the $3d$ states with radial function $R_{32}(r)$. **Sketch** $R_{32}(r)$. **Construct** $P_{32}(r)$ (the 3d state), **sketch** $P_{32}(r)$, and **find** the most probable distance of finding the electron in the $3d$ states. Comment on the similarity and difference between QM result here and Bohr's prediction.

SQ6 *Reduced Mass μ emerges when the* **relative separation** *is introduced - Relevant to the Hydrogen atom and Diatomic Molecules*

Background: In SQ2, TA showed that using the reduced mass μ instead of the electron mass gives the ionization energy of a hydrogen atom that is in better agreement with experimental data. This SQ reminds you of how the reduced mass comes up. In physics, including quantum physics, we often deal with a system of two or more particles. Three-body problems are typically not exactly solvable (both in classical and quantum physics). However, two-body problems can be dealt with readily. There are many examples in physics – planets orbiting around the Sun is a difficult problem, but only the Earth orbiting around the Sun (and ignoring the other planets) is easier. We solved the hydrogen atom problem by assuming the proton being fixed at the origin. In principle, the hydrogen atom problem is a two-body problem with a proton and an electron. Similarly, replacing the proton by an Atom A and the electron by another atom B (doesn't mean Boron here), we have an AB molecule. Thus, a diatomic molecule, being viewed in the simplest viewpoint of two balls connected by a spring (or a stick), is also a two-body system. Here, the idea of reducing a two-body problem to a one-body problem plus a centre of mass problem is reviewed. The result is important in handling all many-body systems.

A simple classical mechanical model of a diatomic molecule (molecule consisting of two atoms) is that of two balls of masses m_1 and m_2 connected by a spring with a natural length r_0 and spring constant K. To make life easier, let the molecule lives only on the x-axis. Instantaneously, the coordinates of m_1 and m_2 are x_1 and x_2, respectively.

TA: **Show that** the two equations of motion are:

$$m_1 \frac{d^2x_1}{dt^2} = K(x_2 - x_1 - r_0) \tag{4}$$

$$m_2 \frac{d^2 x_2}{dt^2} \quad = \quad -K(x_2 - x_1 - r_0) \tag{5}$$

By manipulating these equations, **demonstrate clearly** that the equation of motion for the Center of Mass (CM) corresponds to the CM moving uniformly in time with a constant momentum, **obtain** the equation of motion for the **relative coordinate** $x = x_2 - x_1$, and **illustrate** that the standard harmonic oscillator equation

$$\mu \frac{d^2 r}{dt^2} + Kr = 0 \tag{6}$$

emerges, where μ is the reduced mass. **Show** clearly what r is about. **Give the expressions** for the characteristic angular frequency ω, frequency ν and wavenumber $\overline{\nu}$.

Remarks: We could have allowed rotations as well (not restricted to be on a line). The picture so emerges is similar. It is related to the 2D or 3D rotor problem in QM. It is also interesting to start with the Hamiltonian $H(x_1, p_1, x_2, p_2)$ for the problem given in Eqs.(4) and (5), and work out the separation into CM and relative coordinate problems at the Hamiltonian level. [TA: don't need to work this out.]