PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 2 EXERCISE CLASSES (18-22 January 2021)

TA will discuss the **SAMPLE QUESTIONS** in exercise classes every week. The Sample Questions are designed to serve several purposes. They review what you have learnt in previous courses that are needed in AQM, tell a physics story, enrich discussions in lectures, and some are *closed related* to the questions in an upcoming Problem Set. They also served as worked examples. Students should be able to do the homework problems independently after attending the exercise class. **You should attend one exercise class session.** You are encouraged to work out (or at least think about) the sample questions before attending exercise class and ask the TA questions. Over the semester, the TAs welcome your questions.

SQ1 - Precision spectroscopy is key to developments in quantum mechanics
SQ2 - A relativistic correction term in the kinetic energy term of a Hamiltonian
SQ3 - Two-body problem reduces to CM problem plus relative motion problem

SQ1 *Physics is an experimental science – Atomic spectrum or spectroscopy is key to quantum physics developments*

Background - Physics is an **experimental science** and its developments are often driven by experimental observations and measurements of increasing precision. Atomic and moelcular spectroscopy (“light” (EM waves or photons) being absorbed or emitted) had led the developments in quantum mechanics. The Balmer series of hydrogen spectrum was known in the 19th century. Rydberg played with the known data at the time including Balmer and the other series and came up with a description that the energy correspondence of the spectral lines are given by differences of terms of the form $\sim -\frac{1}{n^2}$. Bohr took it as a statement of the conservation of energy and then came up with the Bohr’s model in 1913. Einstein put together Bohr’s model and Planck’s black-body radiation formula and came up with the idea of stimulated emission and thus laser (to be discussed in the course). Heisenberg wanted to explain the observed intensities of the spectral lines and founded his matrix version of quantum mechanics. Schrödinger wanted to replace the ad hoc rule that Bohr imposed (quantizing the orbital angular momentum to $n\hbar$) by the more natural boundary conditions that matter wave functions ought to be properly behave (continuous, single-valued, can be normalized, etc.) and came up with the time-independent Schrödinger equation in 1926. As spectrometer became more precise, what regarded as one spectral line in the past often came up to be two closely-spaced lines – **fine structure**. Highly accurate spectroscopy in the 20th century had further revealed the hyper-fine structure, and the Lamb shift that eventually led to the development of quantum electrodynamics (QED) - the first successful quantum field theory. All these are only about the hydrogen atom. Many more useful applications were developed when precision spectroscopy was applied to other atoms and molecules. The first thing to realize is – **we should have great respect towards good experimentalists!** The 2014 Nobel Physics Prize was awarded to scientists who succeeded in getting blue lights (blue laser). Two Nobel Chemistry Prizes in the past 4 years (2014 and 2017) were also awarded for clever manipulation of light in high-resolution microscopy.

(a) The simplest version of the Bohr model or solving the Schrödinger equation for a hydrogen atom with the proton fixed at the origin gives the energies of a hydrogen atom as

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2}\frac{1}{n^2} \qquad n = 1, 2, \ldots \tag{1}$$

or you might have seen this in terms of $\hbar$ instead of h. Here, let's say m is the mass of an electron. First, **we learn to speak the spectroscopists' language**. **Show that** the **wave number** $\overline{\nu}$ that has the units of cm^{-1} is given by

$$\overline{\nu} = \frac{me^4}{8\epsilon^2 ch^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \ . \tag{2}$$

Evaluate R_H (the Rydberg constant) in units of cm^{-1}. The value turns out to be 109,7xx cm^{-1}. The time was 1913 and 1926. The Rydberg constant R_H is sometimes written as R_∞.

(b) Precision spectroscopy gives us many data. The National Institute of Standards and Technology (NIST) of USA has measured, updated, and published data for various atomic transitions to very high accuracy. See the site http://www.nist.gov/pml/data/handbook/index2.cfm (Click here on soft copy to link to site). From the site, select "element name" and then "hydrogen" and you will see some atomic data. Then select "energy levels", you will see accurate data of the hydrogen energy levels as measured as absorption and emission. (Click here on soft copy to link to page) **Collect what** R_H **is** from the data. The value turns out to be 109,6xx cm^{-1}. The tables there also give you the wavelengths of the stronger spectral lines.

(c) For ordinary purposes (e.g. learning QM), the difference is tiny and not something to be bothered with. But for serious works, the difference is indicative. There are many reasons for the difference. In PHYS 3021 (2020-21 Term 1) notes, you learned that the Hydrogen Atom (H-atom) problem is actually a two-body problem consisting of the nucleus and the electron. After separating out the center-of-mass motion (moves freely as there is no external force), the electron picks up the **reduced mass** μ instead of m. **Evaluate** R_H again using μ instead of m and see if the value is closer to data.

(d) **Motivating further discussions on the H-atom in PHYS 3022**. In QM I, we solved for the H-atom wavefunctions $\psi_{n\ell m}$ carrying three labels (three quantum numbers, ignoring spin here), but the energy E_n depends only on n. Let's check with real data and see if it is really the case.

TA: Use the energy levels table in NIST website to **illustrate** that (i) the previous observation of the Lyman, Balmer, and other series is actually quite correct; and (ii) if we care about the fine details, there are actually some very tiny splitting of, say, the $n = 2$ levels into very closely-spaced levels, and similarly for the higher n levels. In PHYS3022, we will explain the reasons behind **some (but not all)** of the splitting, e.g. due to spin-orbit coupling, and we need some approximation methods as well. However, some remaining discrepancy requires QED for its explanation which is beyond the scope of our course.

Key points: There are established (regularly updated) tables of spectroscopic data for all atoms. This is a serious business. The reduced mass does have some effects.

SQ2 *A relativistic correction to the kinetic energy term in the Hamiltonian*

We just saw in SQ1 that high-precision H-atom data indicate there are more to be considered. In the standard Hamiltonian, $\hat{p}^2/2m$ comes from the leading term in expanding $E = \sqrt{m^2c^4 + c^2p^2}$. We discussed in class that we always encounter the form

$$\hat{H} = \hat{H}_0 + \hat{H}' \tag{3}$$

where $\hat{H}_0$ is exactly solvable (e.g. H-atom in QM I) and $\hat{H}'$ represents a small correction term to the Hamiltonian. Let's say we want to get one correction term for relativistic effect to $\hat{p}^2/2m$. **Find an expression** for $\hat{H}'$. The remaining question is whether there are some ways to handle such a correction term (a topic to discuss in our course).

To further justify that we are not looking for things to do, **take the speed** of an electron in the $n = 1$ orbit (Bohr model, say) and **illustrate** that v/c is not entirely negligible.

SQ3 *Classical Mechanics: The Reduced Mass μ emerges when the Relative Separation is introduced - Vibrations of Diatomic Molecules.*

We used the reduced mass μ in SQ1. Here is a reminder of what it is. A simple classical mechanical model of diatomic molecule 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. For simplicity, let the molecule be on the x-axis. Instantaneously, the coordinates of m_1 and m_2 are x_1 and x_2, respectively. **Show that** the two equations of motion are:

$$\begin{aligned} m_1 \frac{d^2 x_1}{dt^2} &= k(x_2 - x_1 - r_0) \\ m_2 \frac{d^2 x_2}{dt^2} &= -k(x_2 - x_1 - r_0) \end{aligned}$$

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

$$\mu \frac{d^2 r}{dt^2} + kr = 0$$

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

[Remark: The result here will be used in discussing the vibrational motion of diatomic molecules. As a result, we have specific vibriational molecular spectrum for every molecule.]