

PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 1 EXERCISE CLASSES (7-11 January 2019)

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, you are welcome to go to the TAs for help.

SQ1 - Classical Mechanics: Two-body problem reduces to CM (center-of-mass) problem plus relative motion problem

SQ2 - Two-problem quantum mechanics problem also reduces to CM problem and relative motion problem [a question in PHYS3021 mid-term exam]

SQ3 - Precision spectroscopy is key to developments in quantum mechanics

SQ1 *Classical Mechanics: The Reduced Mass μ emerges when the **relative separation** is introduced - Relevant to the Hydrogen atom, Diatomic Molecules, and more*

Background: Besides the simplest problems such as particle-in-a-box or harmonic oscillator, more often than not we have to deal with a system of two or more particles. Three-body problems, for example, are typically not exactly solvable (both in classical and quantum physics). However, two-body problems can be handled readily. There are many examples in physics – planets orbiting around the Sun is a difficult model, but only the Earth orbiting around the Sun (and ignore all the other planets) is easier. We solved the hydrogen atom problem last Term 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 (not meaning Boron), we have an AB molecule. Thus, a diatomic molecule, the simplest of which is H_2 , is also a two-body system. We mentioned last Term that in QM, we focus on the relative motion (thus assuming the nucleus to be fixed at the origin) and the hydrogen atom problem becomes a one-body (one electron) problem with the mass of the electron replaced by the reduced mass. Here, we review the idea of reducing a two-body problem to a one-body problem plus a centre of mass problem. The result is important in handling all many-body systems. The results are useful in the treatment of a gas of diatomic molecules (the N_2 and O_2 in the classroom), as will be discussed in statistical mechanics.

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 . For simplicity, let the molecule be on the x -axis, and motions can only be along the x -direction. Instantaneously, the coordinates of m_1 and m_2 are x_1 and x_2 , respectively. Using Newton's law, **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 the equations, **demonstrate clearly** that the equation of motion for the Center of Mass (CM) implies that the CM moves uniformly in time with a constant momentum

(thus moving freely). **Obtain** the equation of motion for the **relative coordinate** $x = x_2 - x_1$, and **illustrate** that the standard harmonic oscillator equation

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

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 $\bar{\nu}$.

Remark: Technically, the freely moving center-of-mass motion is the **translation motion**. The relative motion corresponds to the vibration of the two masses. We could have allowed rotations as well (not restricted to be on a line). The picture that would emerge is similar. [TA: don't need to work this out.]

SQ2 *Reduced Mass μ , transformation, and separation of variables*

The results in SQ1 also work in Quantum mechanics. Consider a two-particle system in 1D. A simple case is that the mass m of the two particles are the same (identical mass). The two-particle interaction can be represented by a potential energy function $U(x_1 - x_2)$, i.e., depends only on the combination $(x_1 - x_2)$ of the positions x_1 and x_2 of the two particles. An example is that of two particles connected by a spring (as in a diatomic molecule) as in SQ1. The time-independent Schrödinger equation (TISE) is

$$\underbrace{\left\{ \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} \right] + U(x_1 - x_2) \right\}}_{\hat{H}} \psi(x_1, x_2) = E \psi(x_1, x_2), \quad (1)$$

where the Hamiltonian \hat{H} is marked.

- (a) We want to do a transformation from the variables x_1 and x_2 to two new variables

$$X \equiv \frac{mx_1 + mx_2}{2m} = \frac{x_1 + x_2}{2}, \quad x \equiv x_1 - x_2. \quad (2)$$

Obviously, X is the center of mass coordinate and x is the relative coordinate. **Carry out the transformation** of the second derivatives and **show that** the Hamiltonian \hat{H} becomes

$$\hat{H} = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} + U(x), \quad (3)$$

and **identify** what M and μ are in terms of m .

- (b) Hence, writing $\psi = \Phi(X) \cdot \phi(x)$, apply the **method of separation of variables** to TISE to **obtain** two equations, one for $\Phi(X)$ and another for $\phi(x)$. Inspect the equation for $\Phi(X)$ and **comment** on its solutions (freely moving?).

This is a question in PHYS3021 mid-term exam in Nov 2018.

SQ3 *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 molecular spectroscopy (seeing “light” (EM waves or photons) being absorbed or emitted) had led to key 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 show great respect towards good experimentalists!** 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

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} \quad n = 1, 2, \dots \quad (4)$$

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

$$\bar{\nu} = \frac{me^4}{8\epsilon^2 ch^3} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right). \quad (5)$$

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.

- (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. The NIST site <http://www.nist.gov/pml/data/handbook/index2.cfm> (Click here on soft copy to link to site) has many data. **Unfortunately due to the partial closing down of the US Government, the site is closed temporarily**. When it is working, you could 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) **TA: Show the data for R_H collected earlier**.
- (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. Based on SQ1 and SQ2, the simplest correction is to use the reduced mass μ instead of the electron mass m , because hydrogen atom is a two-body system. **Evaluate** R_H again using μ instead of m and see if the value is closer to data.

- (d) In QM I (PHYS3021), we solved the hydrogen atom Schrödinger equation exactly. Although the wavefunctions $\psi_{n\ell m}$ carry three labels (three quantum numbers), the energy E_n depends only on n . Let's see if it is really the case.

TA: Show the highly accurate measured energy levels table of hydrogen atom to **illustrate** that (i) the previous observation of the Lyman, Balmer, and other series is actually rather 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** of these splitting in our course, e.g. due to spin-orbit coupling, and we need some approximation methods as well. However, some remaining discrepancy is hard to explain at our level.

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