PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 12 EXERCISE CLASSES (8 - 12 April 2019)

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 Set. 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 think about (or work out) the sample questions before attending exercise class and ask the TA questions.

Progress: In Week 11, we discussed molecular spectrum, including rotation spectrum (in microwave range) and vibrational-rotational spectrum (often in IR range). The former arises from transitions between rotational levels (different ℓ in the same vibrational level (usually $n = 0$) and the latter arises from transitions between rotational levels belonging to different ($\Delta n = \pm 1$) vibrational levels. It turns out that our background in Quantum Mechanics I on harmonic oscillator handles the vibrational motions of nuclei and on 3D rigid rotor handles the rotational motions. And the story goes, the electronic part of the molecular problem (bonding) gives a curve $E_{el}(R)$ that shows a preferred bond length at $R = R_0$ such that $E_{el}(R_0)$ is a minimum. Near the minimum, the profile $E_{el}(R)$ is parabola (harmonic oscillator) and the curvature gives the force constant K of the bond characterizing the harmonic oscillator in the **radial direction**. Recall that we have a 3D problem. The radial direction harmonic oscillator corresponds to a 3D **spherically symmetrical potential** and the rotational motion (assuming a fixed R_0 separation between the two nuclei) is readily handled by the angular parts. For molecular states in the lowest electronic state, the possible energies are

$$E^{(molecule)} = E_{el}(R_0) + (n + \frac{1}{2})\hbar\omega + \frac{\ell(\ell+1)\hbar^2}{2I} \qquad (1)$$

where the second term gives the vibrational levels with $\omega = \sqrt{K/\mu}$ being the characteristic angular frequency of the bond (spring) with μ the reduced mass of the two atoms (diatomic molecule), and the third term gives the rotational levels with $I \approx \mu R_0^2$ being the moment of inertia related to the bond length. It is important to realize that the energy scales are very different. The difference of electronic terms (first term to the next curve of $E_{el}(R)$) is of the order several eV to 10 eV (visible to UV). The vibrational term (second term) is 1% of the first term and thus of the order 0.1 eV (IR). The rotational term (third term) is another 1%. Thus, it is of the order of 10^{-4} to 10^{-3} eV (microwave to far IR). Finally, transitions between the allowed molecular energy levels give molecular spectrum. There are selection rules.

We also started to discuss travelling waves in quantum mechanics and their normalization. We will then discuss the probability current density and tunnelling. We motivated the necessity of tunnelling through α-particle decays in nuclei. There are many phenomena and applications based on tunnelling.

SQ27 - Characteristic frequency for vibrations and Rotational Spectrum
SQ28 - Probability Current Density

SQ27 **Rotational Spectrum**

The characteristic frequency ω (in Eq.(1)) for vibrational levels is typically in the IR range. Spectroscopists sometimes quote the numbers in cm^{-1}. For $H^{35}Cl$, the value is 2990.94 cm^{-1}.

(a) **Argue** that almost all the molecules are in the $n = 0$ vibrational level at room temperature. [Here, a bit of statistical physics is needed. The probability that a state of energy ϵ is occupied is proportional to $\exp(-\epsilon/kT)$ at a temperature T (thermal equilibrium).]

(b) **Calculate** the force constant K from the characteristic frequency.

(c) It is easier to see that microwave cannot excite molecules from $n = 0$ to $n = 1$ vibrational level. However, something does happen when microwave is incident upon the molecules. This is related to transitions between rotational levels associated with the $n = 0$ vibrational level. These transitions are related to the third term in Eq. (1). The selection rule is $\Delta\ell = \pm 1$. Thus, molecules at $\ell = 0$ can absorb a photon to go to $\ell = 1$, and those in $\ell = 1$ to $\ell = 2$, and so on, as far as absorption is concerned. **Show** that there will be a series of lines with equal spacing $\hbar^2/I$. In $H^{35}Cl$, the microwave spectrum of $H^{35}Cl$ consists of equally spaced lines of separation of 6.350×10^{11} Hz. **Estimate** the bond length R_0 of $H^{35}Cl$.

[Remark: Putting together the information, one can anticipate how the vibrational-rotational spectrum of $H^{35}Cl$ (needs higher resolution) looks like. The spectrum is shown in class notes.]

SQ28 Probability Current Density

The probability current density $\vec{J}$ in quantum mechanics is given in general by

$$\vec{J} = \frac{\hbar}{2mi}\left(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*\right) \tag{2}$$

The first thing to note is that $\vec{J}$ is a vector.

Of course, the expression becomes simpler (but very often mistakes are still made) in 1D problems. It is important to recall that $\nabla \to \hat{i}\frac{\partial}{\partial x}$ in 1D.

(a) Let's start with $\Psi_{right}(x,t) = A\, e^{ikx - i\omega t}$. **Obtain** $\vec{J}_{right}$.

(b) **Obtain** $\vec{J}_{left}$ for $\Psi_{left}(x,t) = B\, e^{-ikx - i\omega t}$.

(c) Consider $\Psi(x,t) = A\, e^{ikx - i\omega t} + B\, e^{-ikx - i\omega t}$. **Obtain** $\vec{J}$. **Relate** the answer to $\vec{J}_{right}$ and $\vec{J}_{left}$.

(d) For the simplified case of $\Psi(x,t) = e^{ikx - i\omega t} + r\, e^{-ikx - i\omega t}$, **what is** $\vec{J}$?

(e) For the further simplified case form of $\psi(x) = e^{ikx} + r\, e^{-ikx}$, **what is** $\vec{J}$?

(f) Consider $\Psi_{\vec{k}}(\vec{x},t) = Ae^{i\vec{k}\cdot\vec{x} - i\omega t}$, where $\vec{k} = k_x\hat{i} + k_y\hat{j} + k_z\hat{k}$ or (k_x, k_y, k_z) and $\vec{x} = x\hat{i} + y\hat{j} + z\hat{k}$. Apply Eq. (2) to **obtain** $\vec{J}_{\vec{k}}$. Note that $\vec{k}$ is the wave vector giving the direction of propagation.

(g) Hence, **obtain** $\vec{J}$ for $\Psi_{\pm\vec{k}}(\vec{x},t) = A\, e^{i\vec{k}\cdot\vec{x} - i\omega t} + B\, e^{-i\vec{k}\cdot\vec{x} - i\omega t}$.