PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 5 EXERCISE CLASSES (8 - 10 Feb 2021)

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.

SQ8: The "minimal substitution rule" in generating the $-\vec{\mu}_L \cdot \vec{B}$ term and more
SQ9: The rule of adding two angular momenta gives the right number of states
SQ10: Effect of a weak static electric field on $n = 2$ hydrogen atom states

SQ8 *The "minimal substitution rule" in generating the* $-\vec{\mu}_L \cdot \vec{B}$ *term in Hamiltonian and more*

Background: When an **external magnetic field** is applied to an atom, a magnetic interaction energy coming from the interaction between the magnetic dipole moment $\vec{\mu}_L$ accompanying the orbital angular momentum $\vec{L}$ of the electron and the applied magnetic field $\vec{B}$ (or $\vec{B}_{ext}$ to be explicit) is added to the Hamiltonian. The interaction energy carries the form $-\vec{\mu}_L \cdot \vec{B}$. In QM, this term becomes an operator and it is added to the Hamiltonian. The $\vec{\mu}_L$ becomes $\hat{\vec{\mu}}_L$. A consequence is the normal Zeeman effect. **Note that spin angular momentum is ignored here.** All is fine. This follows from the "think classical" and then "go quantum" procedure.

We ask a more general question: "Is there a standard procedure to incorporate the effect of an applied $\vec{B}$ field in QM?" The answer is yes. Here, we introduce **a standard procedure** in QM to include the effect of $\vec{B}$ and to generate the $-\vec{\mu}_L \cdot \vec{B}$ term **automatically**. The procedure is applicable to many other occasions, e.g. incorporating EM fields quantum mechanically into the Dirac equation and in quantum field theories.

In QM, the **vector potential** $\vec{A}$ plays a more important role than the magnetic field $\vec{B}$. Recall that $\vec{B} = \nabla \times \vec{A}$. In QM, when an applied magnetic field acts on a charged particle of charge q, the effect is captured by (i) writing down the Hamiltonian *without* the magnetic field effect; and (ii) **replacing the linear momentum** $\vec{p}$ in the Hamiltonian **by** $\vec{p} - q\vec{A}$, i.e., making the substitution $\vec{p} \to \vec{p} - q\vec{A}$, where $\vec{A}$ is the vector potential that can generate the field $\vec{B}$. When we apply the procedure to the electron in a hydrogen atom in the presence of an applied field $\vec{B} = B\hat{z}$, we have

$$\hat{H} = \frac{(\vec{p} + e\vec{A})^2}{2m} + V(r) \tag{1}$$

where $V(r) = -e^2/(4\pi\epsilon_0 r)$ is the Coulomb potential energy term for a hydrogen atom, and $V(r)$ is a spherically symmetrical potential for other atoms.

TA: For $\vec{B} = B\hat{z}$ (no loss of generality), **choose** a proper $\vec{A}$ that works and **show** that a term of the form $-\vec{\mu}_L \cdot \vec{B}$ emerges (without *a priori* knowing there is an orbital magnetic moment)! Identify $\vec{\mu}_L$. Also **show** that an extra term of the order A^2 (thus B^2) also emerges as a by-product.

Physics remarks: (a) Physically, the term $-\vec{\mu}_L \cdot \vec{B}$ is a **paramagnetic** response, as it prefers the alignment of the magnetic dipole moment with $\vec{B}$. The extra $\sim A^2$ term is a **diamagnetic response** of the orbiting electron. It can be treated by the 1st order perturbation theory. It is analogous to the Lenz law. The response in a loop threaded through by a changing magnetic field is a current that opposes the change. Since the magnetic field is typically not big, the paramagnetic term is more important than the diamagnetic term. In some cases where $L = 0$ (so $\vec{\mu}_L = 0$) (closed-shell), the diamagnetic term becomes important. (b) If we have a scalar potential

ϕ in addition to $\vec{A}$, you may immediately think that there should be a term $q\phi$ added to the energy (Hamiltonian). You are right! (c) The magical thing is that the substitution **generates how a charged particle interacts with an external field**. For EM interaction, the Maxwell's equations and the Lorentz force govern the behavior of EM fields and how a charge interacts with EM fields. Thus the substitution rule gives nothing new. It simply confirms what is known. However, for the cases where the form of the interaction term is not clearly known (e.g. other interactions in particle physics), this substitution serves as a guiding principle in key developments in quantum (gauge) field theories. (d) The nucleus also has a spin magnetic moment. Hence, it creates a $\vec{B}$ field and thus $\vec{A}$. This $\vec{A}$ field will interact with the electron's $\vec{L}$ when the substitution rule is applied. The result is the hyperfine structure.

SQ9 *The rule of adding two angular momenta gives the right number of states*

In class, we illustrated that for p states ($\ell = 1$) including spin ($s = 1/2$), there are 6 states. Changing the descriptions to $j = 3/2$ and $j = 1/2$, there are also 6 states – no more and no less!

In general, it is unnecessary for one of the angular momenta quantum numbers to be 1/2. We could add an angular momentum of quantum number j_1 and another angular momentum of quantum number j_2 to form a total angular momentum for which the quantum number j takes on a range of values defined by j_1 and j_2. While deriving the rule of adding two angular momenta in QM is beyond the scope of our course, applying the rules helps understand features in systems consisting of many electrons such as atoms and molecules. We will make use of the results later.

Here, the TA will show that counting the states by the labels $(j_1, m_{j_1}, j_2, m_{j_2})$ and by the labels (j_1, j_2, j, m_j) account for the same number of states.

TA: Try $j_1 = 5/2$ and $j_2 = 1$. **Show** that the two schemes label the same number of states. Hence, **show** that for general j_1 and j_2, the two schemes are just different ways of describing the same number of states.

SQ10 *Effect of a weak static electric field on $n = 2$ states of hydrogen atom*

We discussed the effects of applied an external magnetic field to a hydrogen atom (Zeeman effect). How about applying an **electric field**? There are several effects. The "electron cloud" will be shifted and hence there will be polarization (electric dipole moment). Here, we study the effect of a **static electric field** $\vec{\mathcal{E}} = \mathcal{E}\hat{z}$ on the degenerate $n = 2$ (2s and 2p) states of a hydrogen atom.

Background: The electron's $(-e)$ charge interacts with the electric potential of an electric field $\vec{\mathcal{E}} = \mathcal{E}\hat{z}$ gives an energy term $\hat{H}' = e\mathcal{E}z$. Recall that for $n = 2$, the states can be 2s, $2p_x$, $2p_y$, $2p_z$. In the unperturbed hydrogen atom problem, these 4 states are degenerate with the same energy $-13.6/4$ eV. Thus, the first thing came to mind is to apply the degenerate perturbation theory, with $\hat{H}'$ being the perturbation. Given that there are 4 degenerate states, the matrix to be considered carefully is 4×4 in size. The problem is actually *simpler*. The results are related to the **Stark effect**.

TA: (Pretend to) **Set up** the problem as a 4×4 matrix (or determinant) problem and **point out/explain** that the problem reduces effectively to 2×2 for the $\hat{H}'$ under consideration. Hence, **show** that two of the 4 states are unaffected by $\hat{H}'$ while the other two split with an extent that is linearly dependent on the field strength $\mathcal{E}$. **Also point out** that the results hold even if the electric field is applied in the $\hat{x}$ or $\hat{y}$ direction. Finally, either evaluate the matrix element $\langle\psi_{200}|\hat{H}'|\psi_{210}\rangle$ explicitly or state the result with a reference.

[**Remarks**: (TA: don't need to do anything) This SQ is related to the **Stark effect**. The effect is the **splitting of spectral line in the presence of an electric field**. It should be contrast with the **Zeeman effect** for splitting of spectral line in the presence of a **magnetic field**. The effect can be understood after working out this SQ. When $\mathcal{E} = 0$, there is a spectral line due to transition between $n = 2$ states (actually 2p states) and $n = 1$ state (1s state). When an electric field is applied, we saw that one p state in $n = 2$ will split from the other two p states, giving rise to splitting of spectral line. Stark was awarded the 1919 Nobel Physics Prize.

What if the applied electric field is very strong (but not tearing the atom apart) as in low-frequency intense laser pulses? To get a sense of the problem, think about an electron barely go out quite far from the nucleus but then the oscillation tilts back the potential energy function so that the electron rushes back towards the nucleus, and so on. What will happen? What will be generated in such electron re-collision processes? This is an area of research in atomic and molecular physics using ultrafast and intense laser.]