PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 4 EXERCISE CLASSES (28 Jan - 1 Feb 2019)

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 in Hamiltonian and more
SQ9: Some expectation values of $f(r)$ for hydrogen atomic states
SQ10: Counting the states of three spin-1/2 particles in three different states in two different ways

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 $\vec{\mu}_L = 0$), 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 *Some expectation values of $f(r)$ for hydrogen atomic states*

In applying perturbation theory (even 1st order approximation as in SQ7), we need to evaluate **expectation value** of some quantity $f(r)$ such as r, $1/r$, $1/r^2$, with respect to a hydrogen atomic state $R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)$. Since $f(r)$ does not depend on θ and ϕ, the integrals over angles $\int(\cdots)d\Omega$ can easily be handled by the normalization of the spherical harmonics. It is an integral of $\int_0^\infty R^*_{n\ell}(r)f(r)R_{n\ell}(r)r^2dr$ that matters at the end. In class notes, a few standard results are listed.

TA: **Evaluate** $\langle r\rangle$ for $2s$ ($R_{20}(r)$) and for $2p$ ($R_{21}(r)$) and illustrate that the results are consistent with the general formula

$$\langle r\rangle_{n\ell m_\ell} = \frac{a_0}{2}\left(3n^2 - \ell(\ell+1)\right) \tag{2}$$

where a_0 is the Bohr radius. [Note: We studied the most probable r_{mp} at which $P(r) = r^2|R(r)|^2$ peaks in QMI. The quantity $\langle r\rangle$ is different, though related.]

TA: **Evaluate** $\langle 1/r\rangle$ for $2s$ and $2p$, and illustrate that the results are consistent with the general result

$$\langle\frac{1}{r}\rangle_{n\ell m_\ell} = \frac{1}{n^2a_0} \tag{3}$$

Important remark: Some students wonder whether $\langle 1/r\rangle \stackrel{?}{=} 1/\langle r\rangle$. The results show that it is **NOT THE CASE**.

SQ10 *Counting the states of three spin-1/2 particles in three different states in two different ways*

We studied how to add an orbital angular momentum of quantum number ℓ to a spin $s = 1/2$ angular momentum to form a total angular momentum. The quantum number j for the magnitude squared J^2 is given by $j = \ell + 1/2$ and $j = \ell - 1/2$. Here, we extend the application of this rule to study the states of three spin-half particles in three different states.

Method 1: Consider there are three spin-1/2 particles (electrons) and there are three states (e.g. $1s$, $2s$, $2p_x$). There is one particle in each state. [The set up avoids complications due to the Pauli Exclusion Principle, a topic to be discussed.] Each particle can be of "spin-up" or "spin-down". We may think that particle 1 is in state 1, particle 2 in state 2, and particle 3 in state 3. A possible state of the system is "up, up, up". TA: **List** all the states.

Method 2: So far, we only know how to add some angular momentum to a spin-1/2 angular momentum. But that is sufficient. TA: By adding two spin-1/2 angular momenta first, and then add in the remaining spin-1/2 angular momentum, **group** the states by the total spin angular momentum quantum number S that gives the eigenvalues $S(S+1)\hbar^2$ of the total spin angular momentum squared $\hat{S}^2_{tot}$. Note that for each value of S, there are accompanying values of M_S for the eigenvalues of $\hat{S}_{tot,z}$. Hence, **illustrate** that the number of states labelled by (S, M_S) is the same as that listed in Method 1.