

DEPARTMENT OF PHYSICS, CHINESE UNIVERSITY OF HONG KONG
PHYS3021 QUANTUM MECHANICS I

SAMPLE QUESTIONS FOR WEEK 12 EXERCISE CLASSES (20 - 24 November 2017)

Read me: TA will discuss the **SAMPLE QUESTIONS** (SQs) and answer your questions in exercise classes every week. The SQs are designed to review what you have learnt, tell a physics story, enrich our discussions, and help you work out the upcoming Problem Set. **Your time table should allow you to attend one exercise class session. The Exercise Classes are an integrated part of the course.** You are encouraged to work out (or think about) the SQs before attending exercise class and ask the TA questions. Over the semester, you are welcome to seek help from TAs/me.

SQ30 - Mid-term weaknesses (Lithium atom Hamiltonian, Sketching wavefunctions in tilted well, constructing \hat{P}^2)

SQ31 - Vector analogy of Schmidt orthogonal procedure for two and three vectors

SQ32 - $Y_{1,1}$, $Y_{1,-1}$ and p_x , p_y

SQ30 *Weak points in the mid-term exam*

Here are some parts in the mid-term exam that many students showed weaknesses. They are more on the conceptual parts rather than the calculation parts. Rough solutions have been posted. In this SQ, TA will discuss the following parts.

- (a) **Write down the Hamiltonian** that goes into the Schrödinger Equation for a **Lithium atom**.

[Hint: It is a 3-electron problem (nucleus fixed at origin). Therefore, each electron has its kinetic energy term. There are many potential energy terms, including electron-nucleus Coulombic attraction, and electron-electron Coulombic repulsion. A further remark is that the wavefunction is then $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$, a three-body wavefunction. The mid-term question concerned only the Hamiltonian. With the Hamiltonian, we **know the TISE** for Lithium atom (and any atom). No one knows how to solve it exactly. But there are many well-established methods to solve it accurately.]

- (b) **Sketch** the ground state wavefunction for two cases so as to stress the difference. Case A is an infinite well. Case B is a tilted infinite well with potential energy function $U(x) = \beta x$ inside the well.

[Hint: Ground state is meant to be the state of the lowest energy. So in a tilted well, how to spread the probability (wavefunction is related to probability density) so as to get at a low energy? Will the particle be found more on the side with lower potential energy or the other way round?]

- (c) Given $\hat{P} = \frac{d}{dx} + x$, **find an expression** for the operator \hat{P}^2 .

[Hint: The standard (and safe) way is to introduce an arbitrary function $f(x)$ and carry out the operations slowly. Some students simply that $(\frac{d}{dx} + x)^2$ and expand it as if it is $(a + b)^2$. This is WRONG! And you can feel how frustrating it could be in grading the papers.]

SQ31 *Schmidt orthogonal procedure* (See Problem 5.4(d))

In class notes, we showed that if two functions are not orthogonal, one can always construct two related functions that are orthogonal. This is particularly useful for degenerate states. The end result is that degenerate states of an operator can always be made orthogonal. Together with the statement that eigenstates for different eigenvalues are orthogonal, we have *eigenstates of a Hermitian operator can be made orthogonal to each other*. This is important in expanding any wavefunction in terms of the eigenstates.

In Problem 5.4(d), students are asked to compose two orthogonal functions. In class notes, a possible combination was given. TA: Read Problem 5.4(d) first and think about an interpretation of the procedure and result for two vectors.

- (a) **Vector analogy:** Let \vec{v}_1 and \vec{v}_2 be two vectors. They are not co-linear (they are not parallel to each other). So they live on a plane. They may NOT be orthogonal. They could be of unit length (normalized in the function language). Interpret the Schmidt orthogonal procedure and **illustrate** in a picture why the resulting vectors are orthogonal.
- (b) **Extend** the discussion to three vectors \vec{v}_1 , \vec{v}_2 , and \vec{v}_3 . They are non-coplanar and they may not be orthogonal. Illustrate how one can compose three orthogonal vectors in a systematic way.

SQ32 $Y_{1,1}$, $Y_{1,-1}$ and p_x , p_y (QM is physics, math, and chemistry beautifully combined)

In solving QM spherically symmetric problems, we got $Y_{\ell m_\ell}(\theta, \phi)$ and the pictures of the spherical harmonics (google them) do not resemble those atomic orbitals you saw in chemistry courses. As discussed, they are related.

- (a) **Show clearly that** combinations of $Y_{1,1}$ and $Y_{1,-1}$ are those of p_x and p_y orbitals. They have the same shape as p_z but directed in different directions.
- (b) **Show that** p_x and p_y are orthogonal to each other, using the orthogonality property of spherical harmonics. [Remark: It is easier to visualize that p_x and p_y are orthogonal as they are directed in orthogonal directions. This comes from the orthogonal property of spherical harmonics. Realizing that \hat{L}^2 and \hat{L}_z are Hermitian operators, their eigenstates can be made orthogonal as illustrated by the spherical harmonics $Y_{\ell m_\ell}$ for the orbital angular momentum.]

[Remark: Quantum Mechanics was established to understand the atomic world. It is physics. However, we need the mathematics to solve the Schrödinger Equation. Imposing boundary conditions (well-behaving wavefunctions) by physical consideration gives us the spherical harmonics. The functions $Y_{\ell m_\ell}$ are not easy to visualize. The mathematics of spherical harmonics gives us the directional p -orbitals, which are important in understanding bonding in molecules and solids. I hope that you see the point. If you only “like” physics but not math and chemistry, you can’t solve the equation and can’t move forward to appreciate the world made of atoms, molecules, and solids. If you only “like” math but not physics and chemistry, you only get many solutions but don’t know how to select the physically allowed ones and make use of them to appreciate the world around us. If you only “like” chemistry but not physics and math, probably you have to memorize all these p_x , p_y , p_z stuff without knowing what they actually are. Therefore, I hope that you will have a good balance in your appreciation and your skills in physics, mathematics, and chemistry.]