PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 7 EXERCISE CLASSES (24 Feb - 1 March 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 our course: For many-electron atoms (and molecules), we made approximations to turn the problems into single-electron problems. Self-consistency is often invoked in these methods. The end results are **atomic orbitals**. We then introduced the requirement that **many-electron wavefunctions must be anti-symmetric** with respect to interchanging any two electrons. This is a more general statement than the Pauli Exclusion Principle. This anti-symmetric requirement must be satisfied when we fill electrons into the atomic orbitals. This step leads to the Pauli Exclusion Principle. **Atomic orbitals** (self-consistency methods) and **Pauli Exclusion Principle** are the key concepts in understanding the periodic table.

SQ15 Slater determinant for three fermions in three different states
SQ16 Two non-interacting particle in 1D harmonic oscillator

SQ16 *Three-electron wavefunctions - Slater determinants* (See Problem 4.1)

Consider three electrons (three fermions) in three **different** single-particle states (after using IPA say) labelled a, b, c with wavefunctions ϕ_a, ϕ_b and ϕ_c. [Note: Sometimes, the label a could already carry a spin information, e.g. "1s-up" or "1s↑". For example, the ground state of lithium atom can be thought to have electrons in 1s-up, 1s-down, and 2s-up (could be 2s-down).]

A wavefunction that has the correct anti-symmetric property is given by a **Slater determinant**

$$\psi(1,2,3) \propto \begin{vmatrix} \phi_a(1) & \phi_b(1) & \phi_c(1) \\ \phi_a(2) & \phi_b(2) & \phi_c(2) \\ \phi_a(3) & \phi_b(3) & \phi_c(3) \end{vmatrix} \tag{1}$$

Here, 1, 2, and 3 are the coordinates of particles 1, 2, 3, respectively. This SQ reminds you of some basic determinant properties and illustrates that determinants are useful (thus why you need to learn them in other courses).

(a) **Find the normalization factor** in front of the expression, given that each single-particle state ϕ is properly normalized. [Remark: This is a counting problem. The normalization factor is related to the number of terms in the right-hand side of Eq. (1).]

(b) **Show** that $\psi(1,2,3)$ is anti-symmetric with respect to interchanging any two particles.

(c) There is a problem if we assign two particles into the **same** single-particle state. **Illustrate** what the problem is when two of the three states are identical. Hence, **point out** that the Pauli Exclusion Principle stating "two electrons cannot occupy the same state" also follows from Eq. (1).

(d) Another important and interesting observation from Eq. (1) is that two fermions tend to **avoid each other**. Let's take the coordinates to be **spatial coordinates** $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$

for three fermions and hence ψ is the spatial part of a 3-fermion wavefunction. In this case, Eq. (1) becomes

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \propto \begin{vmatrix} \phi_a(\mathbf{r}_1) & \phi_b(\mathbf{r}_1) & \phi_c(\mathbf{r}_1) \\ \phi_a(\mathbf{r}_2) & \phi_b(\mathbf{r}_2) & \phi_c(\mathbf{r}_2) \\ \phi_a(\mathbf{r}_3) & \phi_b(\mathbf{r}_3) & \phi_c(\mathbf{r}_3) \end{vmatrix} \tag{2}$$

Show that when any two fermions take on the same location in real space, the spatial wavefunction vanishes. By invoking the Born's interpretation of the wavefunction, **state what it means**. [Remarks: This is NOT a big problem, as for other choices of the coordinates, the wavefunction does not vanish. Thus, an **antisymmetric spatial wavefunction has the property that the particles tend to avoid each other**. This is an important concept. Note that this property comes entirely from the antisymmetric form of the wavefunction. This avoidance of particles is there **even there is no physical interaction** between particles. This is why ideal (non-interacting) Fermi gas and ideal (non-interacting) Bose gas behave differently. This takes us to SQ17.]

[Remark: Students may want to generalize the problem to N electrons in N different states.]

[Remarks: John C. Slater made important contributions to the understanding of matter (atoms, molecules, solids) using quantum mechanics. He wrote several classics textbooks. See *Quantum Theory of Atomic Structure* (2 volumes), *Quantum Theory of Matter*, *Quantum Theory of Molecules and Solids* (2 volumes) **all** by Slater. There are other books on Mechanics and Electromagnetism. Slater was the Physics Department Chairman of MIT from 1930-1950 and built it up to what we know it now.]

SQ17 *Two non-interacting particles in 1D harmonic oscillator and Plots* (See Problem 4.2)

This SQ illustrates the important effect of symmetry in two-particle spatial wavefunctions.

Consider two **non-interacting** but indistinguishable particles under the influence of a 1D parabolic potential energy function, i.e., 1D harmonic oscillator (HO). The oscillator ground state wavefunction is ψ_0, the 1st excited state is ψ_1, etc. We know the energy eigenvalues and eigenstates for 1D harmonic oscillator. We focus on two-particle spatial wavefunction here. We ignore the spin part in this problem.

(a) For the situation of the two particles both in the HO ground state, **write down** the 2-particle wavefunction $\psi(x_1, x_2)$ and **show** that it must be **symmetric**. [Remark: Thus it must go with an anti-symmetric spin part.]

(a') At this point, TA will introduce a way to make 3D plots. We will need to do 3D plots in Problem Set 4. There are many ways to do that and you are welcome to use your favorite way.

(b) **Plot** $\psi(x_1, x_2)$ and $|\psi(x_1, x_2)|^2$ as a function of x_1 and x_2. Note that it is a 3D plot with x_1 and x_2 along two axes and $\psi(x_1, x_2)$ in the third axis. [TA: Lead students to see from the figure what a symmetric $\psi(x_1, x_2)$ means.]

(c) Consider the case that one particle is in HO ground state ϕ_0 and another in the first excited state ϕ_1. **Construct** a two-particle spatial wavefunction $\psi^{(sym)}(x_1, x_2)$ which is symmetric with respect to interchanging the two particles. **Plot** $\psi^{(sym)}(x_1, x_2)$ and $|\psi^{(sym)}(x_1, x_2)|^2$.

(d) Consider the same case that one particle is in HO ground state ϕ_0 and another in the first excited state ϕ_1. **Construct** a two-particle spatial wavefunction $\psi^{(antisym)}(x_1, x_2)$ which is symmetric with respect to interchanging the two particles. **Plot** $\psi^{(antisym)}(x_1, x_2)$ and $|\psi^{(antisym)}(x_1, x_2)|^2$ [TA: Lead students to see from the figure what a antisymmetric $\psi(x_1, x_2)$ means.]

(e) **Discuss the key features** in the plots. In particular, locate where the two particles are more likely and less likely to be found and how these places vary according to the symmetry of the 2-particle wavefunction.

[Important Remarks: Again, the two particles do NOT interact in any way. Nonetheless, depending on the symmetry of the spatial wavefunction, they tend to come together or they tend to avid each other! This is an **entirely quantum** effect. It is as if there is an *effective interaction* induced by the required symmetry of the many-particle wavefunction.]