PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 8 EXERCISE CLASSES (8 - 12 March 2021)

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 discussed how approximations could be made to turn the quantum many-electron problem 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 single-electron 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.

SQ16 Slater determinant for three fermions in three different states
SQ17 Two non-interacting particles in 1D harmonic oscillator (seeing the effects of symmetry of wavefunction)

SQ16 *Three-electron wavefunctions - the Slater determinants*

The Slater Determinant is a convenient way to construct an anti-symmetric wavefunction (also called Totally Antisymmetric State/Wavefunction) for N-electron systems occupying N single-electron states. 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) (Optional for exam purposes.) It is also educational to write $\psi(1,2,3)$ in Eq. (1) explicitly as a linear combination of six terms. **Do it.** Then **make connection** to another way of writing the three-particle antisymmetric wavefunction as

$$\psi(1,2,3) = \frac{1}{\sqrt{3!}} \sum_{P} (-1)^P P \, \phi_a(1)\phi_b(2)\phi_c(3) \tag{2}$$

where the summation is over all permutations of the coordinates 1, 2, 3. [That is to say, (1,2,3), (1,3,2), etc.] The symbol $(-1)^P$ is $+1$ when P is an even permutation and -1 when P is an odd permutation. This form is often used in advanced quantum mechanics treatment of many-electron systems.

(e) Another important and interesting observation from Eq. (1) is that two fermions tend to **avoid each other**. To illustrate this point, let's take the coordinates to be **spatial coordinates** $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ for three fermions (ignoring spin in this discussion). In this case, Eq. (1) becomes

$$\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \propto \begin{vmatrix} \phi_a(\mathbf{r}_1) & \phi_b(\mathbf{r}_1) & \phi_c(\mathbf{r}_1) \\ \phi_a(\mathbf{r}_2) & \phi_b(\mathbf{r}_2) & \phi_c(\mathbf{r}_2) \\ \phi_a(\mathbf{r}_3) & \phi_b(\mathbf{r}_3) & \phi_c(\mathbf{r}_3) \end{vmatrix} \tag{3}$$

Note that the states are still different. **Show** that when any two fermions take on the same location in real space, the spatial wavefunction vanishes. [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 anti-symmetric 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 point will be further illustrated in SQ17.]

(f) **How about N-boson wavefunction?** Let's say we have three bosons in three states labelled a, b, c, as above. We want to construct a **symmetric 3-particle wavefunction**. Referring to the linear combination of six terms in part (d), **write down** a symmetric wavefunction $\psi_S(1,2,3)$.

[Remark: Students should note that the symmetric many-boson wavefunction is equally "complicated" in the sense that it has the same structure as many-fermion wavefunction, but it is "simpler" in the sense that we don't need to worry about the signs of the terms due to permutations.]

[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. Closer to our course Slater studied the self-consistent field and the structure of atoms (Hartree method) in his Physical Review 1928 paper and introduced the Slater Determinant in his 1929 paper on the theory of complex spectra also in the Physical Review.]

SQ17 *Two non-interacting but indistinguishable particles in 1D harmonic oscillator and Plots*

This SQ illustrates the important effect of symmetry in two-particle spatial wavefunctions. You will work out a similar problem in Problem Set 4.

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 eigenstates and eigenvalues for 1D harmonic oscillator. We focus on the 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 if we are to include spin.]

(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: 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.]

[Remark: TAs may want to introduce how 3D plots can be made.]