Physics 852 **Problem Set 8** **Spring 2023**

1. The Carbon atom has 2 valence electrons in the $2p$ shell.

   (a) What are the allowable total LSJ values for states with 2 electrons in the $2p$ shell? (Hint: First couple the s_1 and s_2 of the two electrons to find allowed S values, noting the symmetry of the spin states. Then, do the same for orbital angular momenta l_1 and l_2 to obtain allowed L values. Finally, combine these to obtain allowed J values.)

   (b) Given that there are 6 allowed orbitals for each electron in the $2p$ shell, determine the possible number of 2-electron states in this shell, keeping in mind that the states must be antisymmetric for fermions. Verify that the number of states found in part (a) agree with this result.

2. Consider the normalized antisymmetric two-fermion states,

$$|ab\} \equiv \frac{1}{\sqrt{2}} \left(|ab\rangle - |ba\rangle \right) .$$

   Show that the matrix element of a two-particle operator, V, (such as the electron-electron coulomb potential) can be written as

$$\begin{aligned} \{ab|V|cd\} &= \langle ab|V|cd\rangle - \langle ab|V|dc\rangle \\ &= \langle ab|V|cd\rangle - \langle ba|V|cd\rangle . \end{aligned}$$

3. Consider N non-interacting fermions in a 1d harmonic oscillator potential well. You may assume the fermions are spin-polarized so that they all have $S_z = +1/2$, which in practice means you can drop the spin indices in the following.

   (a) We can express this system in 2^{nd} quantized notation using annihilation/creation operators, a_n and $a_n^\dagger$, that annihilate/create an electron in the n^{th} 1-particle oscillator level. Express the Hamiltonian for this system in 2nd quantized notation.

   (b) Write down the ground state of the system using 2nd quantized notation.

   (c) Express the field operators $\widehat{\psi}(x)$ and $\widehat{\psi}^\dagger(x)$ in terms of a_n and $a_n^\dagger$.

   (d) Calculate the density matrix $\rho(x, x')$ for the ground state, defined as the expectation value of the bilinear product of field operators $\widehat{\psi}^\dagger(x)\widehat{\psi}(x')$. Your final result should be expressed as a sum over oscillator wave functions.

4. Work out the 2nd-quantized version of the following operators in the $(\mathbf{r}, m_s)$ basis (i.e., in terms of Fermion field operators)

   (a) The density operator

$$\hat{\rho}_N(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \hat{\mathbf{r}}_i)$$

(b) The current density operator

$$\hat{\mathbf{j}}_N(\mathbf{r}) = \frac{1}{2m}\sum_{i=1}^{N}\Big[\hat{\mathbf{p}}_i\delta(\mathbf{r}-\hat{\mathbf{r}}_i) + \delta(\mathbf{r}-\hat{\mathbf{r}}_i)\hat{\mathbf{p}}_i\Big]$$

(c) The spin density operator

$$\hat{\mathbf{S}}_N(\mathbf{r}) = \sum_{i=1}^{N}\hat{\mathbf{S}}_i\delta(\mathbf{r}-\hat{\mathbf{r}}_i)$$