PC4902: Elements of QMBT, Pt 2 Problems 3

Key: **E**asy; **M**oderate; **D**ifficult

1. [EM] Verify explicitly that the angular momentum commutation relations are satisfied by the following combinations of Fermi operators:

$$\hat{S}^{+} = \hat{c}^{\dagger}_{\uparrow}\hat{c}_{\downarrow}, \quad \hat{S}^{-} = \hat{c}^{\dagger}_{\downarrow}\hat{c}_{\uparrow}, \quad \hat{S}^{z} = \tfrac{1}{2}\big(\hat{c}^{\dagger}_{\uparrow}\hat{c}_{\uparrow} - \hat{c}^{\dagger}_{\downarrow}\hat{c}_{\downarrow}\big),$$

where $\hat{S}^{\pm}$ are related to $\hat{S}^{x}$ and $\hat{S}^{y}$ in the usual way for spin raising and lowering operators,

$$\hat{S}^{\pm} = \hat{S}^{x} \pm i\hat{S}^{y}.$$

The "spin operators" defined as above commute with the fermion number operator

$$\hat{n} \equiv \hat{n}_{\uparrow} + \hat{n}_{\downarrow} = \hat{c}^{\dagger}_{\uparrow}\hat{c}_{\uparrow} + \hat{c}^{\dagger}_{\downarrow}\hat{c}_{\downarrow},$$

which suggests that $\hat{n}$ should be closely related to the square of the spin operator. If you have time, show explicitly that

$$\hat{\mathbf{S}} \cdot \hat{\mathbf{S}} = \tfrac{3}{4}\big(2\hat{n} - \hat{n}^{2}\big).$$

[To reduce the expression to this form it is helpful to use the fact that $\hat{n}^{2}_{\sigma} = \hat{n}_{\sigma}$ for each value of the spin projection, σ.] Explain the final result by considering what the total S must be when there are 0, 1 and 2 fermions present.

2. [M] Suppose that the interactions of three electrons in a triangular molecule can be described by the Heisenberg Hamiltonian

$$\hat{H} = J(\hat{\mathbf{S}}_{1} \cdot \hat{\mathbf{S}}_{2} + \hat{\mathbf{S}}_{2} \cdot \hat{\mathbf{S}}_{3} + \hat{\mathbf{S}}_{3} \cdot \hat{\mathbf{S}}_{1}).$$

Express $\hat{H}$ in terms of $(\hat{\mathbf{S}}_{1} + \hat{\mathbf{S}}_{2} + \hat{\mathbf{S}}_{3})^{2}$, and show that the ground state energy is $\frac{3}{4}J$ in the ferromagnetic case $J < 0$. What is the degeneracy of the ground state? Write down one of the ground state wave functions: it corresponds classically to all the spins being parallel.

The case $J > 0$ is usually described as *frustrated* because on a triangle you cannot arrange for all pairs of adjacent spins to be "antiparallel". Show that the ground state energy in this case is $-\frac{3}{4}J$, and try to interpret the ground-state wave function.