Exercise 1 – Heitler-London method

In the following, we want to illustrate the emergence of ferromagnetic and antiferromagnetic ordering in materials. To this end, we consider two adjacent atoms separated by $R = R_1 - R_2$, with each atom having an outermost electron described by the wave-function $\phi_1(r)$, $\phi_2(r)$, which are eigenstates of the isolated atoms, i.e. $(i = 1, 2)$

$$H_i\phi_i(r_i) = \left[ \frac{p_i^2}{2m} - \frac{e^2}{|r_i - R_i|} \right] \phi_i(r_i) = E_0\phi_i(r_i).$$

The full Hamiltonian of the system reads

$$\mathcal{H} = H_1 + H_2 + \frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|R_1 - R_2|} - \frac{e^2}{|r_1 - R_2|} - \frac{e^2}{|r_2 - R_1|}.$$ 

(a) Since $\mathcal{H}$ does not depend on spin, the eigenfunctions can be chosen as eigenfunctions of $S^2$ and $S_z$ (where $S = S_1 + S_2$). Write down all possibilities (one singlet + 3 triplet states) for the spin-part of the wave-function.

(b) We can now make the following ansatz for that spatial part of the wave-function:

$$\phi_{\pm}(r_1, r_2) \propto \phi_1(r_1)\phi_2(r_2) \pm \phi_1(r_2)\phi_2(r_1).$$ (1)

Since the wave function has to be anti-symmetric with respect to exchange of the two electrons, how does the spatial part of the wave function look like when the system is in the singlet state and in the triplet state?

(c) Find the energies associated with singlet and triplet states by evaluating the expectation values $E_s = \langle \phi_s | \mathcal{H} | \phi_s \rangle$ and $E_t = \langle \phi_t | \mathcal{H} | \phi_t \rangle$, respectively. Determine the energy difference $-J = E_t - E_s$ as a function of Coulomb and exchange integral.

Remark: Remember that $|\phi_s\rangle$ and $|\phi_t\rangle$ should be properly normalized.
Exercise 2 – Spin-waves in a Heisenberg magnet

We consider the Heisenberg model of localized spin-$S$ moments

$$\mathcal{H} = -\frac{1}{2} \sum_{R,R'} J(R - R') S(R) \cdot S(R') - g\mu_B H \sum_R S_z(R)$$

with the ferromagnetic couplings $J(R - R') = J(R' - R) > 0$.

In the following, we work with the eigenstates of $S_z$, i.e. $S_z(R) | S_z \rangle_R = S_z | S_z \rangle_R$.

(a) We introduce the ladder operators $S_{\pm}(R) = S_x(R) \pm i S_y(R)$ with the property $S_{\pm}(R) | S_{\pm} \rangle_R = \sqrt{(S_\pm S_z)(S + 1 \pm S_z)} | S_{\pm} \pm 1 \rangle_R$, as you should know from your quantum mechanics course. Express $\mathcal{H}$ in terms of $S_z(R)$ and $S_{\pm}(R)$.

(b) In the ground state, all spins are in the same state so that $|0 \rangle = \prod_R | S \rangle_R$. What is the ground state energy $E_0$?

Now we are looking for low lying excitations, so we consider the state where only a single spin at position $R$ is excited, i.e. $| R \rangle = \frac{1}{\sqrt{2S}} S_- (R) | 0 \rangle$. However, since our spin-model has discrete translation invariance, we expect the eigenmodes (=spin-waves) to be

$$| k \rangle = \frac{1}{\sqrt{N}} \sum_R e^{ikR} | R \rangle.$$ 

(analogous to what is used to obtain the phonon modes)

(c) What is the total spin when the system is in the state $| k \rangle$?

(d) Show that $| k \rangle$ are indeed eigenstates of $\mathcal{H}$ and determine the spin-wave dispersion $\epsilon_k = E_k - E_0$ where $\mathcal{H} | k \rangle = E_k | k \rangle$. Show that for small $k$, the dispersion $\epsilon_k$ is quadratic in $k$.

(e) At low temperatures, only spin-waves with small $k$ are excited, so we use the quadratic approximation for $\epsilon_k$. In analogy to phonons, spin-waves behave as Bosons and the average occupation number at temperature $T$ is given by

$$n(k) = \frac{1}{e^{\epsilon_k/k_B T} - 1},$$

so that the magnetization at temperature $T$ is given by

$$M(T) = M(0) \left[ 1 - \frac{1}{NS} \sum_k n(k) \right].$$

In the limit of vanishing magnetic field $H \to 0$, show that the saturation magnetization $M(T \ll T_c)$ is reduced by a term proportional to $T^{3/2}$ for low temperatures ($T^{3/2}$-law of Bloch).