Exercise 1. ***Playing around with wave functions in second quantization.***

In the formalism of second quantization, a general state of N particles at positions $\vec{r}_1$, $\vec{r}_2$, ... is given by

$$|\vec{r}_1, \vec{r}_2, ..., \vec{r}_N\rangle = \frac{1}{\sqrt{N!}} \hat{\Psi}^\dagger(r_N) \cdots \hat{\Psi}^\dagger(r_1)|0\rangle \ , \tag{1}$$

where $|0\rangle$ is the vacuum state and the field operators $\hat{\Psi}(\vec{r})$ are defined as

$$\hat{\Psi}(\vec{r}) = \sum_k \phi_k(\vec{r})\ \hat{a}_k \ , \tag{2}$$

with $\hat{a}_k$ the annihilator of mode k and $\phi_k(\vec{r})$ the one-particle wave function of mode k.

Consider a state $|\psi\rangle$ of three particles in modes k_1, k_2, and k_3. Consider its wave function

$$\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \langle \vec{r}_1, \vec{r}_2, \vec{r}_3|\psi\rangle = \langle \vec{r}_1, \vec{r}_2, \vec{r}_3|\hat{a}^\dagger_{k_3}\hat{a}^\dagger_{k_2}\hat{a}^\dagger_{k_1}|0\rangle \ . \tag{3}$$

(a) First calculate the vacuum expectation value

$$\langle 0|\hat{a}_{\ell_1}\hat{a}_{\ell_2}\hat{a}_{\ell_3}\hat{a}^\dagger_{k_3}\hat{a}^\dagger_{k_2}\hat{a}^\dagger_{k_1}|0\rangle \ , \tag{4}$$

for bosons and for fermions.

(b) Determine $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ for bosons and for fermions. What symmetries does the wave function possess?

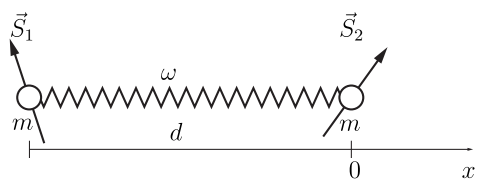
(c) Determine the normalization of the wave function for fermions and for bosons. First consider the case where k_1, k_2 and k_3 are all different, and then study the case where two or more modes are the same. What do you observe?

Note: for the lazy, it is also possible to do the whole exercise with two particles only. For the motivated, calculate it for N particles.

Exercise 2. ***Magnetostriction in a Spin-Dimer-Model.***

As in Exercise 2.3, we consider a dimer consisting of two spin-1/2 particles with the Hamiltonian

$$\mathcal{H}_0 = J\left(\vec{S}_1 \cdot \vec{S}_2 + 3/4\right) \ ,$$



with $J > 0$ (note that the energy levels are shifted as compared to Ex. 2.3). This time, however, the distance between the two spins is not fixed, but they are connected to a spring. The spin–spin coupling constant depends on the distance between the two sites such that the Hamilton operator of the system is

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + J(1 - \lambda\hat{x})\left(\vec{S}_1 \cdot \vec{S}_2 + 3/4\right) \ , \tag{5}$$

where $\lambda \geq 0$, m is the mass of the two constituents, $m\omega^2$ is the spring constant and where x denotes the displacement from the equilibrium distance d between the two spins (in the case of no spin-spin interaction).

(a) Write the Hamiltonian (5) in second quantized form and calculate the partition sum, the internal energy, the specific heat and the entropy. Discuss the behavior of the entropy in the limit $T \to 0$ for different values of λ.

Hints. Set $\hbar = 1$. Rewrite the Hamiltonian using the total spin as in Exercise 2.3, and bring it by completing the square to the form

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2 + \tilde{J}\,\hat{n}_t \ , \tag{6}$$

where $\hat{n}_t$ is the projector on the triplet subspace, and $\hat{X}$ and $\tilde{J}$ are appropriately shifted quantities $\hat{x}$ and J ($\hat{X}$ may depend on $\hat{n}_t$). Recall then the creation and annihilation operators of a harmonic oscillator.

(b) Calculate the expectation value of the distance between the two spins, $\langle d + \hat{x} \rangle$, as well as the fluctuation, $\langle (d + \hat{x})^2 \rangle$. How are these quantities affected by a magnetic field in z-direction, i.e., by adding an additional term in (5) of the form

$$\mathcal{H}_m = -g\mu_B H \sum_i \hat{S}_i^z \quad ?$$

Hints. Write first those averages in terms of $\langle \hat{n}_t \rangle$, which you can calculate explicitly. Recall that for a harmonic oscillator, $\langle \hat{X} \rangle$ vanishes, as well as $\langle a \rangle$, $\langle a^2 \rangle$ etc.

Recalculate the partition function adding the magnetic field term and see how this affects $\langle \hat{n}_t \rangle$.

(c*) If the two sites are oppositely charged, i.e., $\pm q$, the dimer forms a dipole with moment $P = q\,\langle d + \hat{x} \rangle$. This dipole moment can be measured by applying an electric field E along the x-direction, resulting in the additional Hamiltonian term

$$\mathcal{H}_{\mathrm{el}} = -q(d + \hat{x})E \ .$$

Calculate the susceptibility of the dimer at zero electric field,

$$\chi_0^{(\mathrm{el})} = - \left. \frac{\partial^2 F}{\partial E^2} \right|_{E=0} ,$$

and compare your result with the simple form of the fluctuation-dissipation theorem, which asserts that

$$\chi_0^{(\mathrm{el})} \propto \left\langle (d + \hat{x})^2 \right\rangle - \left\langle d + \hat{x} \right\rangle^2 \ . \tag{7}$$

Hint. Proceeding as in Section 1.5.3 of the lecture notes or Exercise 2.1 (e), find out which step no longer applies. How should (7) be "corrected"?

Plot the susceptibility at zero electric field as a function of an applied magnetic field H and discuss your result.