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Problem sheet 12

12.1 Multipole expansion: C_{3v} symmetry

We consider a system of three equal charges which possesses C_{3v} symmetry. During the lecture we derived the modified multipole expansion according to the A_1 representation of C_{3v}.
Two problems, that had not been solved during the lecture, shall be treated in this exercise.

a. What is the direction of the z-axis?

b. For $l = 3$ we need two irreducible basis functions of the A_1 representation of C_{3v}. We conjectured that they are given by $Y_{3,0}$ and $Y_{3,3} - Y_{3,-3}$. Show, that this is indeed the case.

12.2 Tight-binding model

The Hubbard model of a one-dimensional chain is given by the following Hamiltonian

$$\underset{\sim}{H} = -t \sum_{j=1}^{L} \sum_{\sigma=\pm 1/2} \left(\underset{\sim}{c}^{\dagger}_{j,\sigma} \underset{\sim}{c}_{j+1,\sigma} + \underset{\sim}{c}^{\dagger}_{j+1,\sigma} \underset{\sim}{c}_{j,\sigma} \right) + U \sum_{j=1}^{L} \underset{\sim}{n}_{j,1/2}\, \underset{\sim}{n}_{j,-1/2} \ . \tag{1}$$

Here $\underset{\sim}{c}^{\dagger}_{j,\sigma}$ are the creation operators of fermions with spin 1/2 at site j and m-quantum number $m = \sigma$. $\underset{\sim}{c}_{j,\sigma}$ are the respective annihilation operators, $\underset{\sim}{n}_{j,\sigma} = \underset{\sim}{c}^{\dagger}_{j,\sigma} \underset{\sim}{c}_{j,\sigma}$ denote the occupation number operators. $t, U \in \mathbb{R}$. L gives the number of sites.
Creation and annihilation operators follow the canonical anticommutation relations

$$\left\{ \underset{\sim}{c}^{\dagger}_{j,\sigma}, \underset{\sim}{c}^{\dagger}_{j',\sigma'} \right\} = \left\{ \underset{\sim}{c}_{j,\sigma}, \underset{\sim}{c}_{j',\sigma'} \right\} = 0 \tag{2}$$

$$\left\{ \underset{\sim}{c}_{j,\sigma}, \underset{\sim}{c}^{\dagger}_{j',\sigma'} \right\} = \delta_{jj'} \delta_{\sigma\sigma'} \ . \tag{3}$$

In the case of $U = 0$ the Hamiltonian (1) simplifies to the Hamiltonian of the *tight-binding* model. This translationary invariant Hamiltonian could be diagonalized by introducing the eigenbasis of the shift operator (as done before). But in cases of single-particle operators such as the Hamiltonian of the tight-binding model one can diagonalize the Hamiltonian directly by transforming the creation and annihilation operators as follows

$$\underset{\sim}{d}^{\dagger}_{k,\sigma} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} \exp\left[i \frac{2\pi k j}{L} \right] \underset{\sim}{c}^{\dagger}_{j,\sigma} \ , \quad k = 0, 1, \dots L-1 \ . \tag{4}$$

a. How are the annihilation operators transformed?

b. Show that the canonical anticommutation relations (2) also hold for the new creation and annihilation operators.

c. Provide the inverse transformation.

d. How does the tight-binding Hamiltonian look like using the new operators? Give the eigenvalues and eigenstates.