Topology in condensed matter physics
Exercise sheet 5

University of Hamburg
Thore Posske

5.1 Bogoliubov transformations

A Bogoliubov transformation is used to diagonalize a second quantized, quadratic Hamiltonian with anomalous terms. These are terms of the form creation operator times creation operator and annihilation operator times annihilation operator, which appear in the mean-field description of superconductors and in the solution of the interacting fermion problem in one dimension.
Given the annihilation operators c_i for i in a countable index set I, we introduce the transformed annihilation operator

$$d_j = \sum_{i \in I} A_{j,i} c_i + B_{j,i} c_i^\dagger, \tag{1}$$

for each $j \in I$.

1. Assume that the operators c_i for $i \in I$ are fermionic, i.e., $\{c_i, c_j\} = 0$, $\left\{c_i^\dagger, c_j\right\} = \delta_{i,j}$. Derive (necessary and sufficient) conditions for the matrices A and B such that the d_j are fermionic as well.
2. Assume that the operators c_i for $i \in I$ are bosonic, i.e., $[c_i, c_j] = 0$, $\left[c_i, c_j^\dagger\right] = \delta_{i,j}$. Derive (necessary and sufficient) conditions for the matrices A and B such that the d_j are bosonic as well.

Solution: Here, the index + denotes the anticommutator (for fermions) and the minus sign the normal commutator (for bosons), with $\zeta = 1$ for the anticommutator and $\zeta = -1$ for the commutator.

1. $$[d_j, d_k^\dagger]_\pm = [\sum_l A_{jl} c_l + B_{jl} c_l^\dagger,\ \sum_i A_{ik}^* c_i^\dagger + B_{ik}^* c_i]_\pm$$

$$\Bigg| \quad [c_l^\dagger, c_i^\dagger]_\pm = 0 = [c_l, c_i]$$

$$\Bigg| \quad [c_l, c_i^\dagger]_\pm = \delta_{li}, \quad [c_l^\dagger, c_i]_\pm = \pm\delta_{li}$$

$$= A_{jl} A_{ik}^* \delta_{il} + \zeta_\pm B_{jl} B_{ik}^* \delta_{li}$$

$$= A_{ji} A_{ik}^* + \zeta_\pm B_{ji} B_{ik}^* \overset{!}{=} \delta_{kj}$$

$$k = j: \quad \underline{\underline{\sum_i |A_{ji}|^2 + \zeta_\pm |B_{ji}|^2 = 1}}$$

$$k \neq j: \quad \underline{\underline{\sum_i A^*_{ik} A_{ji} + \zeta_\pm B^*_{ik} B_{ji} = 0}}$$

2. $$[d_j, d_k]_\pm = [\sum_i A_{jl} c_l + B_{jl} c_l^\dagger, \sum_k A_{ki} c_i + B_{ki} c_i^\dagger]_\pm$$
$$= \sum_{l,i} A_{jl} B_{ki} \delta_{li} + \zeta_\pm B_{jl} A_{ki} \delta_{li}$$
$$= \sum_i A_{ji} B_{ki} + \zeta_\pm B_{ji} A_{ki} \delta_{li} \stackrel{!}{=} 0$$
$$\Leftrightarrow \quad \underline{\underline{\sum_i A_{ji} B_{ki} = -\zeta_\pm \sum_i B_{ji} A_{ki}}}$$

The conditions therefore are

$$AA^\dagger + \zeta_\pm BB^\dagger = \mathbb{I}$$

and

$$AB^T + \zeta_\pm BA^T = 0 \ .$$

3. Find a parametrization for the matrices A and B of the Bogoliubov transformation of a single bosonic mode (i.e., $I = \{1\}$).

Solution: With $i = k = 1$, we find

$$|A_{11}|^2 - |B_{11}|^2 = 1$$
$$A_{11} B_{11} = B_{11} A_{11} \ .$$

A possible parametrization is

$$A = e^{i\phi_1} \cosh(\vartheta)$$
$$B = e^{i\phi_2} \sinh(\vartheta) \ ,$$

with $\phi_1, \phi_2, \vartheta \in \mathbb{R}$.

4. (* points) Diagonalize

$$H = \alpha b^\dagger b + b^\dagger b^\dagger + bb, \tag{2}$$

where $\alpha \in \mathbb{R}$ and b is a bosonic annihilation operator, by finding a boson d such that

$$H = \epsilon d^\dagger d + \text{const.} \tag{3}$$

For which values of α is such a diagonalization impossible?
Hint: Use $[d, H] = \epsilon d = \epsilon(Ab + Bb^\dagger)$ to obtain linear equations for the coefficients A and B. Interpretation: If the Hamiltonian is not diagonalizable by a Bogoliubov transformation, it describes an unstable equilibrium.

Solution: We want to diagonalise

$$H = \alpha b^\dagger b + b^\dagger b^\dagger + bb = \begin{pmatrix} b^\dagger & b \end{pmatrix} \begin{pmatrix} \frac{\alpha}{2} & 1 \\ 1 & \frac{\alpha}{2} \end{pmatrix} \begin{pmatrix} b \\ b^\dagger \end{pmatrix}$$

$$\begin{aligned} [d, H] &= A\alpha[b, b^\dagger b^\dagger] + A[b, b^\dagger b^\dagger] + B\alpha[b^\dagger, b^\dagger b] + B[b^\dagger, bb] \\ &= \alpha Ab + 2Ab^\dagger - \alpha Bb^\dagger - 2Bb \\ &\overset{!}{=} \epsilon(Ab + Bb^\dagger) \end{aligned}$$

Comparing the conditions yields

$$\epsilon \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \alpha & -2 \\ 2 & -\alpha \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} .$$

This is an eigenvalue problem, with

$$\epsilon = \pm\sqrt{\alpha^2 - 4} .$$

If $\alpha^2 < 4$, we do not get real eigenvalues. Hence, if $\alpha^2 < 4$, there is no diagonalizing Bogolibuov transformation.

The eigenvectors are

$$v_+ = c_+ \begin{pmatrix} \frac{1}{2}\left(\alpha - \sqrt{\alpha^2 - 4}\right) \\ 1 \end{pmatrix}, \quad v_- = c_- \begin{pmatrix} \frac{1}{2}\left(\alpha + \sqrt{\alpha^2 - 4}\right) \\ 1 \end{pmatrix}, \quad c_-, c_+ \in \mathbb{C}$$

Applying the bosonic conditions

$$|A|^2 - |B|^2 = |c_\pm|^2 \; \frac{1}{4}\left(2\alpha^2 - 4 \pm 2\alpha\sqrt{\alpha^2 - 4}\right) - |1|^2 \overset{!}{=} 1 ,$$

we find that $\alpha = \pm 2$ is also invalid because this would result in invalid values of c_+/c_- .
We define

$$\Gamma_\pm(\alpha) := \frac{1}{4}\left(2\alpha^2 - 4 \pm 2\alpha\sqrt{\alpha^2 - 4}\right) - |1|^2 .$$

and realize that $\Gamma_\pm(\alpha)$ needs to be positive in order to fulfill $|A|^2 - |B|^2 = 1$.

Here, we could check for another constraint.

5. Define the Nambu spinor $c = (c_1, c_2, \ldots, c_n, c_1^\dagger, c_2^\dagger, \ldots, c_n^\dagger)$. Express the conditions as a condition on the linear operator that transforms the Nambur spinor.

5.2 Symmetry reduction of Hamiltonians

Consider the following set of Hamiltonians, a two-site tight-binding model for spinful fermions, for instance, describing the valence electrons of a binary molecule in a magnetic field

$$\mathcal{H} = BS_x + t \sum_{\sigma \in \{\uparrow,\downarrow\}} c^\dagger_{1,\sigma} c_{2,\sigma} + c^\dagger_{2,\sigma} c_{1,\sigma}, \tag{4}$$

with the real parameters $t, B \in \mathbb{R}$ describing electron transfer between the two sites and the magnetic field in x-direction, respectively, and $S_x = \frac{\hbar}{2} \sum_{i=1}^{2} c^\dagger_{i,\uparrow} c_{i,\downarrow} + c^\dagger_{i,\downarrow} c_{i,\uparrow}$ being the total x-spin of the particles.

1. Show that $\mathcal{H}$ conserves the total x-spin, i.e., $[\mathcal{H}, S_x] = 0$. Does that remain true for an inhomogeneous magnetic field in x-direction?

Solution: We find the information about the magnetic field in the first term. Because B is not an operator and same operators commute, a change in the magnetic field still conserves the total x-spin. We therefore only examine the other term.

$$[\mathcal{H}, S_x]_- = \Big[BS_x + t \sum_{\sigma \in \{\uparrow,\downarrow\}} c^\dagger_{1,\sigma} c_{2,\sigma} + c^\dagger_{2,\sigma} c_{1,\sigma},\ S_x\Big]_-$$

$$= \Big[t \sum_{\sigma \in \{\uparrow,\downarrow\}} c^\dagger_{1,\sigma} c_{2,\sigma} + c^\dagger_{2,\sigma} c_{1,\sigma}\ ,\ \frac{\hbar}{2} \sum_{i=1}^{2} c^\dagger_{i,\uparrow} c_{i,\downarrow} + c^\dagger_{i,\downarrow} c_{i,\uparrow}\Big]_-$$

$$= \frac{\hbar t}{2} \Big[\sum_{\sigma, k \neq l} c^\dagger_{k\sigma} c_{l\sigma}\ ,\ \sum_{i, m \neq n} c^\dagger_{im} c_{in} \Big]_-$$

$$[AB, CD]_\pm = A[B,C]_- D + \cancel{AC[B,D]_-} + \cancel{[A,C]_- DB} + C[A,D]_\pm B \quad \text{(only cross-terms survive)}$$

$$= \frac{\hbar t}{2} \sum_{\sigma, k \neq l} \sum_{i, m \neq n} \Big\{ c^\dagger_{k\sigma} \underbrace{[c_{l\sigma}, c^\dagger_{im}]_-}_{\delta_{li}\delta_{\sigma m}} c_{in} + c^\dagger_{im} \underbrace{[c^\dagger_{k\sigma}, c_{in}]_-}_{-\delta_{ki}\delta_{\sigma n}} c_{l\sigma} \Big\} \quad = \quad \underline{\underline{0}}$$

2. What is the corresponding unitary symmetry of the family of Hamiltonians?

Solution: The operator S_x is hermitian. The corresponding unitary symmetry is $e^{i\lambda S_x} = U(\lambda)$, the symmetry of total spin rotation around the x-axis.

3. Derive the single particle Hamiltonian by writing $\mathcal{H}$ in the form

$$\sum_{a,b=1}^{4} C^\dagger_a h_{a,b} C_b. \tag{5}$$

with $c = (c_{1,\uparrow}, c_{2,\uparrow}, c_{1,\downarrow}, c_{2,\downarrow})$. Here, h is the single particle Hamiltonian.

Solution: We can choose one of the following two bases:

$$\begin{pmatrix} c^\dagger_{1,\uparrow} & c^\dagger_{2,\uparrow} & c^\dagger_{1,\downarrow} & c^\dagger_{2,\downarrow} \end{pmatrix} \begin{pmatrix} 0 & t & B & 0 \\ t & 0 & 0 & B \\ B & 0 & 0 & t \\ 0 & B & t & 0 \end{pmatrix} \begin{pmatrix} c_{1,\uparrow} \\ c_{2,\uparrow} \\ c_{1,\downarrow} \\ c_{2,\downarrow} \end{pmatrix}$$

Here seems to be a problem:

$$\begin{pmatrix} c^\dagger_{1,\uparrow} & c^\dagger_{1,\downarrow} & c^\dagger_{2,\uparrow} & c^\dagger_{2,\downarrow} \end{pmatrix} \begin{pmatrix} 0 & B & 0 & t \\ B & 0 & t & 0 \\ 0 & t & 0 & B \\ t & 0 & B & 0 \end{pmatrix} \begin{pmatrix} c_{1,\uparrow} \\ c_{1,\downarrow} \\ c_{2,\uparrow} \\ c_{2,\downarrow} \end{pmatrix}$$

4. Block diagonalizes the Hamiltonian by rotating the spin basis into x-direction. Can you represent this transformation and the result in the matrix formulation introduced in Eq. (5)? *Hint: This can be done by introducing the rotated quasi-particles* $\tilde{c}_{i,\uparrow} = \frac{1}{\sqrt{2}}(c_{i,\uparrow} + c_{i,\downarrow})$ *and* $\tilde{c}_{i,\downarrow} = \frac{1}{\sqrt{2}}(-c_{i,\uparrow} + c_{i,\downarrow})$. *(This has an insightful explanation. Which?)*

Solution: We want to transform the Hamiltonian into the x-spin basis. The transformation is performed with the field operators for the eigenmodes for S_x. The new basis is

$$\vec{d}_i = \frac{1}{\sqrt{2}} \begin{pmatrix} c_{i\uparrow} + c_{i\downarrow} \\ -c_{i\uparrow} + c_{i\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} .$$

For $i \in \{1, 2\}$, we can write

$$\vec{d} = \begin{pmatrix} d_{1\uparrow} \\ d_{1\downarrow} \\ d_{2\uparrow} \\ d_{2\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \overbrace{\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix}}^{U} \overbrace{\begin{pmatrix} c_{1\uparrow} \\ c_{1\downarrow} \\ c_{2\uparrow} \\ c_{2\downarrow} \end{pmatrix}}^{\vec{c}} ,$$

and

$$\vec{d}^\dagger = \begin{pmatrix} d^\dagger_{1\uparrow} & d^\dagger_{1\downarrow} & d^\dagger_{2\uparrow} & d^\dagger_{2\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \overbrace{\begin{pmatrix} c^\dagger_{1\uparrow} & c^\dagger_{1\downarrow} & c^\dagger_{2\uparrow} & c^\dagger_{2\downarrow} \end{pmatrix}}^{\vec{c}^\dagger} \overbrace{\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix}}^{U^\dagger} .$$

The matrix U is unitary. We therefore insert $UU^\dagger = U^\dagger U = \mathbb{I}$ and obtain

$$H = \overbrace{\begin{pmatrix} c^\dagger_{1,\uparrow} & c^\dagger_{1,\downarrow} & c^\dagger_{2,\uparrow} & c^\dagger_{2,\downarrow} \end{pmatrix} U^\dagger}^{=\sqrt{2}\ \vec{d}^\dagger} \ U \begin{pmatrix} 0 & B & 0 & t \\ B & 0 & t & 0 \\ 0 & t & 0 & B \\ t & 0 & B & 0 \end{pmatrix} U^\dagger \ \overbrace{U \begin{pmatrix} c_{1,\uparrow} \\ c_{1,\downarrow} \\ c_{2,\uparrow} \\ c_{2,\downarrow} \end{pmatrix}}^{=\sqrt{2}\ \vec{d}}$$

$$= \vec{d}^\dagger \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} 0 & B & 0 & t \\ B & 0 & t & 0 \\ 0 & t & 0 & B \\ t & 0 & B & 0 \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \vec{d}$$

$$= \underline{\underline{\vec{d}^\dagger \overbrace{\begin{pmatrix} B & 0 & t & 0 \\ 0 & -B & 0 & -t \\ t & 0 & B & 0 \\ 0 & -t & 0 & -B \end{pmatrix}}^{=h'} \vec{d}}}\,.$$

The new matrix h' is block diagonal and the Hamiltonian is block diagonalizable for all $B, t \in \mathbb{R}$. The rotation of the spin from the z-representation to the x-representation is done by rotating the spin around the y-axis with $\phi = \frac{\pi}{2}$. The general transformation is the spin representation of the rotation group

$$e^{\frac{i\phi}{2}} = \cos\frac{\phi}{2} + i\sin\frac{\phi}{2}\sigma_y$$

$$\Bigg| \quad \phi = \frac{\pi}{2}\mathbb{I}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \ .$$

End