Theoretische Festkörperphysik – Herbstsemester 2010 **Exercise series 5**
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Jordan-Wigner transformation and Majorana fermions

Motivation There is currently much excitement in parts of the condensed matter community because of a potential observability of Majorana fermions in solid state systems. Majorana fermions are are linear combinations of particle and antiparticle states (in condensed matter: particles and holes) such that the Majorana particle is its own antiparticle. In the second quantized language, the Majorana operators c are thus hermitian, $c^\dagger = c$ (hence they are often called "real" fermions). While such a fermion was over decades just a sometimes convenient theoretical trick for representing fermions, the mere possibility of actually observing such a state is already intriguing. In addition, however, there are by now proposals that build on Majorana fermions for the so-called topological quantum computation, which is a further driving force for many physicists.

In this exercise set, you will start from a simple spin-chain model. By a Jordan-Wigner (JW) transformation you will map it onto a fermionic system, which has Majorana edge states. Based on this insight, you are encouraged to speculate about what conditions must be fulfilled for a true electron system to exhibit similar physics.

Exercise 1: Spin chain and sketch of the phase diagram (2 points) Consider a one-dimensional system of spins $S = 1/2$ described by the Hamiltonian

$$H = \sum_i \left[J\sigma_i^x \sigma_{i+1}^x - h\sigma_i^z \right], \tag{1}$$

where i runs over the lattice sites and $\sigma_i^{x,y,z}$ are the Pauli matrices for the spin operators (the true spins are given by $S_i^{x,y,z} = \frac{\hbar}{2}\sigma_i^{x,y,z}$, but for simplicity we use the Pauli matrices with eigenvalues ± 1 here). Nearest neighbor spins interact by an antiferromagnetic exchange coupling $J > 0$, and h is a uniform external field in the x direction.

Determine the ground state spin configuration in the limits $J \gg |h|$ and $J \ll |h|$, and then give an argument at which ratio $J/|h|$ the transition from one to the other phase occurs.

Exercise 2: Jordan-Wigner transformation (2 points) The JW transformation is the mapping of the spin chain onto a system of spinless fermions. It is given by

$$\sigma_i^z = 2a_i^\dagger a_i - 1, \qquad \sigma_i^x = (a_i^\dagger + a_i)\prod_{j<i}\sigma_j^z, \qquad \sigma_i^y = -i(a_i^\dagger - a_i)\prod_{j<i}\sigma_j^z. \tag{2}$$

Show that these fermion operators a_i obey the anticommutation relations $\{a_i, a_j\} = 0$ and $\{a_i, a_j^\dagger\} = \delta_{ij}$. Explain why the $\prod_{j<i}\sigma_j^z$ is required and compare this with the definition of fermionic creation and annihilation operators given in the lectures. Show then that the Hamiltonian can be written as

$$H = \sum_i \left[-J(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + J(a_i a_{i+1} - a_i^\dagger a_{i+1}^\dagger) - 2h a_i^\dagger a_i \right], \tag{3}$$

and give an interpretation of the different terms.

Exercise 3: Spectrum for an infinite chain (3 points) Assume an infinite chain with lattice constant a. Show that the Hamiltonian can then be written in the form

$$
\begin{aligned}
H &= \sum_p \left\{ -2[h + J\cos(ap)]a_p^\dagger a_p - J(\mathrm{e}^{iap} a_p^\dagger a_{-p}^\dagger + \mathrm{e}^{-iap} a_{-p} a_p) \right\} \\
&= \sum_{p>0} (a_p^\dagger, a_{-p}) \begin{pmatrix} -2[h + J\cos(ap)] & 2iJ\sin(ap) \\ -2iJ\sin(ap) & +2[h + J\cos(ap)] \end{pmatrix} \begin{pmatrix} a_p \\ a_{-p}^\dagger \end{pmatrix},
\end{aligned} \tag{4}
$$

with p restricted to the first Brillouin zone $-\frac{\pi}{a} < p < \frac{\pi}{a}$. The diagonalization of such a Hamiltonian is known as a Bogoliubov transformation. For now, however, we are only interested in the spectrum. Calculate it (eigenvalues of the 2×2 matrix in Eq (4)) and show that there is a gap given by $\Delta = \min\{|J+h|, |J-h|\}$ such that all eigenvalues ϵ_p fulfill $\epsilon_p > \Delta$ or $\epsilon_p < -\Delta$.

Exercise 4: Majorana fermions (3 points) Note that σ_i^x and σ_i^y depend on the hermitian combinations $a_i^\dagger + a_i$ and $-i(a_i^\dagger - a_i)$. These are the combinations we can use to define Majorana fermions,

$$c_i^1 = a_i^\dagger + a_i, \qquad c_i^2 = -i(a_i^\dagger - a_i). \tag{5}$$

Show that $\{c_i^a, c_j^b\} = 2\delta_{ab}\delta_{ij}$ and that the Hamiltonian becomes

$$H = -i \sum_i \left[J c_i^2 c_{i+1}^1 - h c_i^2 c_i^1 \right] + \text{const.} \tag{6}$$

For a chain of finite length, $i = 1, \ldots, N$, most of the eigenstates have energies $\epsilon_n > \Delta$ or $\epsilon_n < -\Delta$ (with Δ given above), but there are in addition precisely 2 states of energies $\epsilon \approx 0$, one located near $i = 1$ and one near $i = N$. For simplicity, we consider here a semi-infinite system ($N \to \infty$), where only one bound state remains that has exactly $\epsilon = 0$. Show then that the bound state is of the form $|b_1\rangle = A(c_1^1 + \lambda c_2^1 + \lambda^2 c_3^1 + \ldots)|\rangle$. Show that it is a Majorana fermion, determine λ, and give the conditions necessary for the existence of the normalization constant A (i.e., such that the bound state can exist). For finite length N, estimate then the energy splitting between the bound states on both ends (remember the splitting between bonding and antibonding states in the H^2 molecule). In the limit $\lambda \to 0$, to which state does the bound state at $i = 1$ correspond?

Exercise 5: Majorana fermions with electrons (bonus) Reconsider now Eq. (4) and assume that the a_p describe real electrons. Speculate what type of interaction, band structure, etc. is necessary to obtain such a Hamiltonian. [Hint: Expressions of the form $a_p a_{-p}$ appear whenever superconductivity is involved, and they represent 2 electrons that are bound together in a Cooper pair. For conventional superconductors, the Cooper pairs are in a spin-singlet state and so the operators are complemented by spin indices $\sigma = \uparrow, \downarrow$ as $a_{p\uparrow} a_{-p\downarrow}$. What does this imply for the $a_{p\sigma}^\dagger a_{p\sigma}$ terms of the kinetic energy?]