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Exercise sheet 2

This exercise will be discussed on 3.12.2020

2. Majorana boundary state in the Kitaev's chain

Consider a chain consisting of $L \gg 1$ sites. Each site can be empty or occupied by an electron (with the fixed spin direction). The Hamiltonian of such chain reads

$$H = -\frac{w}{2}\sum_x (c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x) - \mu \sum_x c_x^\dagger c_x + \frac{\Delta}{2}\sum_x (c_x c_{x+1} + c_{x+1}^\dagger c_x^\dagger). \tag{1}$$

Here $w > 0$ is the hopping amplitude, μ is a chemical potential, and $\Delta > 0$ is the induced superconducting gap. To start, let us assume periodic boundary conditions and infinitely long chain with $L \gg 1$.

a) By introducing Fourier transform of electron operators $c_k = \frac{1}{\sqrt{L}}\sum_k c_k e^{ikx}$, verify that the Hamiltonian up to a constant term can be written in the Nambu form

$$H = \sum_{k>0} (c_k^\dagger, c_{-k}) \begin{pmatrix} \xi_k & \Delta_k \\ \Delta_k^* & -\xi_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}, \tag{2}$$

where $\xi_k = -(\mu + w\cos k)$ and $\Delta_k = i\Delta \sin k$

b) The Hamiltonian (2) can be diagonalized by the Bogolioubov transformation

$$\begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cos\theta_k & i\sin\theta_k \\ i\sin\theta_k & \cos\theta_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix},$$

where angle $\theta_{-k} = -\theta_k$ is odd function of k. Check that anti-commutation relations $\{\alpha_k, \alpha_{k'}^\dagger\} = \delta_{kk'}$ and $\{\alpha_k, \alpha_{k'}\} = 0$ are preserved for any angle θ_k.

c) Verify that the choice of a rotation angle to be $\sin 2\theta_k = -i\Delta_k/\epsilon_k$ with $\epsilon_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$ brings H to the canonical form

$$H = \sum_{k>0} \epsilon_k(\alpha_k^\dagger \alpha_k - \alpha_{-k}\alpha_{-k}^\dagger) = \sum_k \epsilon_k \alpha_k^\dagger \alpha_k + \text{Const}.$$

(note, that in the 2nd sum a summation goes over all momenta $k \in [-\pi, \pi]$).

Let us further consider a half-infinite chain with $x \in \mathbb{Z}$ and $x \geq 1$ and introduce two Majorana fermions

$$\gamma_x^A = i(c_x^\dagger - c_x), \qquad \gamma_x^B = c_x + c_x^\dagger$$

per each cite.

d) Check anti-commutation relations $\{\gamma_x^s, \gamma_{x'}^{s'}\} = 2\delta_{xx'}\delta_{ss'}$.

e) Show that the lattice Hamiltonian (1) takes the following form

$$H = -\frac{i\mu}{2}\sum_{x=1}^{+\infty}\gamma_x^B\gamma_x^A + \frac{i}{4}\sum_{x=1}^{+\infty}(w+\Delta)\gamma_x^A\gamma_{x+1}^B + \frac{i}{4}\sum_{x=1}^{+\infty}(-w+\Delta)\gamma_x^B\gamma_{x+1}^A,$$

when expressed via Majorana fermions.

In addition to the bulk spectrum ϵ_k, the half-chain may posses the boundary Majorana zero-mode γ_0 such that $[\gamma_0, H] = 0$. To find it one can initially derive a formal solution for the infinite chain.

f) Verify that the ansatz

$$\gamma_0 = \sum_x (C_+ z_+^x + C_- z_-^x)\gamma_x^B$$

solves the equation of motion $[\gamma_0, H] = 0$. Here $C_\pm$ are two arbitrary constants while $z_\pm$ are two roots of the quadratic equation

$$(w+\Delta)z^2 + 2\mu z + (w-\Delta) = 0.$$

Hint: to evaluate the commutator $[\gamma_0, H]$ one may use the relation $[A, BC] = \{A, B\}C - B\{A, C\}$ which is valid for any operators A, B and C.

g) The boundary condition for half-infinite chain put the restriction on $C_\pm$. Check that the latter leads to $C_+ = -C_-$, i.e. a zero-mode becomes

$$\gamma_0 = \mathcal{N}^{-1/2}\sum_{x=1}^{+\infty}(z_+^x - z_-^x)\gamma_x^B. \tag{3}$$

h) The physical zero-energy boundary mode must be localized close to the left end of the half-chain. It is possible only if $|z_\pm| < 1$. Check that the condition for existence of the Majorana boundary modes is $w > |\mu|$. A normalization constant in Eq. (3) then can be chosen from the condition $\gamma_0^2 = 1$ (you are not supposed to find it, this is not essential!).

INFO: In the latter case, one says that the chain is found in the 'topologically non-trivial' state. On other hand, at $w < |\mu|$ the solution γ_0 is non-normalizable and hence the Majonana boundary mode is absent — this corresponds to the 'topologically trivial' state of the Kitaev's chain.