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Exercise sheet 2

Solution

3. 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 the Fourier transform for electron operators $c_x = \frac{1}{\sqrt{L}}\sum_k c_k e^{ikx}$, one needs to show 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 $\Delta_k = -i\Delta \sin k$.

We use the identity $\frac{1}{L}\sum_x e^{ikx - ik'x} = \delta_{kk'}$. Then the 1st term in Eq. (1) becomes

$$-\frac{w}{2L}\sum_{x,kk'} \left(e^{-ikx} e^{ik'(x+1)} c_k^\dagger c_{k'} + \text{h.c.}\right) \overset{k=k'}{=} -\frac{w}{2}\sum_k (e^{-ik} c_k^\dagger c_k + \text{h.c.}) = -w\sum_k \cos k\, c_k^\dagger c_k. \tag{3}$$

In a similar way the term proportional to a chemical potential transforms into

$$-\frac{\mu}{L}\sum_{x,kk'} e^{-ikx} e^{ik'x} c_k^\dagger c_{k'} \overset{k=k'}{=} -\mu \sum_k c_k^\dagger c_k. \tag{4}$$

For the order parameter term one gets

$$\frac{\Delta}{2L}\sum_{x,kk'} \left(e^{ikx} e^{ik'(x+1)} c_k c_{k'} + \text{h.c.}\right) \overset{k=-k'}{=} \frac{\Delta}{2}\sum_k (e^{ik} c_{-k} c_k + \text{h.c.}) \tag{5}$$

$$= \frac{\Delta}{2}\sum_{k>0} (e^{ik} c_{-k} c_k + \text{h.c.}) + \frac{\Delta}{2}\sum_{k<0} (e^{ik} c_k c_{-k} + \text{h.c.}) = i\Delta \sum_{k>0} \sin k (c_{-k} c_k - c_k^\dagger c_{-k}^\dagger). \tag{6}$$

Here, to get the very last expression, one needs to change $k \to -k$ in the 2nd sum. Now, using $c_k^\dagger c_k = 1 - c_k c_k^\dagger$ one can rewrite

$$(3) \quad = \quad -w\sum_{k>0} \cos k\, c_k^\dagger c_k + w\sum_{k>0} \cos k\, c_{-k} c_{-k}^\dagger, \tag{7}$$

$$(4) \quad = \quad -\mu \sum_{k>0} c_k^\dagger c_k + \mu \sum_{k>0} c_{-k} c_{-k}^\dagger. \tag{8}$$

Introducing a dispersion relation $\xi_k = -(\mu + w\cos k)$ and the momentum dependent 'p-wave' order parameter $\Delta_k = -i\Delta \sin k$, Eqs. (7,8) and (6) give the desired Nambu representation, Eq. (2).

b) The next task is to diagonalize the Hamiltonian (2) by the Bogolioubov transformation

$$\begin{pmatrix} \alpha_k \\ \alpha^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} \cos\theta_k & i\sin\theta_k \\ i\sin\theta_k & \cos\theta_k \end{pmatrix} \begin{pmatrix} c_k \\ c^\dagger_{-k} \end{pmatrix},$$

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

Let's introduce $\overrightarrow{c_k} = \begin{pmatrix} c_k \\ c^\dagger_{-k} \end{pmatrix}$ and $\overrightarrow{\alpha_k} = \begin{pmatrix} \alpha_k \\ \alpha^\dagger_{-k} \end{pmatrix}$. Then the Bogolioubov transformation written in a matrix form becomes $\overrightarrow{\alpha_k} = e^{i\theta_k\sigma_1}\overrightarrow{c_k}$ and $\overrightarrow{\alpha_k}^\dagger = \overrightarrow{c_k}^\dagger e^{-i\theta_k\sigma_1}$. It suffices then to discuss the case $k = k'$ only, since for different momenta all operators anti-commute anyway. Thus, omitting k, one can write $\{(\overrightarrow{c})_\mu, (\overrightarrow{c})^\dagger_\nu\} = \delta_{\mu\nu}$, where Greek indices refer to the Nambu space. The latter gives

$$\begin{aligned} &\{(\overrightarrow{\alpha})_\mu, (\overrightarrow{\alpha})^\dagger_\nu\} = \{(e^{i\theta_k\sigma_1}\overrightarrow{c})_\mu, (\overrightarrow{c}^\dagger e^{-i\theta_k\sigma_1})_\nu\} = \{(e^{i\theta_k\sigma_1})_{\mu\rho}(\overrightarrow{c})_\rho, (\overrightarrow{c}^\dagger)_\sigma(e^{-i\theta_k\sigma_1})_{\sigma\nu}\} \\ \overset{\rho=\sigma}{=} \;&(e^{i\theta_k\sigma_1})_{\mu\rho}(e^{-i\theta_k\sigma_1})_{\rho\nu} = \delta_{\mu\nu}. \end{aligned} \tag{9}$$

c) We now 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

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

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

Using vectors $\overrightarrow{\alpha_k}$ the Hamiltonian in its canonical form reads

$$H = \sum_{k>0} \epsilon_k \overrightarrow{\alpha_k}^\dagger \sigma_3 \overrightarrow{\alpha_k}. \tag{10}$$

Expressing the latter in terms of original operators c_k and $c^\dagger_k$ it becomes

$$H = \sum_{k>0} \epsilon_k \overrightarrow{c_k}^\dagger e^{-i\theta_k\sigma_1}\sigma_3 e^{i\theta_k\sigma_1}\overrightarrow{c_k} = \sum_{k>0} \epsilon_k \overrightarrow{c_k}^\dagger \sigma_3 e^{2i\theta_k\sigma_1}\overrightarrow{c_k}. \tag{11}$$

When written explicitly in the Nambu form, it reads

$$H = \sum_{k>0} (c^\dagger_k, c_{-k}) \begin{pmatrix} \epsilon_k\cos 2\theta_k & i\epsilon_k \sin 2\theta_k \\ -i\epsilon_k\sin 2\theta_k & -\epsilon_k\cos 2\theta_k \end{pmatrix} \begin{pmatrix} c_k \\ c^\dagger_{-k} \end{pmatrix}, \tag{12}$$

From here the required relations, $\sin 2\theta_k = -i\Delta_k/\epsilon_k$ and $\epsilon_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$, follow.

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

$$\gamma^A_x = i(c^\dagger_x - c_x), \qquad \gamma^B_x = c_x + c^\dagger_x$$

per each cite.

d) Checking anti-commutation relations $\{\gamma^s_x, \gamma^{s'}_{x'}\} = 2\delta_{xx'}\delta_{ss'}$ is straightforward.

e) Next one can show that the lattice Hamiltonian (1) takes the following form (up to a constant)

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

when expressed via Majorana fermions.

Let's discuss the hopping term as an example.

$$-\frac{w}{2}\sum_{x=1}^{+\infty}(c_x^\dagger c_{x+1} + \text{h.c.}) = -\frac{w}{8}\sum_{x=1}^{+\infty}(\gamma_x^B - i\gamma_x^A)(\gamma_{x+1}^B + i\gamma_{x+1}^A) + \text{h.c.} \tag{13}$$

$$= \quad -\frac{w}{8}\sum_{x=1}^{+\infty}(\gamma_x^B\gamma_{x+1}^B + i\gamma_x^B\gamma_{x+1}^A - i\gamma_x^A\gamma_{x+1}^B + \gamma_x^A\gamma_{x+1}^A) + \text{h.c.} \tag{14}$$

At this stage we use that $\gamma_x^A\gamma_{x+1}^A + \text{h.c.} = \gamma_x^A\gamma_{x+1}^A + \gamma_{x+1}^A\gamma_x^A = \{\gamma_x^A, \gamma_{x+1}^A\} = 0$ and the same for $\gamma_x^B\gamma_{x+1}^B$ term. On other hand $i\gamma_x^B\gamma_{x+1}^A + \text{h.c.} = 2i\gamma_x^B\gamma_{x+1}^A$ and $-i\gamma_x^A\gamma_{x+1}^B + \text{h.c.} = -2i\gamma_x^A\gamma_{x+1}^B$. Therefore the kinetic term reads

$$(14) = \frac{iw}{4}\sum_{x=1}^{+\infty}(\gamma_x^A\gamma_{x+1}^B - \gamma_x^B\gamma_{x+1}^A). \tag{15}$$

Other pieces of the Hamiltonian can be re-expressed in terms of Majorana operators in a similar fashion. For the μ-term one finds

$$\begin{aligned} - \quad & \mu\sum_{x=1}^{+\infty}c_x^\dagger c_x = -\frac{\mu}{4}\sum_{x=1}^{+\infty}(\gamma_x^B - i\gamma_x^A)(\gamma_x^B + i\gamma_x^A) = -\frac{\mu}{4}\sum_{x=1}^{+\infty}(2 + i\gamma_x^B\gamma_x^A - i\gamma_x^A\gamma_x^B) = \\ - \quad & \frac{i\mu}{2}\sum_{x=1}^{+\infty}\gamma_x^B\gamma_x^A + \text{Const.} \end{aligned} \tag{16}$$

And the Δ-term transforms as

$$\frac{\Delta}{2}\sum_{x=1}^{+\infty}(c_x c_{x+1} + \text{h.c.}) = \frac{\Delta}{8}\sum_{x=1}^{+\infty}(\gamma_x^B + i\gamma_x^A)(\gamma_{x+1}^B + i\gamma_{x+1}^A) + \text{h.c.} = \frac{i\Delta}{4}\sum_{x=1}^{+\infty}(\gamma_x^A\gamma_{x+1}^B + \gamma_x^B\gamma_{x+1}^A) \tag{17}$$

Then the sum of (15), (16) and (17) gives the required Hamiltonian.

f) 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 we initially derive a formal solution for the infinite chain. For that we 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

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

To prove it we use the relation

$$[A, BC] = \{A, B\}C - B\{A, C\}, \tag{18}$$

which is valid for any operators A, B and C. Indeed $\{A,B\}C - B\{A,C\} = ABC + BAC - BAC - BCA = ABC - BCA = [A, BC]$.

Let's further assume that $\gamma_0 = \sum_x z^x \gamma_x^B$ and derive the equation for z from $[\gamma_0, H] = 0$ using the relation (18). We apply the latter to each term of H. For the μ-term one finds

$$-\frac{i\mu}{2}\sum_{x,x'=1}^{+\infty} z^x[\gamma_x^B, \gamma_{x'}^B\gamma_{x'}^A] = -\frac{i\mu}{2}\sum_{x,x'=1}^{+\infty} z^x\{\gamma_x^B, \gamma_{x'}^B\}\gamma_{x'}^A \overset{x=x'}{=} -i\mu\sum_{x=1}^{+\infty} z^x\gamma_x^A. \tag{19}$$

The $(w+\Delta)$-term gives

$$\frac{i}{4}(w+\Delta)\sum_{x,x'=1}^{+\infty} z^x[\gamma_x^B, \gamma_{x'}^A\gamma_{x'+1}^B] = -\frac{i}{4}(w+\Delta)\sum_{x,x'=1}^{+\infty} z^x\gamma_{x'}^A\{\gamma_x^B, \gamma_{x'+1}^B\} \overset{x=x'+1}{=}$$
$$-\frac{i}{2}(w+\Delta)\sum_{x'=1}^{+\infty} z^{x'+1}\gamma_{x'}^A \overset{x'\to x}{=} -\frac{i}{2}(w+\Delta)\sum_{x=1}^{+\infty} z^{x+1}\gamma_x^A, \tag{20}$$

while the $(-w+\Delta)$-term brings us

$$\frac{i}{4}(-w+\Delta)\sum_{x,x'=1}^{+\infty} z^x[\gamma_x^B, \gamma_{x'}^B\gamma_{x'+1}^A] = \frac{i}{4}(-w+\Delta)\sum_{x,x'=1}^{+\infty} z^x\{\gamma_x^B, \gamma_{x'}^B\}\gamma_{x'+1}^A \overset{x'=x}{=}$$
$$\frac{i}{2}(-w+\Delta)\sum_{x=1}^{+\infty} z^x\gamma_{x+1}^A \overset{x\to x-1}{=} \frac{i}{2}(-w+\Delta)\sum_{x=2}^{+\infty} z^{x-1}\gamma_x^A. \tag{21}$$

Summing up (19), (20) and (21) we find the commutator

$$[\gamma_0, H] = -i\mu\sum_{x=1}^{+\infty} z^x\gamma_x^A - \frac{i}{2}(w+\Delta)\sum_{x=1}^{+\infty} z^{x+1}\gamma_x^A + \frac{i}{2}(-w+\Delta)\sum_{x=2}^{+\infty} z^{x-1}\gamma_x^A. \tag{22}$$

From here it follows that for all $x \geq 2$ the commutator is zero provided

$$-i\mu - \frac{i}{2}(w+\Delta)z + \frac{i}{2}(-w+\Delta)z^{-1} = 0, \tag{23}$$

which gives the required quadratic equation.

g) The point $x = 1$ is special since the last sum in Eq. (22) starts from a cite $x = 2$. We thus assume that $\gamma_0 = \sum_{x=1}^{+\infty}(C_+ z_+^x + C_- z_-^x)\gamma_x^B$ and find the constrain on $C_\pm$.

The relation (22) at $x = 1$ reduces to

$$-i\mu(z_+C_+ + z_-C_-) - \frac{i}{2}(w+\Delta)(z_+^2C_+ + z_-^2C_-) = 0. \tag{24}$$

But we know that $z_\pm$ are the roots of quadratic equation (23). Hence the relation (24) yields $\frac{i}{2}(-w+\Delta)(C_+ + C_-) = 0$ or $C_- = -C_+$. Hence

$$\gamma_0 \propto \sum_{x=1}^{+\infty}(z_+^x - z_-^x)\gamma_x^B \tag{25}$$

is a possible zero mode up to a normalization constant provided both terms decay at $x \to +\infty$. The latter requires $|z_\pm| < 1$.

h) One needs to check that the condition for existence of the Majorana boundary modes is $w > |\mu|$.

The latter condition guarantees that $|z_\pm| < 1$. Indeed, from the quadratic equation for z it follows that $z_+z_- = (w-\Delta)(w+\Delta)$. Since both $w > 0$ and $\Delta > 0$ (by the initial assumption), we see that $|z_+z_-| < 1$. In particular, at the special point $\mu = w$ one finds that $z_+ = (w-\Delta)/(w+\Delta)$ and $z_- = -1$. Then the direct inspection shows that if $\mu > 0$ then $|z_-| < 1$ at $\mu < w$ and $|z_-| > 1$ otherwise. The case $\mu < 0$ can be analyzed in a similar way.