Problems Day 1 PhD school: Vietri Sul Mare 2018

Problem 1: Majorana fermions and superconductivity

Consider the following toy model (Kitaev chain) of a spinless p-wave superconductor in one dimension (Kitaev 2001)

$$H = -\mu \sum_{i=1}^{N} c_{i}^{\dagger} c_{i} - t \sum_{i=1}^{N-1} \left(c_{i}^{\dagger} c_{i+1} + c_{i+1}^{\dagger} c_{i} \right) - \Delta \sum_{i=1}^{N-1} \left(c_{i} c_{i+1} + c_{i+1}^{\dagger} c_{i}^{\dagger} \right)$$
(1)

Note that not only the hopping terms but also the pairing terms involve products of operators on neighboring sites. This is required of the fact that we consider spinless fermions for which $c_i c_i$ and $c_i^{\dagger} c_i^{\dagger}$ would vanish.

In this problem, we consider a finite chain with N sites.

(a) Introduce Majorana fermion operators γ_{Aj} and γ_{Bj} through

$$c_j = \frac{1}{2} (\gamma_{Bj} + i\gamma_{Aj})$$
 with $\gamma^{\dagger}_{\alpha i} = \gamma_{\alpha i}$

(similar to separating a complex number z = x + iy into real and imaginary part). Show that the fermion anti-commutation relations

$$\{c_i, c_j\} = \left\{c_i^{\dagger}, c_j^{\dagger}\right\} = 0 \qquad \left\{c_i, c_j^{\dagger}\right\} = \delta_{ij}$$

imply for the real or Majorana fermions

$$\{\gamma_{\alpha i}, \gamma_{\beta j}\} = 2\delta_{\alpha\beta}\delta_{ij}$$

Physically, the relation $\gamma_{\alpha i} = \gamma_{\alpha i}^{\dagger}$ says that Majorana fermions are their own antiparticles.

(b) Now consider the Hamiltonian (1) in the special case $\mu = 0$ and $t = \Delta$ and show that it can then be written as

$$H = -\mathrm{i}t \sum_{i=1}^{N-1} \gamma_{Bi} \gamma_{Ai+1}$$

Note that γ_{A1} and γ_{BN} are *not* contained in H!

(c) Now introduce new (conventional) fermion operators

$$d_i = \frac{1}{2} (\gamma_{Bi} - i\gamma_{Ai+1})$$
 $i = 1, ..., N - 1$

(Check that the d_i satisfy the appropriate commutation relations.) Note that there were $N c_i$ operators, but that there are only $(N-1) d_i$ -operators. Show that in terms of the d's

$$H = 2t \sum_{i=1}^{N-1} \left(d_i^{\dagger} d_i - \frac{1}{2} \right)$$

Also express the d_i in terms of the original fermion operators c_i and c_i^{\dagger} .

(d) Discuss the eigenstates and the spectrum of H, paying particular attention to the degeneracy of the ground state. Argue (without explicitly redoing the derivations) whether the degeneracy is stable if one varies the parameters of the model away from $\mu = 0$, $\Delta = t$.

Problem 2: Kitaev chain with periodic boundary conditions

Consider the Kitaev chain with N sites

$$H = -\mu \sum_{i=1}^{N} c_{i}^{\dagger} c_{i} - t \sum_{i=1}^{N} \left(c_{i}^{\dagger} c_{i+1} + c_{i+1}^{\dagger} c_{i} \right) - \Delta \sum_{i=1}^{N} \left(c_{i} c_{i+1} + c_{i+1}^{\dagger} c_{i}^{\dagger} \right)$$

and periodic boundary conditions, i.e., with the identifications $c_{N+1} = c_1$. The purpose of this problem is to look at the bulk spectrum and the phase diagram of the Kitaev chain from the point of view of the Bogoliubov-de Gennes Hamiltonian.

(a) Rewrite the Hamiltonian in momentum space by introducing a_k through

$$c_j = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{\mathrm{i}kj} a_k \,.$$

Show that the a_k satisfy the canonical anti-commutation relations and that the Hamiltonian takes the form

$$H = \sum_{k} \xi_k a_k^{\dagger} a_k - \Delta \sum_{k} \left(e^{ik} a_{-k} a_k + e^{-ik} a_k^{\dagger} a_{-k}^{\dagger} \right) ,$$

where $\xi_k = -2t \cos k - \mu$.

(b) Define Nambu operators

$$\phi_k = \left(\begin{array}{c} a_k \\ a^{\dagger}_{-k} \end{array}\right) \,,$$

where k > 0! Show that the ϕ_k satisfy the expected anti-commutation relations. Show that up to constants, the Hamiltonian takes the form

$$H = \sum_{k>0} \phi_k^{\dagger} \begin{pmatrix} \xi_k & 2i\Delta\sin k \\ -2i\Delta\sin k & -\xi_k \end{pmatrix} \phi_k$$

Explain why the k = 0 mode is not very interesting (and has actually been dropped in this expression for H.)

(c) Show that the excitation spectrum of the Kitaev chain is

$$E_k = \pm \sqrt{\xi_k^2 + 4\Delta^2 \sin^2 k}$$

(d) Draw a phase diagram as function of μ and Δ with the line where the gap (i.e. the smallest $|E_k|$ for any k) vanishes. Note, however, that the gap is nonzero on *both* sides of this line. This is a consequence of a *topological* phase transition in this model. One finds that there are edge Majorana fermions similar to those found in problem 1 throughout one of these phases which are topologically protected as long as the gap does not close.

Problem 3: Kitaev chain near the topological phase transition

Lets now consider $\mu \simeq -2t$ where we can focus our attention on small k (since the gap is minimal at k = 0). Writing $\mu = -2t + \delta\mu$, we can then approximate

$$\xi_k = -2t\cos k - \mu \simeq -\delta\mu + \mathcal{O}\left(k^2\right)$$

2i $\Delta \sin k \simeq 2i\Delta k$

so that the Bogoliubov-de Gennes Hamiltonian takes the form

$$\mathcal{H} = \left(\begin{array}{cc} -\delta\mu & 2\mathrm{i}\Delta k\\ -2\mathrm{i}\Delta k & \delta\mu \end{array}\right)$$

in momentum space or

$$\mathcal{H} = \left(\begin{array}{cc} -\delta\mu & 2\Delta\partial_x \\ -2\Delta\partial_x & \delta\mu \end{array}\right)$$

in real space. This can now be used to investigate the effect of slowly varying chemical potentials. Assume in particular that

$$\delta\mu(x) = \alpha x$$

i.e. the system is nominally on opposite sides of the topological phase transition for x < 0 and x > 0. Show that the spectrum of this Hamiltonian is given by

$$E_n^{\pm} = 4\alpha\Delta\left(n+\frac{1}{2}\right) \mp 2\Delta\alpha$$

Note that $E_0^+ = 0!$ This is reminiscent of the edge Majorana modes of problem 1 and in fact, you can entertain yourself by showing that the corresponding Bogoliubov operator is a Majorana operator!

Hint: To derive the spectrum, you may find it helpful to introduce Pauli matrices in Nambu space and consider \mathcal{H}^2 instead of \mathcal{H} . The latter is not losing any information since by symmetry, the eigenenergies of the BdG Hamiltonian come in pairs $\pm E_k$.