BdG recap

generic meanfield SC Hamiltonian in <u>real space</u> rewritten in with the BdG trick

$$H = \sum_{ij} h_{ij} c_i^\dagger c_j + \Delta_{ij} c_i^\dagger c_j^\dagger + \text{h.c.} = \sum_n E_n d_n^\dagger d_n \tag{1}$$

$$= \frac{1}{2} \begin{pmatrix} \underline{c}^\dagger & \underline{c} \end{pmatrix} \underbrace{\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}}_{\mathcal{H}_{BdG}} \begin{pmatrix} \underline{c} \\ \underline{c}^\dagger \end{pmatrix} + \frac{1}{2}\text{Tr}[h]\mathbb{I} \tag{2}$$

Where we introduced the (Nambu) spinor $\begin{pmatrix} \underline{c} \\ \underline{c}^\dagger \end{pmatrix}$ built from creation and annihilation operators. Remember that hermiticity of H requires $h = h^\dagger$ and $\Delta = -\Delta^\top$. The <u>positive</u> eigenvalues of the BdG matrix give the excitation spectrum.

$$\mathcal{H}_{BdG}\psi_n = E_n \psi_n \tag{3}$$

The BdG trick <u>forces</u> PHS on $\mathcal{H}_{BdG}$ this is not a physical it is built in the formalism. PHS is represented

$$\mathcal{P} = \sigma_x \mathcal{K}_R \tag{4}$$

where σ_x is the appropriate Pauli matrix in Nambu space and the operator $\mathcal{K}_R$ is complex conjugation in <u>real space.</u> The effect of PHS is

$$\mathcal{P}\mathcal{H}_{BdG}\mathcal{P}^{-1} = \sigma_x \mathcal{K}_R \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \mathcal{K}_R \sigma_x = \sigma_x \begin{pmatrix} h^* & \Delta^* \\ -\Delta & -h \end{pmatrix} \sigma_x = \begin{pmatrix} -h & -\Delta \\ \Delta^* & h^* \end{pmatrix} = -\mathcal{H}_{BdG} \tag{5}$$

Kitaev wire

the simplest superconducting model for spinless fermions

$$H_K = \sum_p -\mu c_p^\dagger c_p - t\left(c_p^\dagger c_{p+1} + c_{p+1}^\dagger c_p\right) + \Delta^* c_{p+1}^\dagger c_p^\dagger + \Delta c_p c_{p+1} \tag{6}$$

take a 3 site peace

$$\begin{aligned} H_{3K} &= \mu\left(c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3\right) - t\left(c_1^\dagger c_2 + c_2^\dagger c_3 + c_2^\dagger c_1 + c_3^\dagger c_2\right) + \Delta\left(c_1 c_2 + c_2 c_3\right) + \Delta^*\left(c_2^\dagger c_1^\dagger + c_3^\dagger c_2^\dagger\right) \\ &= \frac{1}{2}\left[\mu\left(c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3\right) - t\left(c_1^\dagger c_2 + c_2^\dagger c_3 + c_2^\dagger c_1 + c_3^\dagger c_2\right) + \Delta\left(c_1 c_2 + c_2 c_3\right) + \Delta^*\left(c_2^\dagger c_1^\dagger + c_3^\dagger c_2^\dagger\right)\right. \\ &\quad \left. - (\circlearrowright)\right] + \frac{3}{2}\mu\mathbb{I} \end{aligned}$$

here $\circlearrowright$ means the reversal of all operator sequences. Let us cast this in the BdG form

$$H_{3K} = \frac{1}{2} C^\dagger \mathcal{H}_{BdG} C + \frac{1}{2}\text{Tr}[h]\mathbb{I} \tag{7}$$

with a slightly different definition for C, namely take $C^\dagger = \begin{pmatrix} c_1^\dagger & c_1 & c_2^\dagger & c_2 & c_3^\dagger & c_3 \end{pmatrix}$ that is group operators acting on the same site together. With this choice

$$\mathcal{H}_{BdG} = \begin{pmatrix} -\mu & 0 & -t & -\Delta^* & & \\ 0 & \mu & \Delta & t & & \\ -t & \Delta^* & -\mu & 0 & -t & -\Delta^* \\ -\Delta & t & 0 & \mu & \Delta & t \\ & & -t & \Delta^* & -\mu & 0 \\ & & -\Delta & t & 0 & \mu \end{pmatrix} = \begin{pmatrix} U & T & \\ T^\dagger & U & T \\ & T^\dagger & U \end{pmatrix} \tag{8}$$

with

$$U = \begin{pmatrix} -\mu & 0 \\ 0 & \mu \end{pmatrix} = -\mu\sigma_z,\ T = \begin{pmatrix} -t & -\Delta^* \\ \Delta & t \end{pmatrix} = -t\sigma_z + \mathrm{i}\left(\text{Im}\left(\Delta\right)\sigma_x - \text{Re}\left(\Delta\right)\sigma_y\right) \tag{9}$$

PHS in this case is given by

$$\mathcal{P}_l = \sigma_x \mathcal{K},\ \mathcal{P} = \begin{pmatrix} \mathcal{P}_l & & \\ & \mathcal{P}_l & \\ & & \mathcal{P}_l \end{pmatrix} = \begin{pmatrix} \sigma_x & & \\ & \sigma_x & \\ & & \sigma_x \end{pmatrix} \mathcal{K} \tag{10}$$

where σ_x acts on the local Nambu spinor $f_p = \begin{pmatrix} c_p \\ c_p^\dagger \end{pmatrix}$ and $\mathcal{K}$ is just a complex conjugation, as one would expect it from a complex conjugation in real space. Note that

$$\mathcal{P}_l U \mathcal{P}_l^{-1} = \sigma_x \mathcal{K} \left(-\mu\sigma_z\right) \mathcal{K} \sigma_x = \mu\sigma_z = -U \tag{11}$$

$$\mathcal{P}_l T \mathcal{P}_l^{-1} = \sigma_x \mathcal{K} \left[-t\sigma_z + \mathrm{i}\left(\mathrm{Im}\left(\Delta\right)\sigma_x - \mathrm{Re}\left(\Delta\right)\sigma_y\right)\right] \mathcal{K}\sigma_x = \left[t\sigma_z - \mathrm{i}\left(\mathrm{Im}\left(\Delta\right)\sigma_x - \mathrm{Re}\left(\Delta\right)\sigma_y\right)\right] = -T \tag{12}$$

here we make use of

$$\sigma_x\sigma_y\sigma_x = -\sigma_y, \;\; \sigma_x\sigma_z\sigma_x = -\sigma_z, \;\; \mathcal{K}\sigma_y\mathcal{K} = -\sigma_y \tag{13}$$

thus we have as we expected

$$\mathcal{P}\mathcal{H}_{BdG}\mathcal{P}^{-1} = \begin{pmatrix} \mathcal{P}_l U \mathcal{P}_l^{-1} & \mathcal{P}_l T \mathcal{P}_l^{-1} & \\ \mathcal{P}_l T \mathcal{P}_l^{\dagger -1} & \mathcal{P}_l U \mathcal{P}_l^{-1} & \mathcal{P}_l T \mathcal{P}_l^{-1} \\ & \mathcal{P}_l T \mathcal{P}_l^{\dagger -1} & \mathcal{P}_l U \mathcal{P}_l^{-1} \end{pmatrix} = -\mathcal{H}_{BdG} \tag{14}$$

let us now consider an infinite chain! It is natural to rewrite the Hamiltonian of the system with the above defined U and T matrices and the local Nambu spinor operators

$$f_p = \begin{pmatrix} c_p \\ c_p^\dagger \end{pmatrix} \tag{15}$$

$$H_K = \frac{1}{2}\sum_p \left(f_p^\dagger U f_p + f_p^\dagger T f_{p+1} + f_{p+1}^\dagger T^\dagger f_p \right) + \text{const} \tag{16}$$

This system has translational invariance and hence we cast it in terms of planewaves.

$$f_k = \sum_p f_p e^{\mathrm{i}kp}, \;\; f_p = \sum_k f_k e^{-\mathrm{i}kp} \tag{17}$$

$$f_k^\dagger = \sum_p f_p^\dagger e^{-\mathrm{i}kp}, \;\; f_p^\dagger = \sum_k f_k^\dagger e^{\mathrm{i}kp} \tag{18}$$

$$H_K = \frac{1}{2}\sum_{pkk'} f_k^\dagger \left(U + T e^{-\mathrm{i}k'} + T^\dagger e^{\mathrm{i}k} \right) f_{k'} e^{\mathrm{i}(k-k')p} \tag{19}$$

$$= \frac{1}{2}\sum_k f_k^\dagger \underbrace{\left(U + T e^{-\mathrm{i}k} + T^\dagger e^{\mathrm{i}k} \right)}_{\mathcal{H}_{BdG}(k)} f_k \tag{20}$$

where we made use of $\sum_p e^{\mathrm{i}(k-k')p} = \delta_{k,k'}$. Fun fact

$$f_k = \sum_p f_p e^{\mathrm{i}kp} = \sum_p \begin{pmatrix} c_p \\ c_p^\dagger \end{pmatrix} e^{\mathrm{i}kp} = \begin{pmatrix} \sum_p c_p e^{\mathrm{i}kp} \\ \sum_p c_p^\dagger e^{\mathrm{i}kp} \end{pmatrix} = \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \tag{21}$$

in k space the momentum of the holes is reversed! Consider the effect of complex conjugation in <u>real space</u> on the momentum space BdG matrix

$$\mathcal{K}_R\mathcal{H}_{BdG}(k)\mathcal{K}_R = \left(U^* + T^* e^{-\mathrm{i}k} + \left(T^\dagger\right)^* e^{\mathrm{i}k} \right) \tag{22}$$

$$= \left(U + T e^{\mathrm{i}k} + \left(T^\dagger\right) e^{-\mathrm{i}k} \right)^* = \mathcal{H}_{BdG}^*(-k) \tag{23}$$

that is real space conjugation flips k as well. Considering now the effect PHS we have

$$\mathcal{P}\mathcal{H}_{BdG}(k)\mathcal{P}^{-1} = \left(-U - T e^{-\mathrm{i}k} - T^\dagger e^{\mathrm{i}k} \right) = -\mathcal{H}_{BdG}(k) \tag{24}$$

note that it is a common practice in literature to give the operator representing PHS in momentum space as

$$\mathcal{P}' = \sigma_x \mathcal{K} \tag{25}$$

here $\mathcal{K}$ is just conjugation, or conjugation defined in momentum space, with this operator PHS is expressed as

$$\mathcal{P}'\mathcal{H}_{BdG}(k)\mathcal{P}'^{-1} = \left(-U - T e^{\mathrm{i}k} - T^\dagger e^{-\mathrm{i}k} \right) = -\mathcal{H}_{BdG}(-k) \tag{26}$$

thus one has to be careful.

For the Kitaev chain we have

$$U = \begin{pmatrix} -\mu & 0 \\ 0 & \mu \end{pmatrix} = -\mu\sigma_z,\ T = \begin{pmatrix} -t & -\Delta^* \\ \Delta & t \end{pmatrix} = -t\sigma_z + \mathrm{i}\left(\mathrm{Im}\left(\Delta\right)\sigma_x - \mathrm{Re}\left(\Delta\right)\sigma_y\right) \tag{27}$$

$$\mathcal{H}_{BdG}(k) = \left(U + Te^{-\mathrm{i}k} + T^\dagger e^{\mathrm{i}k}\right) = \sigma_z\left(-\mu - 2t\cos\left(k\right)\right) + 2\sin\left(k\right)\left(\mathrm{Im}\left(\Delta\right)\sigma_x - \mathrm{Re}\left(\Delta\right)\sigma_y\right) = \vec{h}(k)\cdot\vec{\sigma} \tag{28}$$

$$\vec{h}(k) = \begin{pmatrix} 2\sin\left(k\right)\mathrm{Im}\left(\Delta\right) \\ -2\sin\left(k\right)\mathrm{Re}\left(\Delta\right) \\ \left(-\mu - 2t\cos\left(k\right)\right) \end{pmatrix} \tag{29}$$

note that the elements of this vector must be real to guarantee that the Hamiltonian is hermitian!

$$E_k = \left|\vec{h}(k)\right| \tag{30}$$

since we are only interested in positive energies.

DISCUSS HERE SHAPE OF SPECTRUM!! PICTURES AND NOTEBOOKS!

A generic "2band" BdG matrix will also have the general form

$$\mathcal{H}_{BdG}(k) = \vec{h}(k)\cdot\vec{\sigma} = h_x(k)\sigma_x + h_y(k)\sigma_y + h_z(k)\sigma_z \tag{31}$$

let us see what restrictions does PHS give for this general case

$$\mathcal{P}\mathcal{H}_{BdG}(k)\mathcal{P}^{-1} = \sigma_x\mathcal{K}_R\vec{h}(k)\cdot\vec{\sigma}\mathcal{K}_R\sigma_x = \sigma_x\left[h_x(-k)\sigma_x - h_y(-k)\sigma_y + h_z(-k)\sigma_z\right]\sigma_x \tag{32}$$

$$= \left[h_x(-k)\sigma_x + h_y(-k)\sigma_y - h_z(-k)\sigma_z\right] \stackrel{!}{=} -\vec{h}(k)\cdot\vec{\sigma} \tag{33}$$

thus we require that the x and y component be an odd function of k while the z component should be even.

$$h_{x/y}(-k) = -h_{x/y}(k),\ h_z(-k) = h_z(k) \tag{34}$$

This gives us a possibility for the definition of a topological invariant

DISCUSS HERE 8-0 TOPLOGICAL INVARIANT WITH THE BALL

Majorana fermions

Topological invariants of insulators sign boundary modes. Boundary modes of the Kitaev wire can be cast in terms of MFs. Algebraic properties of Majorana operators

$$b_p = c_p + c_p^\dagger = b_p^\dagger \tag{35}$$

$$a_p = \frac{c_p - c_p^\dagger}{\mathrm{i}} = a_p^\dagger \tag{36}$$

$$c_p = \frac{b_p + \mathrm{i}a_p}{2},\ c_p^\dagger = \frac{b_p - \mathrm{i}a_p}{2} \tag{37}$$

$$b_p b_p = b_p^\dagger b_p = \left(c_p + c_p^\dagger\right)\left(c_p + c_p^\dagger\right) = c_p c_p + c_p^\dagger c_p^\dagger + c_p^\dagger c_p + c_p c_p^\dagger = \mathbb{I} \tag{38}$$

$$a_p a_p = -\left(c_p - c_p^\dagger\right)\left(c_p - c_p^\dagger\right) = -\left(c_p c_p + c_p^\dagger c_p^\dagger - c_p^\dagger c_p - c_p c_p^\dagger\right) = \mathbb{I} \tag{39}$$

$$b_p a_p = \left(c_p + c_p^\dagger\right)\left(\frac{c_p - c_p^\dagger}{\mathrm{i}}\right) = \frac{c_p^\dagger c_p - c_p c_p^\dagger}{\mathrm{i}} = -\left(\frac{c_p - c_p^\dagger}{\mathrm{i}}\right)\left(c_p + c_p^\dagger\right) = -b_p a_p \tag{40}$$

Generally thus

$$\gamma_p = \gamma_p^\dagger,\ \gamma_p\gamma_p = \mathbb{I},\ \{\gamma_p, \gamma_q\} = 2\delta_{pq} \tag{41}$$

$$\gamma_p\gamma_q + \gamma_q\gamma_p = 2\delta_{pq} \tag{42}$$

Two MF-s make a real one!

$$c = \frac{\gamma_p + \mathrm{i}\gamma_q}{2} \tag{43}$$

Note that the two need not originate from the same place!

Kitaev model for real Δ is written

$$H = \sum_p -\mu c_p^\dagger c_p - t\left(c_p^\dagger c_{p+1} + c_{p+1}^\dagger c_p\right) + \Delta\left(c_{p+1}^\dagger c_p^\dagger + c_p c_{p+1}\right) \tag{44}$$

$$c_p^\dagger c_p = \left(\frac{b_p - \mathrm{i}a_p}{2}\right)\left(\frac{b_p + \mathrm{i}a_p}{2}\right) = \frac{b_p b_p + a_p a_p - \mathrm{i}a_p b_p + \mathrm{i}b_p a_p}{4} = \frac{2 + 2\mathrm{i}b_p a_p}{4} = \frac{1 + \mathrm{i}b_p a_p}{2} \tag{45}$$

$$\begin{aligned}\left(c_p^\dagger c_{p+1} + c_{p+1}^\dagger c_p\right) &= \frac{(b_p - \mathrm{i}a_p)(b_{p+1} + \mathrm{i}a_{p+1}) + (b_{p+1} - \mathrm{i}a_{p+1})(b_p + \mathrm{i}a_p)}{4} \\ &= \frac{b_p b_{p+1} + \mathrm{i}b_p a_{p+1} - \mathrm{i}a_p b_{p+1} + a_p a_{p+1} + b_{p+1} b_p + \mathrm{i}b_{p+1} a_p - \mathrm{i}a_{p+1} b_p + a_{p+1} a_p}{4} \\ &= \mathrm{i}\frac{b_p a_{p+1} - a_p b_{p+1}}{2}\end{aligned} \tag{46}$$

$$\begin{aligned}\left(c_{p+1}^\dagger c_p^\dagger + c_p c_{p+1}\right) &= \frac{(b_{p+1} - \mathrm{i}a_{p+1})(b_p - \mathrm{i}a_p) + (b_p + \mathrm{i}a_p)(b_{p+1} + \mathrm{i}a_{p+1})}{4} \\ &= \frac{b_{p+1} b_p - \mathrm{i}b_{p+1} a_p - \mathrm{i}a_{p+1} b_p - a_{p+1} a_p + b_p b_{p+1} + \mathrm{i}b_p a_{p+1} + \mathrm{i}a_p b_{p+1} - a_p a_{p+1}}{4} \\ &= \mathrm{i}\frac{b_p a_{p+1} + a_p b_{p+1}}{2}\end{aligned} \tag{47}$$

$$H = \sum_p \left[-\mu\left(\frac{1 + \mathrm{i}b_p a_p}{2}\right) - t\left(\mathrm{i}\frac{b_p a_{p+1} - a_p b_{p+1}}{2}\right) + \Delta\left(\mathrm{i}\frac{b_p a_{p+1} + a_p b_{p+1}}{2}\right)\right] \tag{48}$$

$$= \frac{\mathrm{i}}{2}\sum_p \left[-\mu b_p a_p + (\Delta + t)\, a_p b_{p+1} + (\Delta - t)\, b_p a_{p+1}\right] - \sum_p \frac{\mu}{2} \tag{49}$$

$$= \frac{\mathrm{i}}{2}\sum_p \left[-\mu\frac{b_p a_p - a_p b_p}{2} + (\Delta + t)\,\frac{a_p b_{p+1} - b_{+1} a_p}{2} + (\Delta - t)\,\frac{b_p a_{p+1} - a_{p+1} b_p}{2}\right] \tag{50}$$

$$H_{3site} - \frac{3\mu}{2} = \frac{\mathrm{i}}{4}\begin{pmatrix} b_1 & a_1 & b_2 & a_2 & b_3 & a_3 \end{pmatrix}\begin{pmatrix} 0 & -\mu & 0 & (\Delta - t) & & \\ \mu & 0 & (\Delta + t) & 0 & & \\ 0 & -(\Delta + t) & 0 & -\mu & 0 & (\Delta - t) \\ -(\Delta - t) & 0 & \mu & 0 & (\Delta + t) & 0 \\ & & 0 & -(\Delta + t) & 0 & -\mu \\ & & -(\Delta - t) & 0 & \mu & 0 \end{pmatrix}\begin{pmatrix} b_1 \\ a_1 \\ b_2 \\ a_2 \\ b_3 \\ a_3 \end{pmatrix} \tag{51}$$

To highlight the two topologically distinct phases let us find the "fully dimerized" limits. The trivial case can be elucidated when all manner of inter-site communications are absent that is $\Delta = t = 0$:

$$H - \sum_p \frac{\mu}{2} = -\frac{\mathrm{i}}{2}\sum_p \left[\mu b_p a_p\right] \tag{52}$$

$$H = \sum_p -\mu c_p^\dagger c_p \tag{53}$$

thus we have proper fermions sitting on their original sites.

In the other phase, assume $\Delta = t$, and $\mu = 0$

$$H = -\frac{\mathrm{i}}{2}\sum_p \left[(\Delta + t)\, a_p b_{p+1}\right] \propto \sum_p \left[\Delta \tilde{c}_p^\dagger \tilde{c}_p\right] \tag{54}$$

here the $\tilde{c}_p$ operators are fermionic operators built from MFs of neighboring sites! Crucially, for a chain of length N two MF operators are missing from the above expression, namely b_1 and a_N! A fermionic operator can be built from them with the usual recipie

$$c_{BM} = \frac{b_1 + \mathrm{i}a_N}{2} \tag{55}$$

however this annihilates a highly unusual non local particle.