

**NOTES: Monte Carlo simulation of topological phase transition in two dimensions**

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## GOAL OF THE PROJECT SPT

In this project, we want to study the interaction driven reduction of the topological classification within the symmetry class A' in two dimensions ( $\mathbb{Z} \rightarrow \mathbb{Z}_4$ ) without breaking any symmetries. The according code can be found in `Hamiltonian_SPT.f90` and compiled as `make SPT` with invokes the file `Compile_SPT`. In the following, we will first discuss the physical part of the model and later also comment of the implementation.

## PRECURSOR

Let's begin with the following topologically non-trivial Dirac Hamiltonian in symmetry class A'

$$\mathcal{H} = \sum_{\mathbf{k}} \chi_{\mathbf{k}} [t \sin k_x \gamma_1 + t \sin k_y \gamma_2 + (2 + \lambda + \cos k_x + \cos k_y) \gamma_3] \chi_{\mathbf{k}}^\dagger \quad (1)$$

where  $\gamma_i$  with  $i = 1, \dots, 5$  are the anticommuting Dirac matrices of dimension 4 acting on the vector  $\chi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow R}, c_{\mathbf{k}\downarrow R}, c_{\mathbf{k}\uparrow L}, c_{\mathbf{k}\downarrow L})^T$ . Any choice of Dirac matrices is equally fine, you can take for example  $\gamma_{1,2} = \sigma_{1,2}\tau_3$ ,  $\gamma_{3,4} = \sigma_0\tau_{1,2}$  and  $\gamma_5 = \sigma_3\tau_3$ . Observe that  $\gamma_{2;4}^* = -\gamma_{2;4}$  which will be assumed through the rest of these notes.

As required by the symmetry class, this model satisfies two time-reversal ( $\mathcal{T}_1$  and  $\mathcal{T}_2$ ) and one particle-hole symmetry ( $\mathcal{C}$ ). In the first quantized language, these symmetries are anti-unitary (e.g.  $\mathcal{T}_1 = \mathcal{K}U_1$ ) and their unitary parts act on the Hamiltonian as  $U_\alpha H^*(-\mathbf{k})U_\alpha^\dagger = \pm H(\mathbf{k})$  with  $(+/-)$  refers to the TRS (PHS). Here we find  $U_1 = \gamma_1\gamma_4$ ,  $U_2 = \gamma_1\gamma_5$  and  $U_C = \gamma_2\gamma_3$  with  $\mathcal{T}_1^2 = \mathcal{C}^2 = 1$  and  $\mathcal{T}_2^2 = -1$ . Combing the anti-unitary symmetries pairwise generates one commuting and two anti-commuting unitary symmetries, namely  $R = \mathcal{T}_1\mathcal{T}_2 = \gamma_4\gamma_5$  and the chiral symmetries  $\mathcal{S}_{1;2} = \mathcal{T}_{1;2}\mathcal{C} = \gamma_{5;4}$ .

Eq. (1) satisfies other symmetry, the four-fold rotations  $C_4$  as  $U_{C_4} H(-k_y, k_x) U_{C_4}^\dagger = H(k_x, k_y)$  with  $U_{C_4} = \frac{1}{\sqrt{2}}(1 + \gamma_1\gamma_2)$  and the two parity symmetries  $P_{x;y}$  acting as  $U_{P_x} H(k_x, -k_y) U_{P_x}^\dagger = H(k_x, k_y)$  with  $U_{P_x} = \gamma_1\gamma_4$  or  $U_{P_x} = \gamma_1\gamma_5$  and  $U_{P_y} H(-k_x, k_y) U_{P_y}^\dagger = H(k_x, k_y)$  with  $U_{P_x} = \gamma_2\gamma_4$  or  $U_{P_x} = \gamma_2\gamma_5$ . The inversion symmetry is generated by applying two  $C_4$  rotation. Combining inversion and TR or PH symmetry leads to anti-unitary symmetries which are local in  $\mathbf{k}$ -space.

In summary, we found the following symmetries:

Trafo of $H$	unitary part	second qu. implementation	Trafo of $i$
$U^\dagger H(\mathbf{k}) U = H(\mathbf{k})$	$U = \gamma_4\gamma_5$	$\mathcal{U}\chi_{\mathbf{k}}\mathcal{U}^{-1} = U\chi_{\mathbf{k}}$	$\mathcal{U}i\mathcal{U}^{-1} = i$
$U^\dagger H(\mathbf{k}) U = -H(\mathbf{k})$	$U = \begin{cases} \gamma_4 \\ \gamma_5 \end{cases}$	$\mathcal{A}\chi_{\mathbf{k}}\mathcal{A}^{-1} = \chi_{\mathbf{k}}^\dagger U^\dagger$	$\mathcal{A}i\mathcal{A}^{-1} = -i$
$U^\dagger H^*(\mathbf{k}) U = H(\mathbf{k})$	$U = \begin{cases} \gamma_2\gamma_4 \\ \gamma_2\gamma_5 \end{cases}$	$\mathcal{A}\chi_{\mathbf{k}}\mathcal{A}^{-1} = U\chi_{\mathbf{k}}$	$\mathcal{A}i\mathcal{A}^{-1} = -i$
$U^\dagger H^*(\mathbf{k}) U = -H(\mathbf{k})$	$U = \gamma_1\gamma_3$	$\mathcal{U}\chi_{\mathbf{k}}\mathcal{U}^{-1} = \chi_{\mathbf{k}}^\dagger U^\dagger$	$\mathcal{U}i\mathcal{U}^{-1} = i$

The unitary symmetries have direct consequences of the spectrum at a given point  $\mathbf{k}$ :

- As  $H(\mathbf{k})$  commutes with  $R = \gamma_4\gamma_5$ , they can simultaneously diagonalized such that  $H(\mathbf{k})\Psi_{\mathbf{k}} = E\Psi_{\mathbf{k}}$  and  $R\Psi_{\mathbf{k}} = r\Psi_{\mathbf{k}}$
- $R^2 = -1$  such that  $r = \pm i$ . Additionally,  $[R, S_{\pm}] = \pm 2iS_{\pm}$  where  $S_{\pm} = \gamma_4 \pm i\gamma_5$ .  $S_{\pm}$  acts as a raising/lowering operator for  $R$ . It also squares to zero, indicating some kind of fermionic nature.
- As  $S_{\pm}$  anti-commutes with  $H(\mathbf{k})$ , one of them can be used to generate a new state  $S_{\pm}\Psi_{\mathbf{k}}$  with the eigenvalues  $-E$  and  $-r$ , hence they are orthogonal even for  $E = 0$ .
- We use one of the anti-unitary (first quantization) symmetries to generate another state orthogonal to  $\Psi_{\mathbf{k}}$  (in some sense as a generalized Kramers pair). To guarantee its orthogonality to  $S_{\pm}\Psi_{\mathbf{k}}$ , the operation has to commute with  $R$  such that it conserves the eigenvalue  $r$ . These requirements are only fulfilled by  $\mathcal{K}\gamma_1\gamma_3$  leading to the state  $\gamma_1\gamma_3\Psi_{\mathbf{k}}^*$ . Observe:

$$\Psi_{\mathbf{k}}^\dagger \gamma_1\gamma_3 \Psi_{\mathbf{k}}^* = \Psi_{\mathbf{k}}^\dagger (\gamma_1\gamma_3)^\dagger (\gamma_1\gamma_3)^2 \Psi_{\mathbf{k}}^* = -(\gamma_1\gamma_3 \Psi_{\mathbf{k}})^\dagger \Psi_{\mathbf{k}}^* = -\Psi_{\mathbf{k}}^\dagger (\gamma_1\gamma_3 \Psi_{\mathbf{k}})^* = -\Psi_{\mathbf{k}}^\dagger \gamma_1\gamma_3 \Psi_{\mathbf{k}}^* \quad (2)$$

Hence we have generated two orthogonal single particle states at energy  $-E$ .

Summarizing the above discussion, we can employ symmetry operation to generate the quadruple of states  $(\Psi_{\mathbf{k}}, S_{-r}\Psi_{\mathbf{k}}, \gamma_1\gamma_3\Psi_{\mathbf{k}}^*, S_{-r}\gamma_1\gamma_3\Psi_{\mathbf{k}}^*)$  with the Eigenvalues  $((E, r), (-E, -r), (-E, r), (E, -r))$ . If the energy  $E$  vanishes, the states with the same  $r$  are still orthogonal to each other due to Eq. (2). Hence the subspace with  $E = 0$  is at least four-fold degenerate at a given point  $\mathbf{k}$ .

If there is a Dirac node at an arbitrary  $\mathbf{k}$ , then there are three additional one generated by the rotation symmetry (TRS and/or PHS would only generate one more node at  $-\mathbf{k}$ ). Applying parity operations guarantees the existence of another set of four Dirac cones. Inverting this statement leads to the following conclusions:

- a single Dirac node has to be at the rotation-, TRS-, and parity-invariant momenta, hence a single cone can only exist at  $\mathbf{k} = (0, 0)$  or at  $\mathbf{k} = (\pi, \pi)$ .
- two Dirac nodes can additionally be located as a pair at TRS-invariant  $\mathbf{k} = (0, \pi)$  and at  $\mathbf{k} = (\pi, 0)$ .

## LATTICE HAMILTONIAN

The Hamiltonian in Eq. (1) mostly gapped, except for  $\lambda \in \{-4, -2, 0\}$  where semi-metals separate topological distinct insulators. It is topologically trivial for  $\lambda > 0$  and for  $\lambda < -4$ . The other two regions are non-trivial with a winding of  $\pm 1$ . To study the topological reduction, we have to connect two sectors with a difference in the winding number of multiples of 4. This is not possible in the current version. We can therefore either replace  $\mathbf{k} \rightarrow 2\mathbf{k}$  or simply add three additional copies of the original Hamiltonian. Following the second path, we refine the above model to

$$\mathcal{H} = \sum_{\mathbf{k}, o} \chi_{\mathbf{k}, o} [t \sin k_x \gamma_1 + t \sin k_y \gamma_2 + (2 + \lambda + \cos k_x + \cos k_y) \gamma_3] \chi_{\mathbf{k}, o}^\dagger \quad (3)$$

with  $o = 1, \dots, 4$ . The interaction which supposedly connects different topological sectors by gaping the semi-metal without breaking the relevant symmetries is given by

$$\mathcal{H}_{\text{int}} = \frac{V}{2} \sum_{\mathbf{r}, \sigma'} \left( S_{\mathbf{r}, \sigma'}^{x,1} S_{\mathbf{r}, \sigma'}^{x,2} + S_{\mathbf{r}, \sigma'}^{y,1} S_{\mathbf{r}, \sigma'}^{y,2} \right) \quad (4)$$

$$= \frac{V}{8} \sum_{\mathbf{r}, \sigma'} \left[ \left( S_{\mathbf{r}, \sigma'}^{x,1} + S_{\mathbf{r}, \sigma'}^{x,2} \right)^2 - \left( S_{\mathbf{r}, \sigma'}^{x,1} - S_{\mathbf{r}, \sigma'}^{x,2} \right)^2 + \left( S_{\mathbf{r}, \sigma'}^{y,1} + S_{\mathbf{r}, \sigma'}^{y,2} \right)^2 - \left( S_{\mathbf{r}, \sigma'}^{y,1} - S_{\mathbf{r}, \sigma'}^{y,2} \right)^2 \right] \quad (5)$$

with  $\mathbf{S}_{\mathbf{r}, \sigma'}^1 = (\chi_{\mathbf{r}, 1}^\dagger, \chi_{\mathbf{r}, 2}^\dagger) \boldsymbol{\sigma} P_{\sigma'} \gamma_5 (\chi_{\mathbf{r}, 1}, \chi_{\mathbf{r}, 2})^T$  and  $\mathbf{S}_{\mathbf{r}, \sigma'}^2 = (\chi_{\mathbf{r}, 3}^\dagger, \chi_{\mathbf{r}, 4}^\dagger) \boldsymbol{\sigma} P_{\sigma'} \gamma_5 (\chi_{\mathbf{r}, 3}, \chi_{\mathbf{r}, 4})^T$  where  $P_{\sigma'} = \frac{1}{2}(1 + i\sigma' \gamma_3 \gamma_4)$  is yet another projector.

## SYMMETRIES AND SOME OTHER IMPORTANT ASPECTS

First of all, the free part (see (3)) still fulfils all symmetries discussed in the precursor with an additional  $SU(4)$  degree of freedom that rotates in the sub-lattice/orbital space  $o$  with the unitary part given as  $U_o \otimes U$ .

For the following, it is more convenient to use the following nomenclature:

$$\chi_{\mathbf{r}}^\dagger = (\chi_{\mathbf{r}, 1}^\dagger, \chi_{\mathbf{r}, 2}^\dagger, \chi_{\mathbf{r}, 3}^\dagger, \chi_{\mathbf{r}, 4}^\dagger) \quad (6)$$

$$\mathbf{S}_{\mathbf{r}, \sigma}^1 = \chi_{\mathbf{r}}^\dagger \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & 0 \end{pmatrix} \otimes P_{\sigma} \gamma_5 \chi_{\mathbf{r}} \quad (7)$$

$$\mathbf{S}_{\mathbf{r}, \sigma}^2 = \chi_{\mathbf{r}}^\dagger \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \otimes P_{\sigma} \gamma_5 \chi_{\mathbf{r}} \quad (8)$$

Using the relation  $P_{\sigma} \gamma_5 = (P_{\sigma} \gamma_5)^* = (P_{\sigma} \gamma_5)^T = (P_{\sigma} \gamma_5)^\dagger$  takes care of possible complex conjugation (anti-unitary part in second quantized version) or possible transpositions whenever  $\chi^\dagger \leftrightarrow \chi$  and the combination of both.

Lets begin with the analysis of the standard unitary operations given by  $\tilde{R} = 1 \otimes \gamma_4 \gamma_5$ ,  $\tilde{S}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes 1$ ,  $\tilde{S}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes 1$ ,  $\tilde{S}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes 1$ . All of them commute with the free part of the system. The first two already leave  $\mathbf{S}_{\mathbf{r}, \sigma}^{1,2}$  invariant whereas the last two exchange one with the other. Hence the full interacting system is invariant under these unitary particle-particle transformation.

We also recover the symmetries from above for the interaction system if we choose  $U_0 = 1$ . This may transform  $P_{\sigma} \gamma_5$  to  $\pm P_{\pm \sigma} \gamma_5$  and the transformation might also invert the position  $\mathbf{r} \rightarrow -\mathbf{r}$ . As both  $\mathbf{S}_{\mathbf{r}, \sigma}^{1,2}$  pick up the overall sign, this part cancels immediately. In a similar fashion, both sign flips in  $\sigma$  and  $\mathbf{r}$  can be absorbed by a substitution as we sum over both

variables. Hence the interacting system still obeys all old symmetries with the trivial extension to the new sub-lattice/orbital space. Additionally it acquires three additional standard unitary symmetries. Most importantly  $\tilde{S}^\alpha$  form a  $SU(2)$  algebra and  $\tilde{S}^x \pm i\tilde{S}^y$  act as ladder operators for  $\tilde{S}^z$ .

As  $H$ ,  $\tilde{R}$  and  $\tilde{S}^z$  mutually commute, we can add another quantum number to the quadruple of states, namely  $\sigma$ , promoting the set to eight symmetry related, linearly independent states.

I think, that the nodes of the Dirac cone has to be 8-fold degenerate such that the rotation symmetry fixes their position to  $(\pi, \pi)$ . Is this correct??? We have to be really sure here, otherwise we might interpret the QMC data wrong and the numerics will not necessarily show us that this reasoning is incorrect.

### TESTS OF THE PROTECTING SYMMETRIES

The set of independent symmetries of the interacting Hamiltonian is given by

Name	Action on operators	Action on scalars
$\mathcal{T}$	$\mathcal{T}\chi_{\mathbf{r},\alpha}\mathcal{T}^{-1} = \gamma_{14}\chi_{\mathbf{r},\alpha}$	$\mathcal{T}i\mathcal{T}^{-1} = -i$
$\mathcal{C}$	$\mathcal{C}\chi_{\mathbf{r},\alpha}\mathcal{C}^{-1} = \chi_{\mathbf{r},\alpha}^\dagger\gamma_{23}^\dagger$	$\mathcal{T}i\mathcal{T}^{-1} = i$
$\mathcal{R}$	$\mathcal{R}\chi_{\mathbf{r},\alpha}\mathcal{R}^{-1} = \gamma_{45}\chi_{\mathbf{r},\alpha}$	$\mathcal{T}i\mathcal{T}^{-1} = i$
$C_4$	$C_4\chi_{\mathbf{r},\alpha}C_4^{-1} = \frac{1}{\sqrt{2}}(1 + \gamma_{12})\chi_{(-r_y, r_x),\alpha}$	$C_4iC_4^{-1} = i$
$P_x$	$P_x\chi_{\mathbf{r},\alpha}P_x^{-1} = \gamma_{15}\chi_{(-r_x, r_y),\alpha}$	$P_xiP_x^{-1} = i$
$S_x$	$S_x\chi_{\mathbf{r}}S_x^{-1} = \sigma_x \otimes 1 \chi_{\mathbf{r}}$	$S_xiS_x^{-1} = i$
$S_z$	$S_\alpha\chi_{\mathbf{r}}S_z^{-1} = \sigma_z \otimes 1 \chi_{\mathbf{r}}$	$S_ziS_z^{-1} = i$
$U_1$	$U_1\chi_{\mathbf{r}}U_1^{-1} = 1 \otimes \sigma_z \chi_{\mathbf{r}}$	$U_1iU_1^{-1} = i$

This allows to define the following operators that are protected by exactly one symmetry and classify them by the acquired sign upon symmetry transformations:

operator $O$	$TOT^{-1}$	$COC^{-1}$	$ROR^{-1}$	$C_4OC_4^{-1}$	$P_xOP_x^{-1}$	$S_xOS_x^{-1}$	$S_zOS_z^{-1}$	$U_1OU_1^{-1}$
$\sum_{\mathbf{k},\alpha} i\chi_{\mathbf{k},\alpha}^\dagger(\sin k_x\gamma_1 + \sin k_y\gamma_2)\gamma_3\chi_{\mathbf{k},\alpha}$	-	+	+	+	+	+	+	+
$\sum_{\mathbf{k}}(n_{\mathbf{k}} - 8)$	+	-	+	+	+	+	+	+
$\sum_{\mathbf{k},\alpha} \chi_{\mathbf{k},\alpha}^\dagger\gamma_4\chi_{\mathbf{k},\alpha}$	+	+	-	+	+	+	+	+
$\sum_{\mathbf{k},\alpha} \chi_{\mathbf{k},\alpha}^\dagger(\sin k_x\gamma_1 - \sin k_y\gamma_2)\chi_{\mathbf{k},\alpha}$	+	+	+	-	+	+	+	+
$\sum_{\mathbf{k},\alpha} \chi_{\mathbf{k},\alpha}^\dagger(\sin k_y\gamma_1 - \sin k_x\gamma_2)\chi_{\mathbf{k},\alpha}$	+	+	+	+	-	+	+	+
$\sum_{\mathbf{k}} \chi_{\mathbf{k}}^\dagger\sigma_z \otimes 1 \gamma_3\chi_{\mathbf{k}}$	+	+	+	+	+	-	+	+
$\sum_{\mathbf{k}} \chi_{\mathbf{k}}^\dagger\sigma_x \otimes 1 \gamma_3\chi_{\mathbf{k}}$	+	+	+	+	+	+	-	+
$\sum_{\mathbf{k}} \chi_{\mathbf{k}}^\dagger 1 \otimes \sigma_x \gamma_3\chi_{\mathbf{k}}$	+	+	+	+	+	+	+	-

Remark: I first thought that the pseudo-spin-spin would already signal a breaking of the  $SU(2)$  symmetry, but a magnetic instability is also forbidden by PHS.