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 ($\mathbb{Z} \to \mathbb{Z}_4$) 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'

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

where γ_i with $i = 1, ..., 5$ 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 $U_\alpha H^*(-\mathbf{k}) U^\dagger_\alpha = \pm H(\mathbf{k})$ with $+(-)$ refers to the TRS (PHS). Here we find $U_1 = \gamma_1\gamma_4$, $U_2 = \gamma_1\gamma_5$ and $U_{\mathcal{C}} = \gamma_2\gamma_3$ with $\mathcal{T}_1^2 = \mathcal{C}^2 = 1$ and $\mathcal{T}_1^2 = -1$. 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 $U_{C_4} H(-k_y, k_x) U^\dagger_{C_4} = H(k_x, k_y)$ with $U_{C_4} = \frac{1}{\sqrt{2}}(1 + \gamma_1\gamma_2)$ and the two parity symmetries $P_{x;y}$ acting as $U_{P_x} H(k_x, -k_y) U^\dagger_{P_x} = H(k_x, k_y)$ with $U_{P_x} = \gamma_1\gamma_4$ or $U_{P_x} = \gamma_1\gamma_5$ and $U_{P_y} H(-k_x, k_y) U^\dagger_{P_x} = H(k_x, k_y)$ 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
$U^\dagger H(\mathbf{k}) U = H(\mathbf{k})$	$U = \gamma_4\gamma_5$	$\mathcal{U}\chi_{\mathbf{k}}\mathcal{U}^{-1} = U\chi_{\mathbf{k}}$	$\mathcal{U}i\mathcal{U}^{-1} = i$
$U^\dagger H(\mathbf{k}) U = -H(\mathbf{k})$	$U = \begin{cases}\gamma_4 \\ \gamma_5\end{cases}$	$\mathcal{A}\chi_{\mathbf{k}}\mathcal{A}^{-1} = \chi^\dagger_{\mathbf{k}} U^\dagger$	$\mathcal{A}i\mathcal{A}^{-1} = -i$
$U^\dagger H^*(\mathbf{k}) U = H(\mathbf{k})$	$U = \begin{cases}\gamma_2\gamma_4 \\ \gamma_2\gamma_5\end{cases}$	$\mathcal{A}\chi_{\mathbf{k}}\mathcal{A}^{-1} = U\chi_{\mathbf{k}}$	$\mathcal{A}i\mathcal{A}^{-1} = -i$
$U^\dagger H^*(\mathbf{k}) U = -H(\mathbf{k})$	$U = \gamma_1\gamma_3$	$\mathcal{U}\chi_{\mathbf{k}}\mathcal{U}^{-1} = \chi^\dagger_{\mathbf{k}} U^\dagger$	$\mathcal{U}i\mathcal{U}^{-1} = i$

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 use 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 it's 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:

$$\Psi^\dagger_{\mathbf{k}}\gamma_1\gamma_3\Psi^*_{\mathbf{k}} = \Psi^\dagger_{\mathbf{k}}(\gamma_1\gamma_3)^\dagger(\gamma_1\gamma_3)^2\Psi^*_{\mathbf{k}} = -(\gamma_1\gamma_3\Psi)^\dagger_{\mathbf{k}}\Psi^*_{\mathbf{k}} = -\Psi^\dagger_{\mathbf{k}}(\gamma_1\gamma_3\Psi_{\mathbf{k}})^* = -\Psi^\dagger_{\mathbf{k}}\gamma_1\gamma_3\Psi^*_{\mathbf{k}} \tag{2}$$

  Hence we have generated to 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 exitence 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 ± 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 $\mathbf{k} \to 2\mathbf{k}$ or simply add three additional copies of the original Hamiltonian. Following the second path, we refine the above model to

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

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

$$\begin{aligned}
\mathcal{H}_{\text{int}} &= \frac{V}{2} \sum_{\mathbf{r},\sigma'} \left(S^{x,1}_{\mathbf{r},\sigma'} S^{x,2}_{\mathbf{r},\sigma'} + S^{y,1}_{\mathbf{r},\sigma'} S^{y,2}_{\mathbf{r},\sigma'} \right) &(4)\\
&= \frac{V}{8} \sum_{\mathbf{r},\sigma'} \left[\left(S^{x,1}_{\mathbf{r},\sigma'} + S^{x,2}_{\mathbf{r},\sigma'} \right)^2 - \left(S^{x,1}_{\mathbf{r},\sigma'} - S^{x,2}_{\mathbf{r},\sigma'} \right)^2 + \left(S^{y,1}_{\mathbf{r},\sigma'} + S^{y,2}_{\mathbf{r},\sigma'} \right)^2 - \left(S^{y,1}_{\mathbf{r},\sigma'} - S^{y,2}_{\mathbf{r},\sigma'} \right)^2 \right] &(5)
\end{aligned}$$

with $\mathbf{S}^1_{\mathbf{r},\sigma'} = (\chi^\dagger_{\mathbf{r},1}, \chi^\dagger_{\mathbf{r},2}) \boldsymbol{\sigma} P_{\sigma'} \gamma_5 (\chi_{\mathbf{r},1}, \chi_{\mathbf{r},2})^T$ and $\mathbf{S}^2_{\mathbf{r},\sigma'} = (\chi^\dagger_{\mathbf{r},3}, \chi^\dagger_{\mathbf{r},4}) \boldsymbol{\sigma} P_{\sigma'} \gamma_5 (\chi_{\mathbf{r},3}, \chi_{\mathbf{r},4})^T$ 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:

$$\chi^\dagger_{\mathbf{r}} = (\chi^\dagger_{\mathbf{r},1}, \chi^\dagger_{\mathbf{r},2}, \chi^\dagger_{\mathbf{r},3}, \chi^\dagger_{\mathbf{r},4}) \tag{6}$$

$$\mathbf{S}^1_{\mathbf{r},\sigma} = \chi^\dagger_{\mathbf{r}} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & 0 \end{pmatrix} \otimes P_\sigma \gamma_5 \chi_{\mathbf{r}} \tag{7}$$

$$\mathbf{S}^2_{\mathbf{r},\sigma} = \chi^\dagger_{\mathbf{r}} \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \otimes P_\sigma \gamma_5 \chi_{\mathbf{r}} \tag{8}$$

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 $\mathbf{S}^{1,2}_{\mathbf{r},\sigma}$ 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 $\mathbf{r} \to -\mathbf{r}$. As both $\mathbf{S}^{1,2}_{\mathbf{r},\sigma}$ pick up the overall sign, this part cancels immediately. In a similar fashion, both sign flips in σ 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 σ, 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 (π, π). 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
$\mathcal{T}$	$\mathcal{T}\chi_{\mathbf{r},\alpha}\mathcal{T}^{-1} = \gamma_{14}\chi_{\mathbf{r},\alpha}$	$\mathcal{T}i\mathcal{T}^{-1} = -i$
$\mathcal{C}$	$\mathcal{C}\chi_{\mathbf{r},\alpha}\mathcal{C}^{-1} = \chi^\dagger_{\mathbf{r},\alpha}\gamma^\dagger_{23}$	$\mathcal{T}i\mathcal{T}^{-1} = i$
$\mathcal{R}$	$\mathcal{R}\chi_{\mathbf{r},\alpha}\mathcal{R}^{-1} = \gamma_{45}\chi_{\mathbf{r},\alpha}$	$\mathcal{T}i\mathcal{T}^{-1} = i$
C_4	$C_4\chi_{\mathbf{r},\alpha}C_4^{-1} = \frac{1}{\sqrt{2}}(1+\gamma_{12})\chi_{(-r_y,r_x),\alpha}$	$C_4 i C_4^{-1} = i$
P_x	$P_x\chi_{\mathbf{r},\alpha}P_x^{-1} = \gamma_{15}\chi_{(-r_x,r_y),\alpha}$	$P_x i P_x^{-1} = i$
S_x	$S_x\chi_{\mathbf{r}}S_x^{-1} = \sigma_x \otimes 1\,\chi_{\mathbf{r}}$	$S_x i S_x^{-1} = i$
S_z	$S_\alpha\chi_{\mathbf{r}}S_z^{-1} = \sigma_z \otimes 1\,\chi_{\mathbf{r}}$	$S_z i S_z^{-1} = i$
U_1	$U_1\chi_{\mathbf{r}}U_1^{-1} = 1 \otimes \sigma_z\,\chi_{\mathbf{r}}$	$U_1 i U_1 = i$

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

operator O	$\mathcal{T}O\mathcal{T}^{-1}$	$\mathcal{C}O\mathcal{C}^{-1}$	$\mathcal{R}O\mathcal{R}^{-1}$	$C_4OC_4^{-1}$	$P_xOP_x^{-1}$	$S_xOS_x^{-1}$	$S_zOS_z^{-1}$	$U_1OU_1^{-1}$
$\sum_{\mathbf{k},\alpha} i\chi^\dagger_{\mathbf{k},\alpha}(\sin k_x\gamma_1 + \sin k_y\gamma_2)\gamma_3\chi_{\mathbf{k},\alpha}$	-	+	+	+	+	+	+	+
$\sum_{\mathbf{k}}(n_{\mathbf{k}} - 8)$	+	-	+	+	+	+	+	+
$\sum_{\mathbf{k},\alpha}\chi^\dagger_{\mathbf{k},\alpha}\gamma_4\chi_{\mathbf{k},\alpha}$	+	+	-	+	+	+	+	+
$\sum_{\mathbf{k},\alpha}\chi^\dagger_{\mathbf{k},\alpha}(\sin k_x\gamma_1 - \sin k_y\gamma_2)\chi_{\mathbf{k},\alpha}$	+	+	+	-	+	+	+	+
$\sum_{\mathbf{k},\alpha}\chi^\dagger_{\mathbf{k},\alpha}(\sin k_y\gamma_1 - \sin k_x\gamma_2)\chi_{\mathbf{k},\alpha}$	+	+	+	+	-	+	+	+
$\sum_{\mathbf{k}}\chi^\dagger_{\mathbf{k}}\sigma_z \otimes 1\,\gamma_3\chi_{\mathbf{k}}$	+	+	+	+	+	-	+	+
$\sum_{\mathbf{k}}\chi^\dagger_{\mathbf{k}}\sigma_x \otimes 1\,\gamma_3\chi_{\mathbf{k}}$	+	+	+	+	+	+	-	+
$\sum_{\mathbf{k}}\chi^\dagger_{\mathbf{k}}1 \otimes \sigma_x\,\gamma_3\chi_{\mathbf{k}}$	+	+	+	+	+	+	+	-
$\sum_{\mathbf{k}}\chi^\dagger_{\mathbf{k}}1 \otimes \sigma_y\chi_{\mathbf{k}}$	+	+	+	+	+	+	+	-

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.