

TR Invariant T.I.

Taper

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Abstract

An incomplete note of dissertation by Taylor Hughes [Hug09].

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	Questions:	
	• Do we have a precise definition of <i>topological phase transition</i> ?	

1 Spectrum of (2+1)d Lattice Dirac Model

sec:2+1d-LDirac Model

$$\begin{aligned} H_{LD} = \sum_{m,n} \Big\{ & i \left[c_{m+1,n}^\dagger \sigma^x c_{m,n} - c_{m,n}^\dagger \sigma^x c_{m+1,n} \right] + i \left[c_{m,n+1}^\dagger \sigma^y c_{m,n} - c_{m,n}^\dagger \sigma^y c_{m,n+1} \right] \\ & - \left[c_{m+1,n}^\dagger \sigma^z c_{m,n} + c_{m,n}^\dagger \sigma^z c_{m+1,n} + c_{m,n+1}^\dagger \sigma^z c_{m,n} + c_{m,n}^\dagger \sigma^z c_{m,n+1} \right] \\ & + (2 - m) c_{m,n}^\dagger \sigma^z c_{m,n} \frac{\hbar}{2} \Big\} \end{aligned} \quad (1.0.1)$$

Above is the lattice model (eq.2.19) of [Hug09]. Here it should be noted that $c_{m,n} = (c_{u,m,n}, c_{v,m,n})$ for two degrees of freedom.

This Hamiltonian is solved here with a infinite cylinder geometry, i.e. the lattice is infinite in x direction while being periodic in y direction. Because of this special setup, the p_x is still a good quantum number. Therefore we can do a fourier expansion in x direction:

$$c_{m,n} = \frac{1}{\sqrt{L_x}} \sum_{p_x} e^{ip_x m} c_{p_x,n} \quad (1.0.2)$$

The resulted Hamiltonian is

$$\begin{aligned}
\tilde{H}_{LD} = \sum_{n,p_x} & 2 \sin(p_x) c_{p_x,n}^\dagger \sigma^x c_{p_x,n} + i \left[c_{p_x,n+1}^\dagger \sigma^y c_{p_x,n} - c_{p_x,n+1}^\dagger \sigma^y c_{p_x,n} \right] \\
& - \left[2 \cos(p_x) c_{p_x,n}^\dagger \sigma^z c_{p_x,n} c_{p_x,n+1}^\dagger \sigma^z c_{p_x,n} + c_{p_x,n}^\dagger \sigma^z c_{p_x,n+1} \right] \\
& + (2-m) c_{p_x,n}^\dagger \sigma^z c_{p_x,n}
\end{aligned} \tag{1.0.3}$$

This Hamiltonian can be solved by acting it on the test wavefunction:

$$|\psi_{p_x}\rangle = \sum_n \psi_{p_x,n,u} c_{p_x,n,u}^\dagger + \psi_{p_x,n,v} c_{p_x,n,v}^\dagger |0\rangle \tag{1.0.4}$$

Note, in choosing the test wavefunction, u and v could not be separated, because there is still interaction between the two component in terms like $c_{p_x,n}^\dagger \sigma^x c_{p_x,n}$. If we calculate $\tilde{H}_{LD} |\psi_{p_x}\rangle = E_{p_x} |\psi_{p_x}\rangle$, we would get after careful calculation:

$$\begin{aligned}
& \sum_n c_{p_x,n}^\dagger A \psi_{p_x,n-1} + c_{p_x,n}^\dagger B \psi_{p_x,n} + c_{p_x,n}^\dagger C \psi_{p_x,n+1} \\
& = E_{p_x} \sum_n c_{p_x,n}^\dagger \psi_{p_x,n}
\end{aligned} \tag{1.0.5}$$

where

$$c_{p_x,n}^\dagger = (c_{p_x,n,u}^\dagger, c_{p_x,n,v}^\dagger) \tag{1.0.6}$$

$$A = i\sigma^y - \sigma^z \tag{1.0.7}$$

$$B = 2 \sin(p_x) \sigma^x - 2 \cos(p_x) \sigma^z + (2-m) \sigma^z \tag{1.0.8}$$

$$C = -i\sigma^y - \sigma^z \tag{1.0.9}$$

$$\psi_{p_x,n} = \begin{pmatrix} \psi_{p_x,n,u} \\ \psi_{p_x,n,v} \end{pmatrix} \tag{1.0.10}$$

Suppose there is N lattice in the y direction. Then the periodic boundary condition implies that $\psi_{N+1} = \psi_{n=1}$, and $\psi_{n=0} = \psi_N$.

Therefore, the eigenvalue equation could be turned into a matrix form:

$$H_{\text{disc}} \psi \equiv \begin{pmatrix} B & C & & A \\ A & B & C & \\ & A & B & C \\ & & \dots & \\ & & A & B & C \\ C & & & A & B \end{pmatrix} \begin{pmatrix} \psi_{p_x,1} \\ \psi_{p_x,2} \\ \dots \\ \psi_{p_x,N} \end{pmatrix} = E_{p_x} \begin{pmatrix} \psi_{p_x,1} \\ \psi_{p_x,2} \\ \dots \\ \psi_{p_x,N} \end{pmatrix} \tag{1.0.11}$$

1.1 Numerical result

sec:Numerical result

Note: Results in this section are contained in the file "Lattice Dirac Model (2+1)-d.nb", and the file "Dirac.Lattice.Model.21.d.m".

Let us take $N = 3$ for simplicity. The eigenvalue problem is solve using Mathematica, and the 6 eigenvalues are:

$$\begin{pmatrix} -\sqrt{m^2 + 4m \cos(px) + 4} \\ \sqrt{m^2 + 4m \cos(px) + 4} \\ -\sqrt{m^2 + 4m \cos(px) - 6m - 12 \cos(px) + 16} \\ -\sqrt{m^2 + 4m \cos(px) - 6m - 12 \cos(px) + 16} \\ \sqrt{m^2 + 4m \cos(px) - 6m - 12 \cos(px) + 16} \\ \sqrt{m^2 + 4m \cos(px) - 6m - 12 \cos(px) + 16} \end{pmatrix} \quad (1.1.1)$$

It is found that at $m = -2$, there is a band crossing at $p_x = 0$:

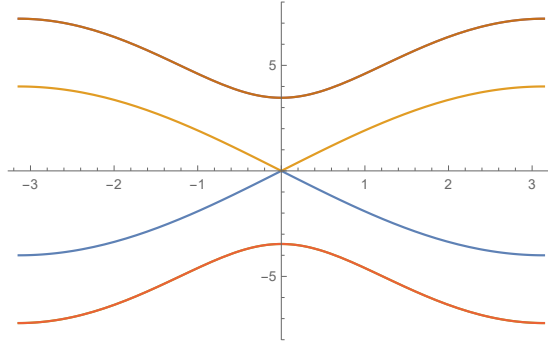


Figure 1: The Eigenvalue plot for $m = -2$. Plotted as $E_{p_x} \vee p_x$

Also, at $m = 2$, there is a band crossing at $p = \pm\pi$:

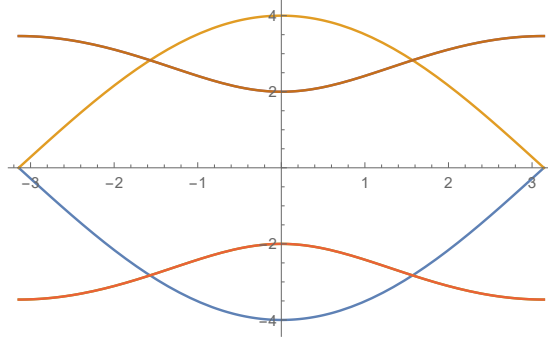


Figure 2: The Eigenvalue plot for $m = 2$. Plotted as $E_{p_x} \vee p_x$

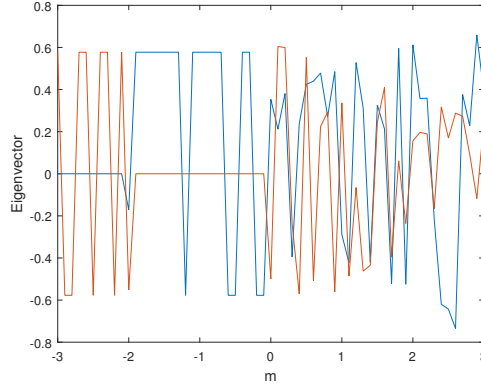
Since the paper will be focusing in points around $p_x = 0$, I will focus in $m = -2$. In this case, I want to find more information about the eigenvectors.

When I looked blindly at the value $(m, p_x) = (-2, 0)$, the Mathematica gave me two eigenvectors both corresponds to the eigenvalue 0:

$$\{0, 1, 0, 1, 0, 1\}, \{1, 0, 1, 0, 1, 0\} \quad (1.1.2)$$

It led me to believe that there are two spin waves, with made with purely spin up waves and another of purely spin down waves. But this is not correct.

It is found later that the matrix H_{disc} is singular (with determinant 0) when $(m, p_x) = (-2, 0)$. Also, a Matlab calculation shows that the eigenvectors of the crossing bands actually flunctuate between ± 1 in a way illustrated as below:



Also, the Mathematica solved eigenvector also demonstrate a drastical change around $m = -2$. For example, one component, when plotted against p_x change from:

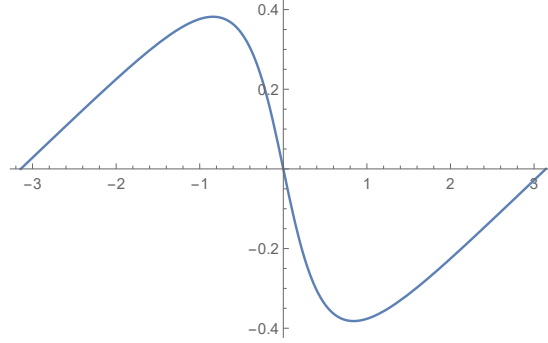


Figure 3: $m = -3$

to

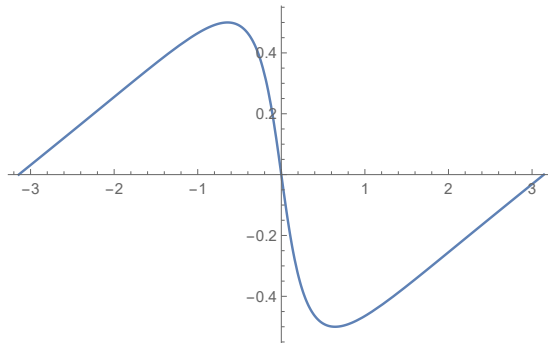


Figure 4: $m = -2.5$

and suddenly to

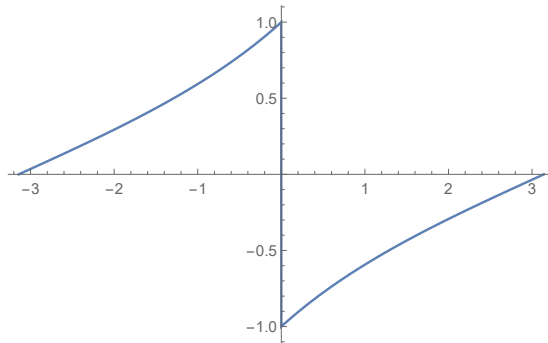


Figure 5: $m = -2$. There is a discontinuity at $p_x = 0$

Finally, it becomes smooth again:

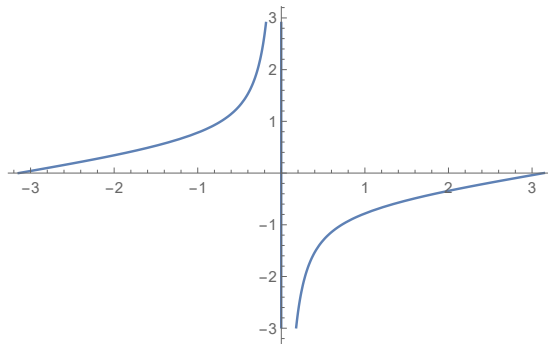


Figure 6: $m = -1.5$

The details can be explored in the Mathematica notebook.

Also, the case of $N = 4$ is also calculated in Mathematica. There are similarly two crossing happening at (m, p_x) equals $(-2, 0)$ and $(2, \pm\pi)$.

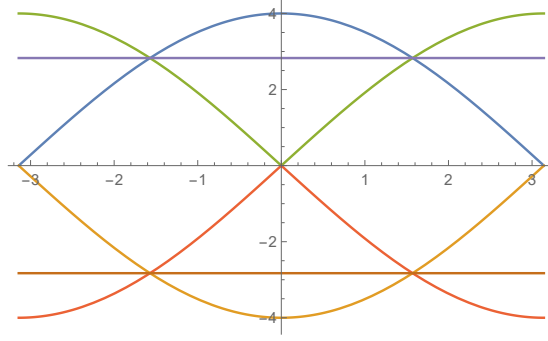


Figure 7: $m = 2$

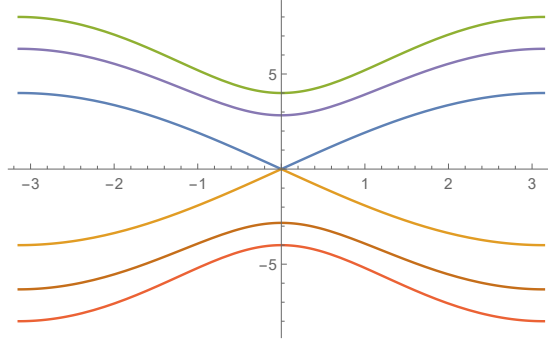


Figure 8: $m = -2$

Surprisingly, the two bands that cross have exactly the same function dependence on p_x and m for the cases of $N = 3$ and $N = 4$.

1.2 Discussion about the Lattice Model

I notice that equation (2.19) transformed according to (2.20) is not exactly equation (2.21), but is:

$$H = \sum_{p_x, p_y} c_{p_x, p_y}^\dagger \times [2 \sin(p_x) \sigma^x + 2 \sin(p_y) \sigma^y + (2 - m - 2 \cos(p_x) - 2 \cos(p_y)) \sigma^z] c_{p_x, p_y} \quad (1.2.1)$$

This result does not become the continuum Dirac Hamiltonian as p_x, p_y goes to zero. Therefore, I suspect that certain constants should be modified so that:

$$\begin{aligned}
H_{LD} = \sum_{m,n} \bigg\{ & \frac{i}{2} \left[c_{m+1,n}^\dagger \sigma^x c_{m,n} - c_{m,n}^\dagger \sigma^x c_{m+1,n} \right] + \frac{i}{2} \left[c_{m,n+1}^\dagger \sigma^y c_{m,n} - c_{m,n}^\dagger \sigma^y c_{m,n+1} \right] \\
& - \frac{1}{2} \left[c_{m+1,n}^\dagger \sigma^z c_{m,n} + c_{m,n}^\dagger \sigma^z c_{m+1,n} + c_{m,n+1}^\dagger \sigma^z c_{m,n} + c_{m,n}^\dagger \sigma^z c_{m,n+1} \right] \\
& + (2-m) c_{m,n}^\dagger \sigma^z c_{m,n} \bigg\} \tag{1.2.2}
\end{aligned}$$

This affects the numerical analysis effectively by the replacement

$$\sigma^i \rightarrow \frac{1}{2} \sigma^i, \quad (2-m) \rightarrow 2(2-m)$$

And the result is similar to previous study, except that the band crossing happens at different values of m . For example, the eigenvalue of original and the modified equation (2.21) are plotted in Mathematica notebook "Eq2.21-Demo.nb". Also, the solution to the infinite cylinder boundary condition has again two band crossings, each at (m, p_x) equals $(0, 0)$ and $(2, \pm\pi)$ (for $N = 3$ case).

References

- [Hug09] Taylor Hughes. *Time-reversal Invariant Topological Insulators*. PhD thesis, Stanford University, 2009. URL: <http://gradworks.umi.com/33/82/3382746.html>.

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