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Abstract

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

Contents

Start with chapter 2.
Questions:

- Do we have a precise definition of *topological phase transition*?

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

sec:2+1d-LDirac Model

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

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.

1.1 Numerical Solution in Infinity Cylinder Geometry

Infinity Cylinder Geometry

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:

$$c_{m,n} = \frac{1}{\sqrt{L_x}} \sum_{p_x} e^{ip_x m} c_{p_x,n} \tag{1.1.1}$$

The resulted Hamiltonian is

$$\begin{aligned}
\tilde{H}_{LD} = \sum_{n,p_x} \quad & 2\sin(p_x) c^\dagger_{p_x,n} \sigma^x c_{p_x,n} + i \left[c^\dagger_{p_x,n+1} \sigma^y c_{p_x,n} - c^\dagger_{p_x,n+1} \sigma^y c_{p_x,n} \right] \\
& - \left[2\cos(p_x) c^\dagger_{p_x,n} \sigma^z c_{p_x,n} c^\dagger_{p_x,n+1} \sigma^z c_{p_x,n} + c^\dagger_{p_x,n} \sigma^z c_{p_x,n+1} \right] \\
& + (2-m) c^\dagger_{p_x,n} \sigma^z c_{p_x,n}
\end{aligned} \tag{1.1.2}$$

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

$$|\psi_{p_x}\rangle = \sum_n \psi_{p_x,n,u} c^\dagger_{p_x,n,u} + \psi_{p_x,n,v} c^\dagger_{p_x,n,v} |0\rangle \tag{1.1.3}$$

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

$$\begin{aligned}
& \sum_n c^\dagger_{p_x,n} A \psi_{p_x,n-1} + c^\dagger_{p_x,n} B \psi_{p_x,n} + c^\dagger_{p_x,n} C \psi_{p_x,n+1} \\
& = E_{p_x} \sum_n c^\dagger_{p_x,n} \psi_{p_x,n}
\end{aligned} \tag{1.1.4}$$

where

$$c^\dagger_{p_x,n} = \left(c^\dagger_{p_x,n,u}, c^\dagger_{p_x,n,v} \right) \tag{1.1.5}$$

$$A = i\sigma^y - \sigma^z \tag{1.1.6}$$

$$B = 2\sin(p_x)\sigma^x - 2\cos(p_x)\sigma^z + (2-m)\sigma^z \tag{1.1.7}$$

$$C = -i\sigma^y - \sigma^z \tag{1.1.8}$$

$$\psi_{p_x,n} = \begin{pmatrix} \psi_{p_x,n,u} \\ \psi_{p_x,n,v} \end{pmatrix} \tag{1.1.9}$$

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:

$$H_{\text{disc}}\psi \equiv \begin{pmatrix} B & C & & & A \\ A & B & C & & \\ & A & B & C & \\ & & \cdots & & \\ & & A & B & C \\ C & & & A & B \end{pmatrix} \begin{pmatrix} \psi_{p_x,1} \\ \psi_{p_x,2} \\ \cdots \\ \\ \\ \psi_{p_x,N} \end{pmatrix} = E_{p_x} \begin{pmatrix} \psi_{p_x,1} \\ \psi_{p_x,2} \\ \cdots \\ \\ \\ \psi_{p_x,N} \end{pmatrix} \tag{1.1.10}$$

Note: Numerical calculations 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:

$$\begin{pmatrix} -\sqrt{m^2 + 4m\cos(\text{px}) + 4} \\ \sqrt{m^2 + 4m\cos(\text{px}) + 4} \\ -\sqrt{m^2 + 4m\cos(\text{px}) - 6m - 12\cos(\text{px}) + 16} \\ -\sqrt{m^2 + 4m\cos(\text{px}) - 6m - 12\cos(\text{px}) + 16} \\ \sqrt{m^2 + 4m\cos(\text{px}) - 6m - 12\cos(\text{px}) + 16} \\ \sqrt{m^2 + 4m\cos(\text{px}) - 6m - 12\cos(\text{px}) + 16} \end{pmatrix} \tag{1.1.11}$$

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

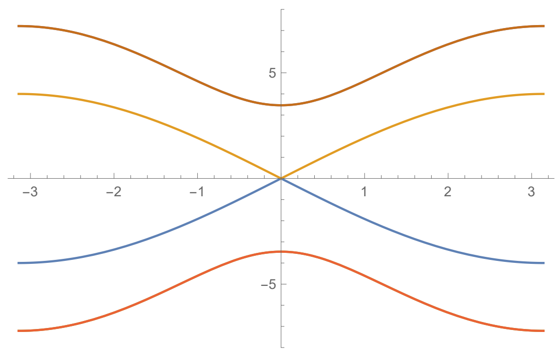


Figure 1: The Eigenvalue plot for $m = -2$. Plotted as E_{p_x}-p_x

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

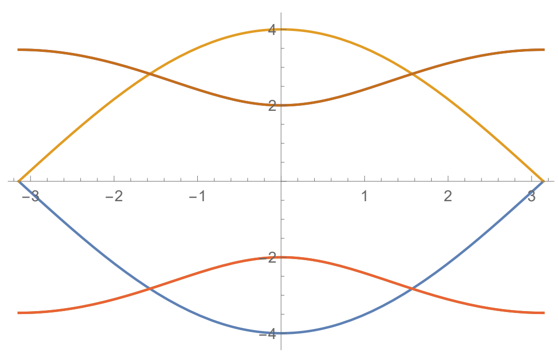


Figure 2: The Eigenvalue plot for $m = 2$. Plotted as E_{p_x}-p_x

When the band crosses, there will be two eigenvectors, corresponds to the two crossed bands, in the form of:

$$\psi_{p_x} = \Big(\psi(p_x), 1, \psi(p_x), 1, \psi(p_x), 1\Big)^T \tag{1.1.12}$$

$$\phi_{p_x} = \Big(\phi(p_x), 1, \phi(p_x), 1, \phi(p_x), 1\Big)^T \tag{1.1.13}$$

where $\psi(p_x)$ and $\phi(p_x)$ are functions of p_x. A look into the plot of $\psi(p_x)$ and $\phi(p_x)$ reveals that they together provide the path way for excited particles to transfer from the lower band to the upper band.

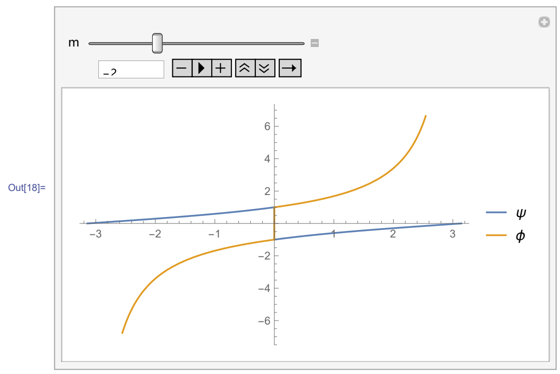


Figure 3: Plot of $\psi(p_x)$ and $\phi(p_x)$ when $m = -2$

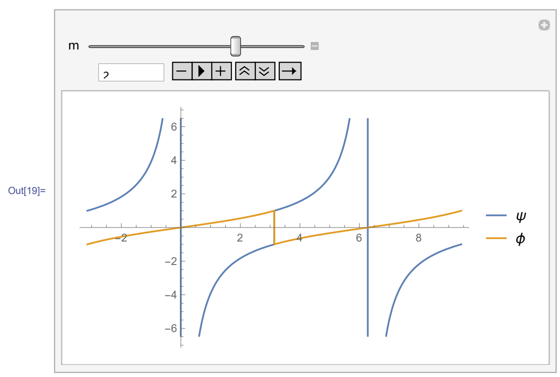


Figure 4: Plot of $\psi(p_x)$ and $\phi(p_x)$ when $m = 2$, where I have extended the plot range s.t. $p_x \in \{-\pi, 3\pi\}$ to make the meaning clear.

Therefore, I think [1] this represents a pure spin-up wave transfering in the point $p_x = 0$ when $m = 2$, and $p_x = \pm\pi$ when $m = 2$.

[1]If I interpret the two component u, v as one for spin up and the other for spin down.

1.2 Why I think the Lattice Model is wrong

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

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

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:

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

This affects the numerical analysis effectively by the replacement

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

The calculated result is similar to that in the previous section, except that the band crossing happens at different values of m. [2] So the essential point is unaltered by the difference in some constants. However, in the correct calculation, the crossing band appears at $m = 0$, which represents a massless spin-$\frac{1}{2}$ particle. I think this should have some theoretical implications.

1.3 Calculation Note unrelated to the main-subject

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

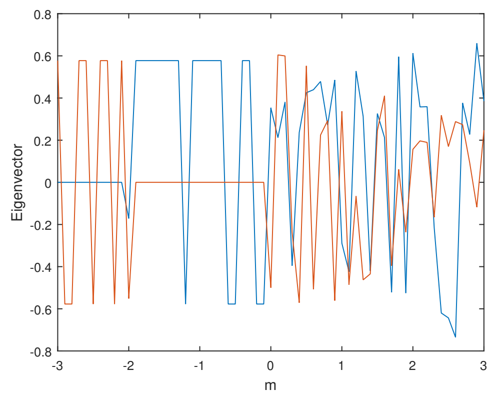
When I looked blindly at the value $(m, p_x) = (-2, 0)$, the Mathematica gave me two eigenvectors both corresponds to the eigenvalue 0:

$$\{0,1,0,1,0,1\}, \{1,0,1,0,1,0\} \tag{1.3.1}$$

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.

[2] 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).

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:

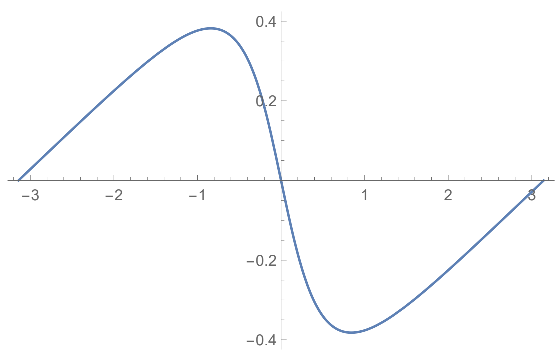


Figure 5: $m = -3$

to

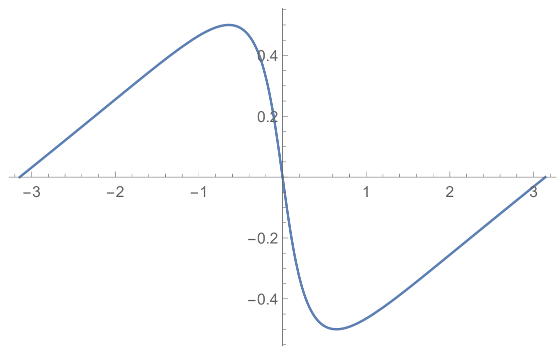


Figure 6: $m = -2.5$

and suddenly to

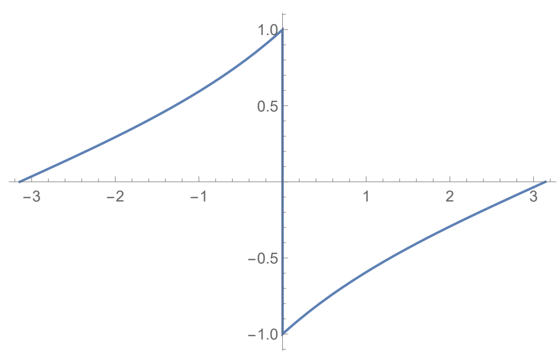


Figure 7: $m = -2$. There is a discontinuity at $p_x = 0$

Finaly, it becomes smooth again:

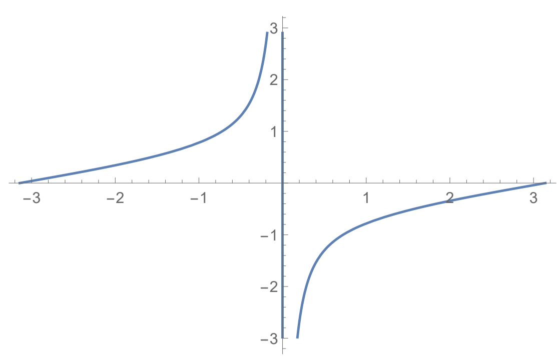


Figure 8: $m = -1.5$

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 $(2, \pm\pi)$.

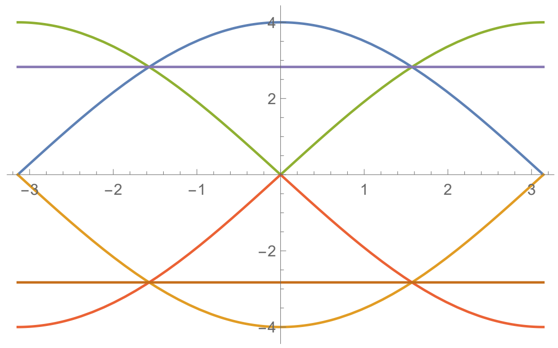


Figure 9: $m = 2$

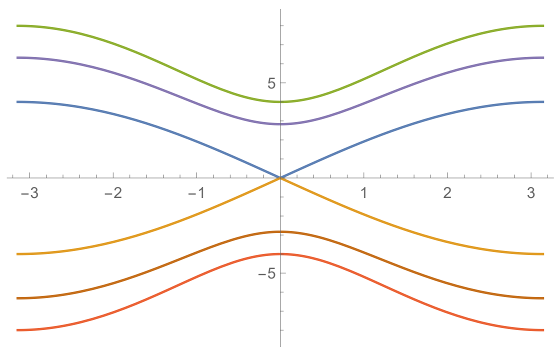


Figure 10: $m = -2$

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

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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