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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

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

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:

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

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

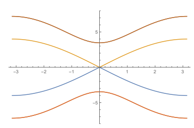


Figure 1: The Eigenvalue plot for $m = -2$. Plotted as E_{p_x}-p_x

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

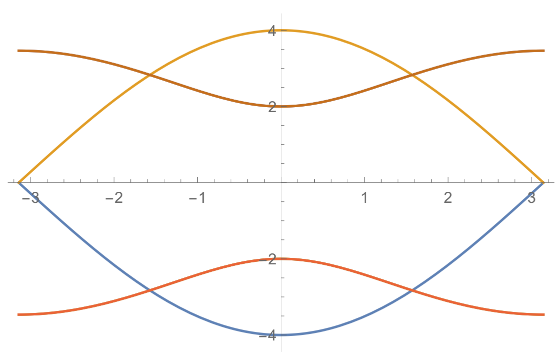


Figure 2: The Eigenvalue plot for $m = 2$. Plotted as E_{p_x}-p_x

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.

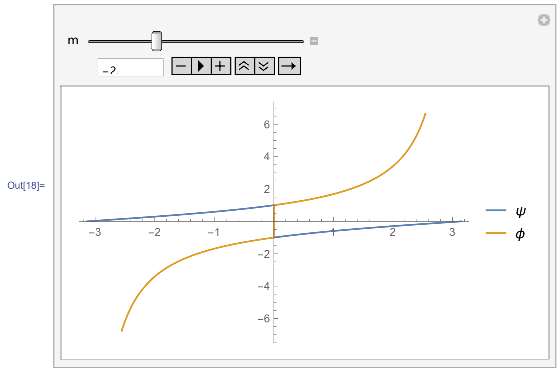


Figure 3: Plot of $\psi(p_x)$ and $\phi(p_x)$ when $m = -2$

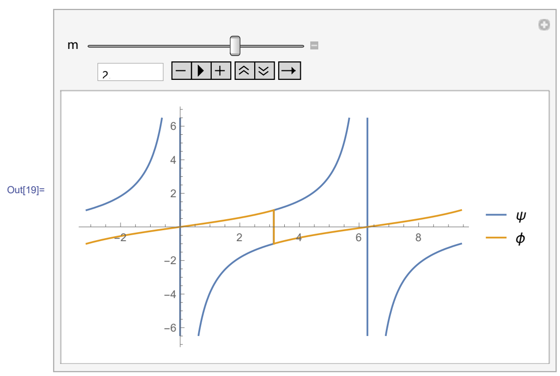


Figure 4: Plot of $\psi(p_x)$ and $\phi(p_x)$ when $m = 2$, where I have extended the range s.t. $p_x \in \{-\pi, 3\pi\}$ to make the meaning clear.

Therefore, one may predict a pure spin-up wave transfering in the point $p_x = 0$ when $m = 2$, and $p_x = \pm\pi$ when $m = 2$.

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:

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

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. [1] 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.

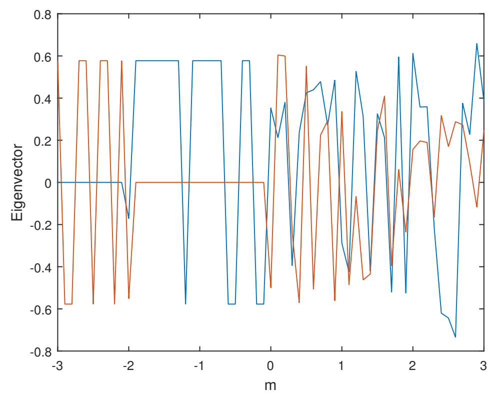
When I looked blindly at the value $(m, p_x) = (-2, 0)$, the Mathematica gave me two eigenvectors both corresponds to the eigenvalue 0:

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

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.

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:

[1] 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).



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

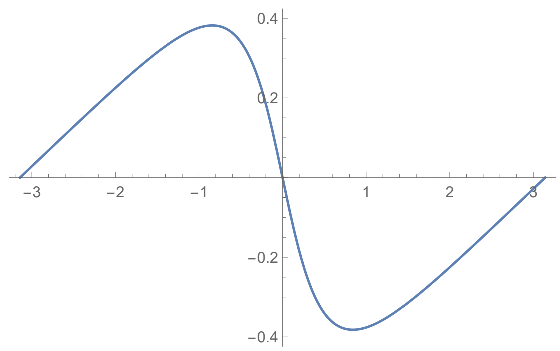


Figure 5: $m = -3$

to

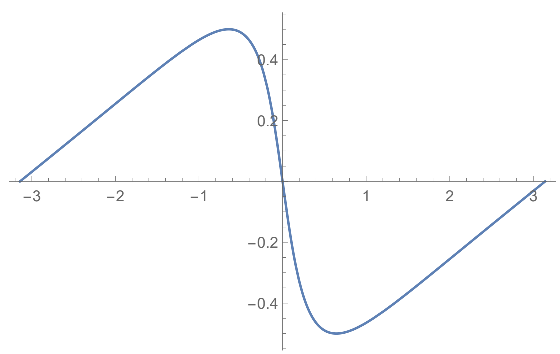


Figure 6: $m = -2.5$

and suddenly to

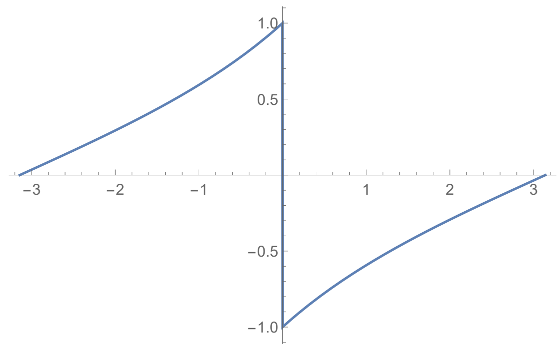


Figure 7: $m = -2$. There is a discontinuity at $p_x = 0$

Finaly, it becomes smooth again:

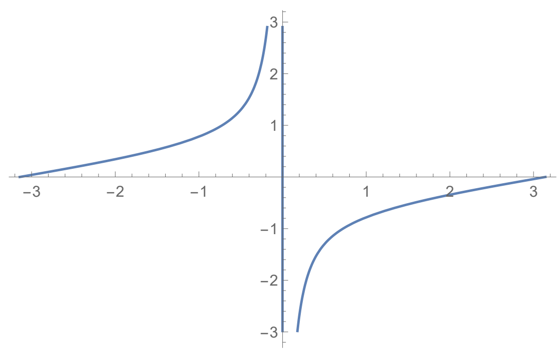


Figure 8: $m = -1.5$

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 $(2, \pm\pi)$.

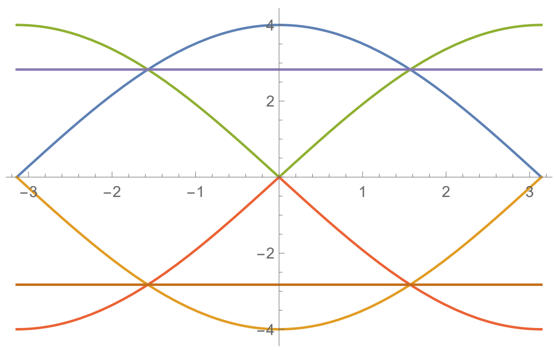


Figure 9: $m = 2$

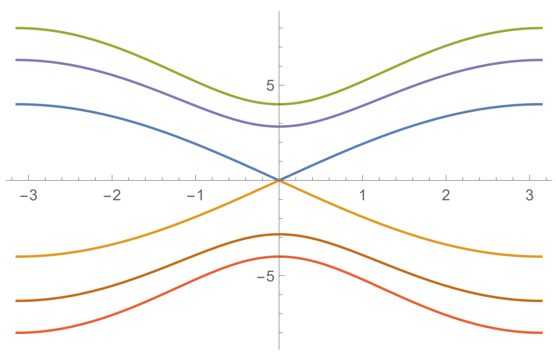


Figure 10: $m = -2$

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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