

TR Invariant T.I.

Taper

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Abstract

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

Contents

1	Spectrum of (2 + 1)d Lattice Dirac Model	1
1.1	Numerical Solution in Infinity Cylinder Geometry	1
1.2	Why I think the Lattice Model Hamiltonian is mildly wrong	5
1.3	Calculation Note I (Not related to the main discussion)	5
1.4	Numerical Solution with open boundary condition in both dimensions	8
2	License	12
	Start with chapter 2.	
	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

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

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.

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:

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

The resulted Hamiltonian is

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

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

$$|\psi_{p_x}\rangle = \sum_n \psi_{p_x,n,u} c_{p_x,n,u}^\dagger + \psi_{p_x,n,v} c_{p_x,n,v}^\dagger |0\rangle \quad (1.1.3)$$

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:

$$\begin{aligned} & \sum_n c_{p_x,n}^\dagger A \psi_{p_x,n-1} + c_{p_x,n}^\dagger B \psi_{p_x,n} + c_{p_x,n}^\dagger C \psi_{p_x,n+1} \\ & = E_{p_x} \sum_n c_{p_x,n}^\dagger \psi_{p_x,n} \end{aligned} \quad (1.1.4)$$

where

$$c_{p_x,n}^\dagger = (c_{p_x,n,u}^\dagger, c_{p_x,n,v}^\dagger) \quad (1.1.5)$$

$$A = i\sigma^y - \sigma^z \quad (1.1.6)$$

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

$$C = -i\sigma^y - \sigma^z \quad (1.1.8)$$

$$\psi_{p_x,n} = \begin{pmatrix} \psi_{p_x,n,u} \\ \psi_{p_x,n,v} \end{pmatrix} \quad (1.1.9)$$

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:

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

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:

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

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

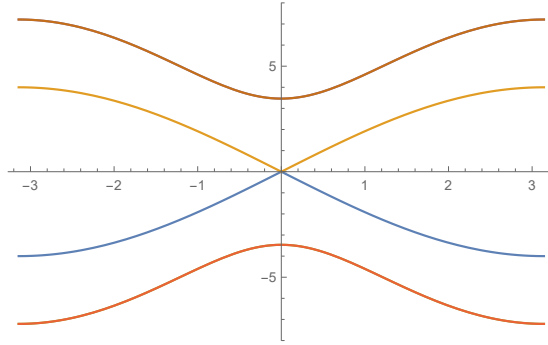


Figure 1: The Eigenvalue plot for $m = -2$. Plotted as $E_{p_x}-p_x$

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

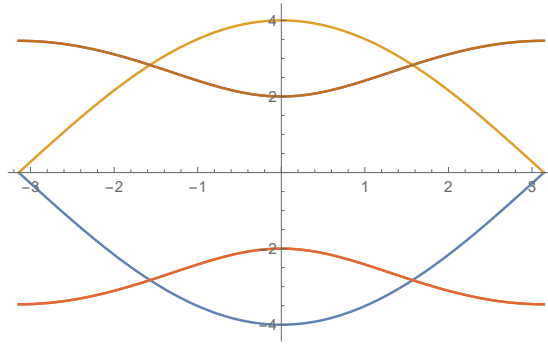


Figure 2: The Eigenvalue plot for $m = 2$. Plotted as $E_{p_x}-p_x$

When the band crosses, there will be two eigenvectors, corresponds to

the two crossed bands, in the form of:

$$\psi_{p_x} = \left(\psi(p_x), 1, \psi(p_x), 1, \psi(p_x), 1 \right)^T \quad (1.1.12)$$

$$\phi_{p_x} = \left(\phi(p_x), 1, \phi(p_x), 1, \phi(p_x), 1 \right)^T \quad (1.1.13)$$

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.

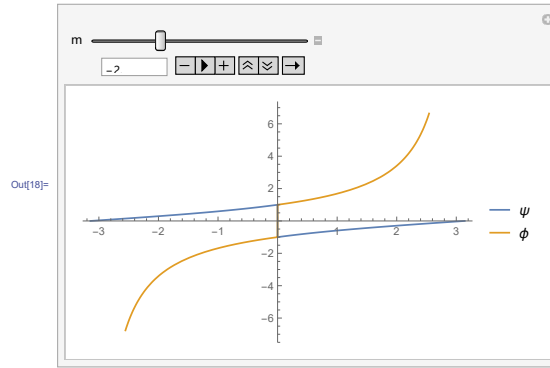


Figure 3: Plot of $\psi(p_x)$ and $\phi(p_x)$ when $m = -2$

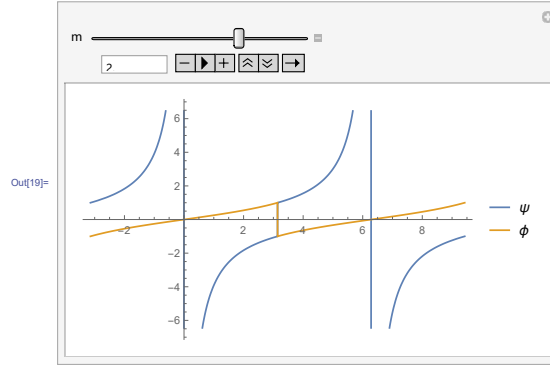


Figure 4: Plot of $\psi(p_x)$ and $\phi(p_x)$ when $m = 2$, where I have extended the plot range s.t. $p_x \in \{-\pi, 3\pi\}$ to make the meaning clear.

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

¹If 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 Hamiltonian is mildly wrong

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

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

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:

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

This affects the numerical analysis effectively by the replacement

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

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 I (Not related to the main discussion)

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.

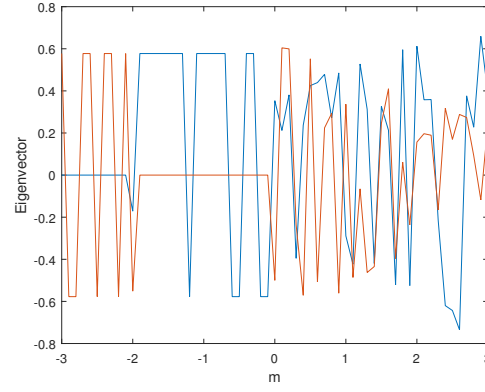
When I looked blindly at the value $(m, p_x) = (-2, 0)$, the Mathematica gave me two eigenvectors both corresponds to the eigenvalue 0:

$$\{0, 1, 0, 1, 0, 1\}, \{1, 0, 1, 0, 1, 0\} \quad (1.3.1)$$

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.

²For 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:

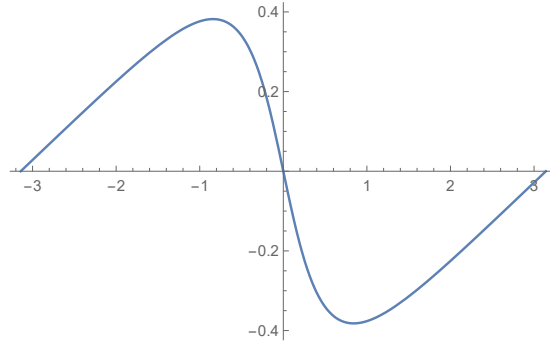


Figure 5: $m = -3$

to

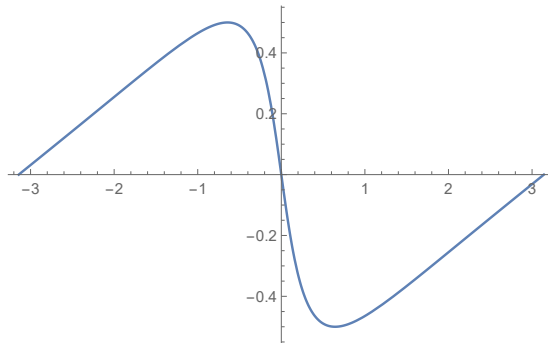


Figure 6: $m = -2.5$

and suddenly to

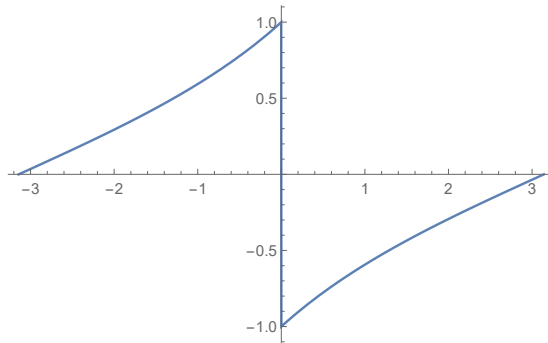


Figure 7: $m = -2$. There is a discontinuity at $p_x = 0$

Finally, it becomes smooth again:

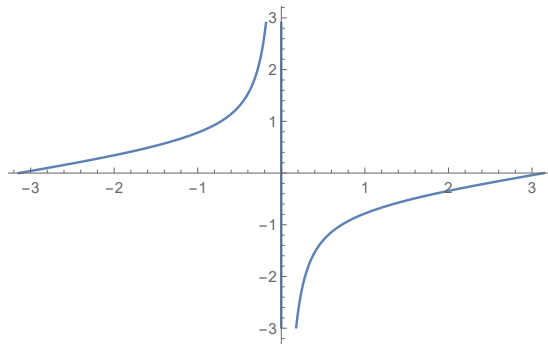


Figure 8: $m = -1.5$

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 $(2, \pm\pi)$.

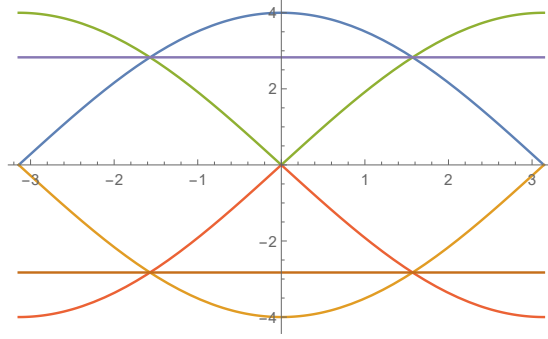


Figure 9: $m = 2$

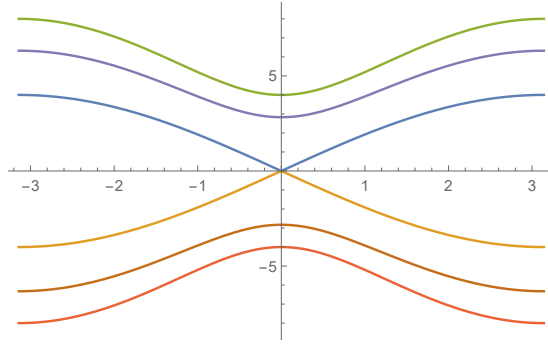


Figure 10: $m = -2$

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>.

1.4 Numerical Solution with open boundary condition in both dimensions

Note 1: Since the essential point is not altered by the minor error in Hamiltonian, as mentioned in Section 1.2. I will continue with the Lattice

Model Hamiltonian that produce correctly the Dirac Hamiltonian in the continuum limit.

Note 2: Calculation in this part is available in the Mathematica notebook "Lattice Dirac Model (2+1)-d-2.nb".

When the two sides are of open boundary, the problem is quite simple and the Fourier-transformed Hamiltonian is (almost) diagonal in momentum space. It is (as calculated in [Hug09], eq.2.21):

$$H = \sum_{p_x, p_y} c_{p_x, p_y}^\dagger \times [\sin(p_x)\sigma^x + \sin(p_y)\sigma^y + (2 - m - \cos(p_x) - \cos(p_y))\sigma^z] c_{p_x, p_y} \quad (1.4.1)$$

The eigenvalues of the Hamiltonian of the form $\mathbf{a} \cdot \boldsymbol{\sigma}$ are:

$$E_1 = |a|, \quad E_2 = -|a| \quad (1.4.2)$$

If plotted in (p_x, p_y) plane, we will find several interesting crossing happening when $m = 0, 2, 4$:

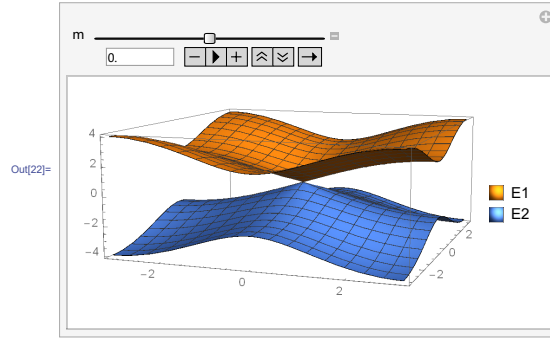


Figure 11: $m = 0$

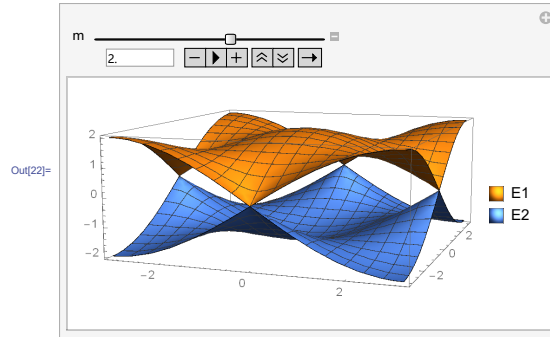


Figure 12: $m = 2$

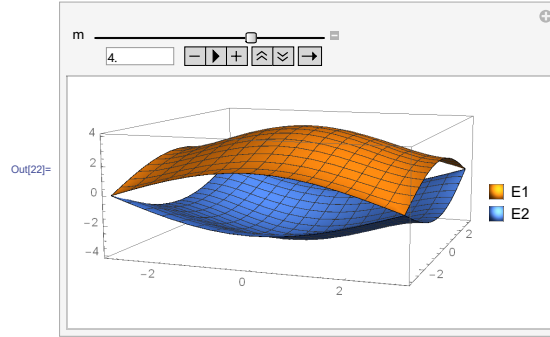


Figure 13: $m = 4$

The eigenvectors are of the form:

$$(\phi, \sin(p_x) + i \cos(p_y)), \quad (\psi, \sin(p_x) + i \cos(p_y)) \quad (1.4.3)$$

where

$$\phi = (2 - m - \cos(p_x) - \cos(p_y)) + E_1 \quad (1.4.4)$$

$$\psi = (2 - m - \cos(p_x) + \cos(p_y)) + E_1 \quad (1.4.5)$$

And they have very interesting behavior from $m = -1$ to $m = 6$, they gradually contact and exchange the position of each other ³:

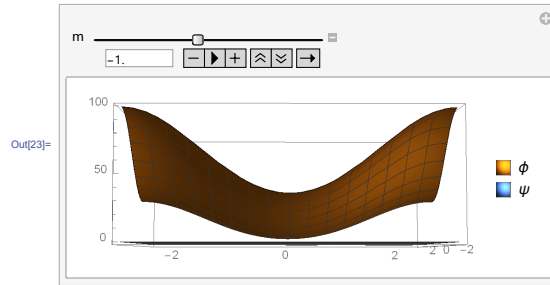


Figure 14: $m = -1$

³You would get more fun if you execute the animation inside the Mathematica notebook

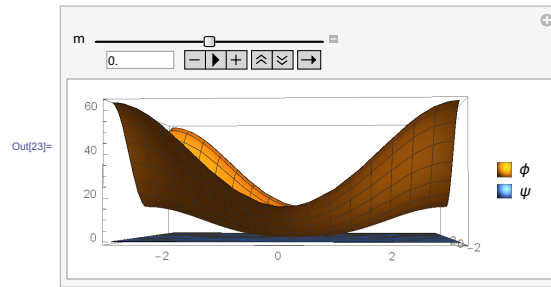


Figure 15: $m = 0$

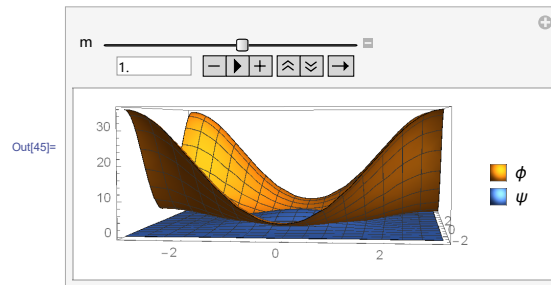


Figure 16: $m = 1$

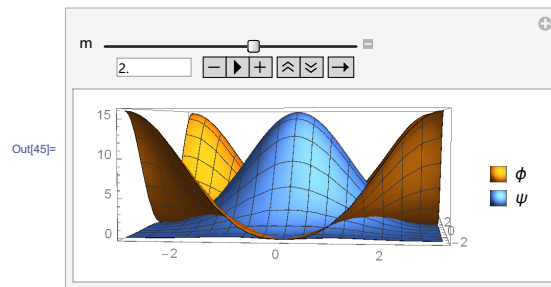


Figure 17: $m = 2$

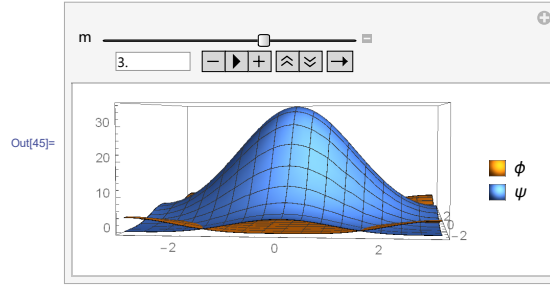


Figure 18: $m = 3$

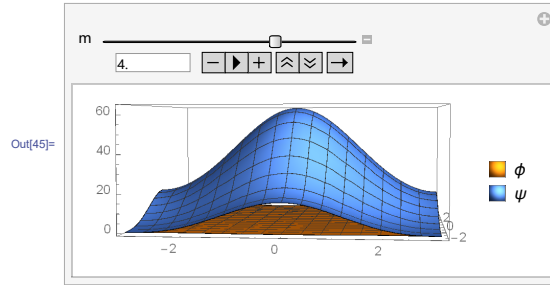


Figure 19: $m = 4$

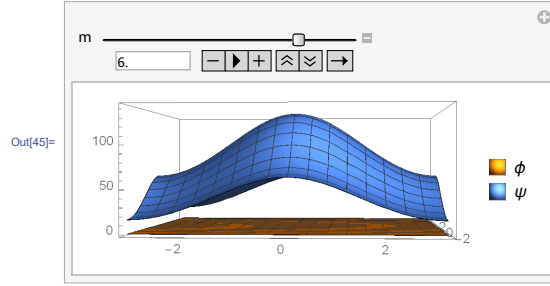


Figure 20: $m = 6$

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