Refresher Course on Quantum Mechanics in Tezpur.

In this part of the course, I plan to do 2 things.

In the first part of my course, I will explain why relativistic quantum mechanics is relevant both in high energy physics and condensed matter physics. Then I will give some recent examples from recent condensed matter physics and show why it is relevant to graphene, topological insulato and other materials like silicene.

In the second part of my course, I will talk about particles responding to a magnetic field and here again, I will connect it up to recent problems in the QHE in both the relativistic and non-relativistic context.

Let us start with the first part, which is relativistic quantum mechanics. Historically, Dirac first introduced his famous Dirac eq^n to describe a free electron satisfying the relativistic dispersion $E^2 = \vec{p}^2 c^2 + m^2 c^4$

E = energy, $\vec{p}$ = mtm and m = mass. and c = velocity of light.

The most important that this eq^n introduced was the concept of $-ve$ energy solutions and its interpretation as an anti-ptcle, or the positron, which was discovered soon after its prediction. The Dirac eq^n in 3+1 dimensions is a 4 component spinor eq^n which described a spin ↑ and ↓ electron and a spin ↑ & ↓ positron. ~~For massless particles, one can at~~ We will come to this along with its cousins — the Weyl equation and the Majorana eq^n shortly.

But let me also explain that today the study of the Dirac eq^n

is also very important in cond. matter systems. Naively, since in CMP, electrons move at low velocities compared to c, one would expect the Dirac eq² not to play a role, and indeed, in most condensed matter systems the Schrödinger eq² « which is the non-relativistic wave eq² » is what is used. But recently, in materials like graphene and its cousins, and topological insulators, it ~~has been found~~ was found that the valence band and the conduction band touch at some points in the Brillouin zone and if we look for the low energy theory around these band-touching points, ~~their~~ ~~spectrum turns~~ ~~out~~ ~~to be linear~~ spectrum turns out to be linear — ~~the velocity~~ and the ~~the velocity~~ velocity of light is replaced by the Fermi velocity $E = v_F |\vec{k}|$ and the mass of the dispersing particle is ~~zero~~ — So we get the massless Dirac eq².

Let me first briefly review the relativistic wave eq^n or Dirac eq^n for massive particles in 3+1 dimensions

The eq^n has to be first order in time so that the wave-fn can be understood as a probability amplitude

And Lorentz invariance implies that space and time should be treated on the same footing.

So ~~naively~~ one ~~can just write~~ ~~$i\frac{\partial \psi}{\partial t} = (\vec{\alpha} \cdot \vec{p})$~~

In the ~~non~~ non-relativistic quantum mechanics, we get the Schrödinger eq^n from

$$H = \frac{\vec{p}^2}{2m}$$

by replacing $\vec{p} = -i\hbar \vec{\nabla}$. H by $i\hbar \frac{\partial}{\partial t}$ and That is why we get

$$i\hbar \frac{\partial \psi (\vec{x}, t)}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi (\vec{x}, t)}{\partial t^2}$$

For the relativistic case, since $E = \pm\sqrt{\vec{p}^2 + m^2}$ has a square root, the straight forward eq we will get by the ~~above~~ above substitution is non-local,

We ~~write~~ down follow the historical path and ~~into~~ down a matrix eq^2

$$i\hbar \frac{\partial \psi}{\partial t} = (\vec{\alpha}\cdot\vec{p} + \beta m)\psi$$

where ψ = column vetor

and α_i, β are fixed so that we get $E^2 = \vec{p}^2 + m^2$.

I won't go thru' this, ~~but~~ since I am sure all of you know This. But just to fix the notation, we have

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij}$$
$$\alpha_i \beta + \beta \alpha_i = 0$$
$$\beta^2 = 1$$

α_i, β are ~~Hermitian~~ 4 anti-commuting even ~~(odd)~~ - dimensional traceless matrices whose eigenvalues are ± 1.

For 3+1 dimensions — they are 4 dim matrices

For 1+1 or 2+1 dimension, they are the 2 dimensional σ matrices.

Also for $m = 0$ case in 3+1 dim, we can do with 2 dim ~~ore~~ matrices

To write it out explicitly once

$$i\hbar \frac{\partial}{\partial t}\begin{pmatrix} \psi_1(\vec{x},t) \\ \psi_2(\vec{x},t) \\ \psi_3 \\ \psi_4 \end{pmatrix} = -i\hbar \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} \frac{\partial \psi_1}{\partial x_1} \\ \frac{\partial \psi_2}{\partial x_1} \\ \frac{\partial \psi_3}{\partial x_1} \\ \frac{\partial \psi_4}{\partial x_1} \end{pmatrix}$$

$$+ \begin{pmatrix} 0 & & 0 & -i \\ & & i & 0 \\ 0 & -i & & 0 \\ i & 0 & & \end{pmatrix} \begin{pmatrix} \frac{\partial \psi_1}{\partial x_2} \\ \frac{\partial \psi_2}{\partial x_2} \\ \frac{\partial \psi_3}{\partial x_2} \\ \frac{\partial \psi_4}{\partial x_2} \end{pmatrix} + \begin{bmatrix} 0 & & 1 & 0 \\ & & 0 & -1 \\ 1 & 0 & & 0 \\ 0 & -1 & & 0 \end{bmatrix} \begin{pmatrix} \frac{\partial \psi_1}{\partial x_3} \\ \frac{\partial \psi_2}{\partial x_3} \\ \frac{\partial \psi_3}{\partial x_3} \\ \frac{\partial \psi_4}{\partial x_3} \end{pmatrix}$$

$$+ \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} m \psi$$

Here we have used

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

One can also use other representations

Most of you probably also remember that the Dirac eq^n can be compactly written in 4 vector notation as

$$\left(i \hbar \gamma^\mu \frac{\partial}{\partial x^\mu} - m \right) \psi(x) = 0$$

with $\gamma^0 = \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ and $\gamma^i = \beta\alpha^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}$

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2 g^{\mu\nu}$$

Besides being explicitly relativistically invariant, the Dirac eq^n is also invariant under charge conjugation C, space-inversion or parity P and time-reversal invariance T

→ Module on graphene

Now let me show how the excitations in a material like graphene behaves like Dirac particles. As you may all have heard, graphene was isolated by peeling of layers using a scotch-tape and what was amazing is that they managed to isolate single layers of graphene, put it on a substrate and characterise it.
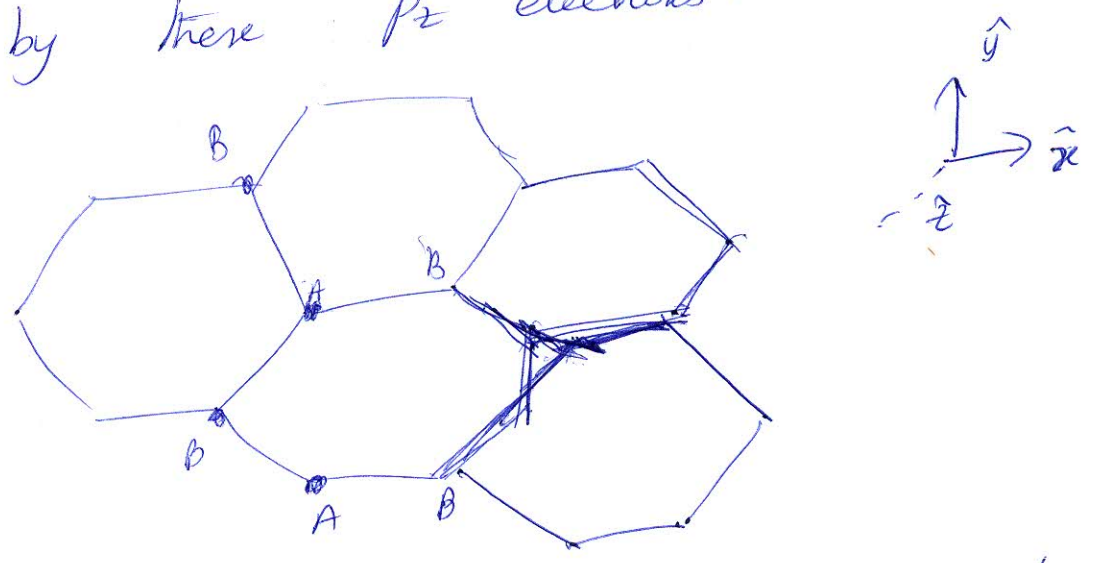
In Manchester, the exptalists put graphene on silicon wafers. The surface reflects colours and the interference pattern depends on the # of atomic layers. So experienced exptalists could identify single layers, double layers, etc, just by looking at it. They then confirmed it by ~~looking~~ putting contacts on it and looking at the conductance, and checking that it had the properties of a single layer.

Before going on to describe details of graphene, let me just mention why it is technologically so important. It is extremely strong ∵ of the carbon bonds (200 times as strong as steel) extremely thin and flexible. 1 sq.m of graphene can hold several kilos of wt. thought it's own weight is barely a mg. It is an extremely good conductor of electricity at room temperature and also of heat. All these properties are mainly ∵ of the electronic structure of graphene, which is very different from that of most materials. We will come to that now.

What is graphene ?

Graphene consists of a honeycomb lattice of carbon atoms. In this structure, each carbon atom has 6 electrons - 2 electrons filling the inner shell $1s^2$, 3 electrons engaged in the 3 - in -plane covalent bonds in the sp^2 configuration, and a single electron occupying the p_z orbital $\perp^r$ to the plane.

Much of the physics of graphene comes from the 2 dim fluid of electron fluid formed by these p_z electrons.
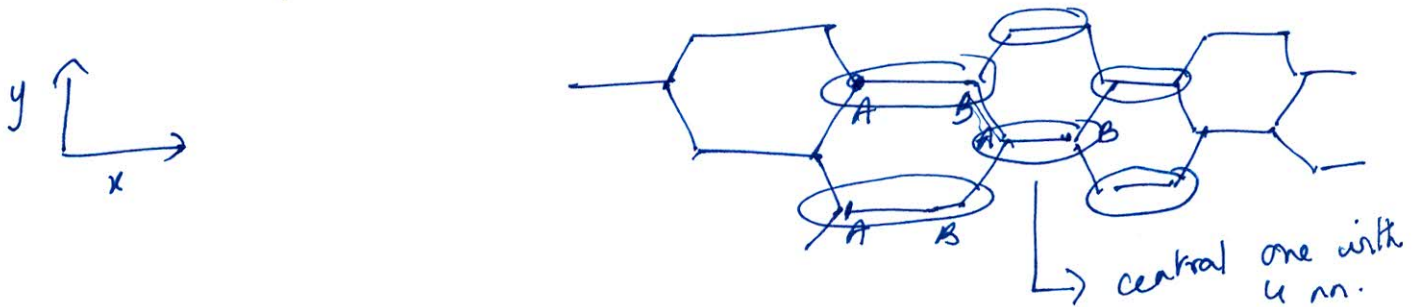

So the ~nearest neighbour tight-binding model has to be written only for the p_z electrons. $t \sim 2.7 eV$ is the hopping amplitude between p_z orbitals of 2 adjacent carbon atoms. We could write down the second quantised Hamiltonian

$$H = t \sum_{\vec{r}_A} \sum_{\alpha=1}^{3} C_B^+ (\vec{r}_A + \vec{\delta}_\alpha) \, C_A(\vec{r}_A)$$

$$+ h.c$$

where the sum over r_A goes over the A sites and the sum over α goes over its ~~neig~~ nearest neighbour B sites.

But ~~let~~ ~~me~~ let me do this using first quantised formalism because that may be ~~easier to~~ easier to use when you are teaching a quantum mechanics course because many students may not be familiar with the second ~~quantised~~ quantisation

So we start with graphene, which is a mono-layer of graphite ~~which~~ with the carbon atoms arranged in a hexagonal lattice, as I already mentioned

$y \uparrow$
$\rightarrow x$

$\rightarrow$ central one with 4 nn.

We first need to choose the unit cell so that the neighbourhood looks the same around each unit.

Now within the unit, we work with any point and choose the corresponding pt. on all the other units.

Now we can write down the nearest neighbour tight-binding Hamiltonian

$$h(\vec{k}) = \sum_m (H_{nm}) e^{i\vec{k}\cdot(\vec{r_m} - \vec{r_n})}$$

where m runs over all the sites. The only ones where $H \neq 0$ is when $m = n$ or m is one of the nearest neighbours of n.

So there are only 5 terms

When $m = n$, it is easy

$$H_{nm} = \begin{matrix} & A & B \\ A & \\ B & \end{matrix}\begin{pmatrix} \epsilon & t \\ t & \epsilon \end{pmatrix}$$

(This is the 2x2 matrix of the unit cell.)

When we choose $m =$ lower right unit (B of n coupled to A of m)

Then $$H_{nm} = \begin{pmatrix} 0 & 0 \\ t & 0 \end{pmatrix}$$

Same for upper right, but with diff. phase part.

Then when we choose lower left, then
$$H_{nm} = \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix}$$ (A of n coupled to B of m)

& upper left = same, but with diff. phase.

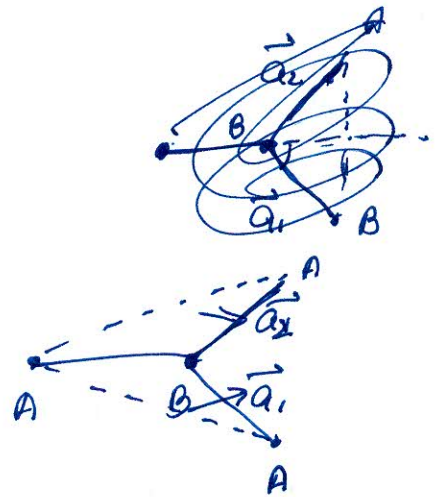Now include the phases.

For $n = m$, $\vec{r}_n = \vec{r}_m$.

For $n \neq m$, adding approp. phases, we get

$$\begin{pmatrix} 0 & 0 \\ t & 0 \end{pmatrix} e^{+i\vec{k}\cdot\vec{a}_1} + \begin{pmatrix} 0 & 0 \\ t & 0 \end{pmatrix} e^{i\vec{k}\cdot\vec{a}_2}$$

and $\begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix} e^{-i\vec{k}\cdot\vec{a}_1} + \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix} e^{-i\vec{k}\cdot\vec{a}_2}$

where

$$\vec{a}_1 = (1 + \cos 60°) a_0 \, \hat{x}$$
$$- \sin 60° \, \hat{y} \, a_0$$

$$\vec{a}_2 = \frac{3}{2} a_0 \, \hat{x} + \frac{\sqrt{3}}{2} a_0 \, \hat{y}$$

$a_0 = C-C$ bond length $\cong 1.42 \, A°$

$= 1.42 \times 10^{-10}$ m. in graphene

So now, we can write the

sum as

$$h(\vec{k}) = \begin{pmatrix} \epsilon & t\left(1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2}\right) \\ t\left(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}\right) & \epsilon \end{pmatrix}$$

$$= \begin{pmatrix} \epsilon & h_0^* \\ h_0 & \epsilon \end{pmatrix}$$

with $\quad h_0 = t \left(1 + e^{i\vec{k}\cdot\vec{a_1}} + e^{i\vec{k}\cdot\vec{a_2}} \right)$

$$= t \left(1 + e^{ik_x a} \, 2\cos k_y b \right)$$

(where $\vec{a_1} = a\hat{x} + b\hat{y}$

and $\vec{a_2} = a\hat{x} - b\hat{y}$)

Now, let us linearise the dispersion around the low energy values, for First, you can direct around the Fermi points points where $h_0 = 0$

(assume :. by these diagonalisup

the Hamiltonian , we will get

$$(\epsilon - \lambda)^2 + |h|^2 = 0 \quad \Longrightarrow \quad \lambda = \epsilon \; E$$

$$= \epsilon \pm |h_0|)$$

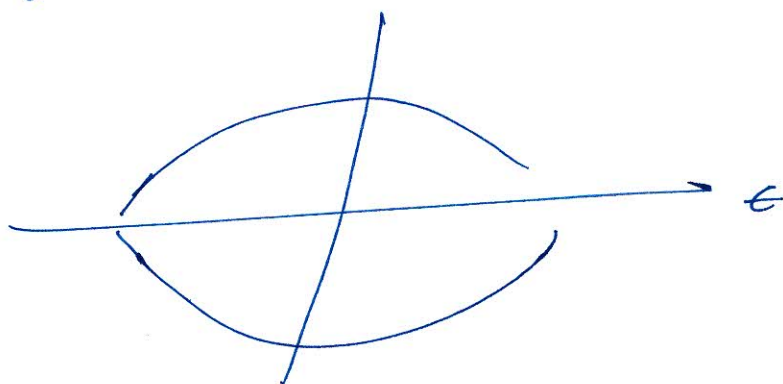Here, since our unit cell contains 2 atoms, we will have 2 branches of dispersion. For N unit cells, we have N branches states per branch And since , we can have $\uparrow$ & $\downarrow$ electrons, the N states can accome $2N$ electrons. Now, we have $2N$ Carbon atoms (N units) and as 1 already said , only one electron per Carbon
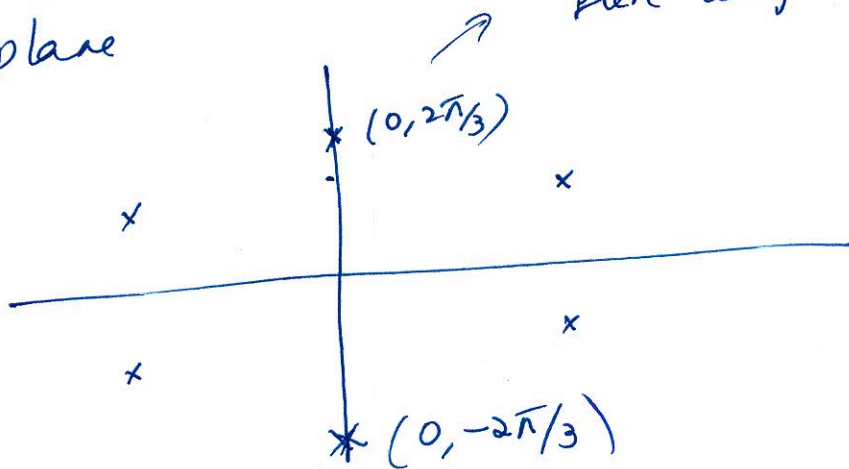
atom is important. So we have $2N$ electrons. So the lower branch is completely filled and the upper branch is completely empty and the Fermi level is at $E = \epsilon$

Now we linearise around the pt. such pts) because they will be closest to the Fermi energy

$$h_o = t \left(1 + 2e^{ik_x a} \cos k_y b \right) = 0$$

at the following pts in the (k_x, k_y) plane $\nearrow$ here $\cos k_y b = -\tfrac{1}{2}$

$\times$ $(0, 2\pi/3)$

$\times$

$\times$

$\times$

$\times$ $(0, -2\pi/3)$

It is easy to get the other points as well.

Now, let us lineause in the vicinity of the point $k_x = 0$, $k_y = \frac{2\pi}{3b}$

Then

$$h_0 = h_0\left(0, \frac{2\pi}{3b}\right) + \frac{\partial h_0}{\partial k_x}(k_x - 0)\bigg|_{\left(k_x = 0, \frac{2\pi}{3b}\right)}$$

$$+ \frac{\partial h_0}{\partial k_y}\bigg|_{k_y = \frac{2\pi}{3b}, k_x = 0}\left(k_y - \frac{2\pi}{3b}\right) + \sim$$

$$= 0 + ita\left(2\cos k_y b \cdot e^{ik_x a}\right)\bigg|_{k_x = 0, k_y = \frac{2\pi}{3b}}$$

$$\phi - 2te^{ik_x a} b \sin k_y b\bigg|_{k_y = \frac{2\pi}{3b}, k_x = 0} + \sim$$

$$\overset{\sim}{\leftarrow} \quad -iat\, k_x - tb\sqrt{3}\left(k_y - \frac{2\pi}{3b}\right)$$

$$b = \sqrt{3}\,a_0 = \frac{\sqrt{3}}{2} \cdot \frac{2}{3}a$$

Using $\quad a = \frac{3a_0}{2}$,

we get $\quad h_0 \sim -iat\left(k_x - i\left(k_y - \frac{2\pi}{3b}\right)\right)$

$$\Rightarrow |h_0| = at\sqrt{k_x^2 + \left(k_y - \frac{2\pi}{3b}\right)^2}$$

$$= at\sqrt{\delta k_x^2 + \delta k_y^2}$$

what is of interest is th $\underline{\quad}$ deviation from the F.P

Hence $\quad t = \epsilon \pm at\sqrt{\delta k_x^2 + \delta k_y^2}$

$$= \epsilon \pm at\,|\delta\vec{k}|$$

Hence the velocity of electrons in graphene is

$$\hbar v_0 = \frac{dE}{d|\vec{k}|} = at = \frac{3}{2} a_0 t$$

Using the value of a_0 & the hopping parameter value $\sim 3eV$, we get

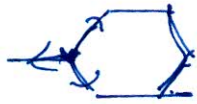$$\hbar v_0 = \frac{3}{2} \times 1.4 \times 10^{-10} m \times 3 \times 1.6 \times 10^{-19} \text{ coulombs}$$

Turns out that $v_0 \sim 10^6$ m/se

$$= \frac{1}{300} \text{ velocity of light.}$$

Note that in graphene, the velocity is constant (like in Dirac eq^n) and does not change with mtm. In the NR case, it is k/m.

One can also expand around the other Fermi points as well. The point is that if we look at the electrons which are conducting, then there will be little pockets around each of the Fermi points which are conducting and one has to add all of them up.
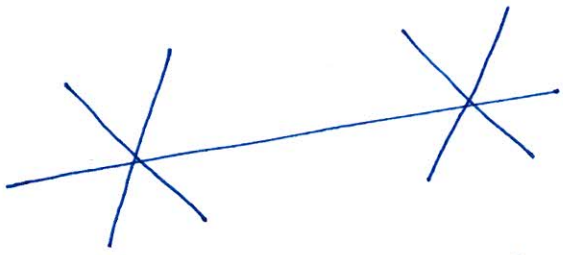
This is what gives rise to the concept of valleys in graphene. So essentially, one can calculate in any one valley and multiply by the degeneracy factor g. The total deg. factor $= 2$ (for spins) $\times$ N (# of valleys.)

Naively, we have 6 Fermi points, so y may think that you have 6 valleys. But if you look at the Brillouin zone of graphene, you notice that each F.P. is shared by 3 zones

So at each point, only $\frac{1}{3}$ of the valley is inside the B.Z. Hence, we have only $\frac{1}{3} \times 6 = 2$ valleys. Another way of saying this is that are 2 inequivalent Fermi points and the other 2 are connected by reciprocal lattice vectors.

So basically what we have are 2 Dirac cones around any of the 2 inequivalent Fermi-points

For graphene E turns out be zero and one gets the dispersion

$$E = \pm \hbar v_0 |\vec{\delta k}|$$
$$= \pm \hbar v_0 \sqrt{k_x^2 + k_y^2}$$
$$= \pm v_0 \sqrt{p_x^2 + p_y^2} = \pm v_0 |\vec{p}|$$

This is precisely the dispersion of a massless Dirac particle.

In fact, if you go back and write

$$h(\vec{k}) = \begin{pmatrix} 0 & t(1 + e^{-ik_x a} 2\cos k_y b) \\ * & 0 \end{pmatrix}$$

linearise, etc around F.P

$$= \begin{pmatrix} 0 & \frac{3}{2} t a_0 (ik_x - k_y) \\ \frac{3}{2} t a_0 (-ik_x - k_y) & 0 \end{pmatrix}$$

$$= i\hbar v_0 \begin{pmatrix} 0 & -k_y + ik_x \\ -k_y - ik_x & 0 \end{pmatrix}$$

is precisely the Dirac eq^2 in 2+1 dimensio