M2 ICFP 2016/2017

Graphene, Dirac fermions and topological matter

by Pascal Simon (pascal.simon@u-psud.fr)

TD No 1 : Klein tunneling in graphene

1 Introduction : plane waves

The goal is to compute the probability transmission T of a graphene electron across a potential step or barrier. We assume the barrier to be smoothed at the lattice scale $a \sim 0.1$ nm but sharp at the wavelength scale λ_F. Why such assumptions ? The single valley hamiltonian is :

$$H = v_F \boldsymbol{p} \cdot \boldsymbol{\sigma} + V(\boldsymbol{r}) \tag{1}$$

where the potential V is constant in some finite area of space. In the following we take $\hbar \equiv 1$ and $v_F \equiv 1$.

1) We first consider a constant potential $V(\boldsymbol{r}) = V_0$. We are looking for plane waves solutions in the graphene sheet of area $\mathcal{A} = 1$. Why can we restrict to the single valley Hamiltonian. Show that the (spinorial) plane wave

$$\psi(\boldsymbol{r}) = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{2}} \begin{pmatrix} 1 \\ \alpha e^{i\theta_{\boldsymbol{k}}} \end{pmatrix} \tag{2}$$

is an eigenvector of the hamiltonian with eigenenergy $E = \alpha k + V_0$ where $\boldsymbol{k}$ is the wavevector (we assume k_x, k_y real), $\tan\theta_{\boldsymbol{k}} = k_y/k_x$ gives the x-axis angle, α is the band index defiend by $\alpha = \mathrm{sgn}(E - V_0)$.

2a) The velocity operator is defined as $\hat{\vec{v}} \equiv \dot{\vec{r}}$. Using the Heisenberg equation of motion for the Dirac Hamiltonian in Eq. (1), express $\hat{\vec{v}}$.

2b) Show that the average velocity of a plane wave of momentum $\vec{k}$ and band index α is

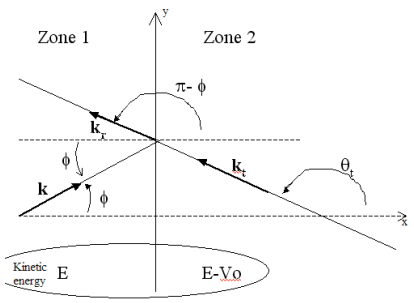
$$\vec{v} \equiv \langle \vec{k}, \alpha | \hat{\vec{v}} | \vec{k}, \alpha \rangle = \alpha \frac{\vec{k}}{k} \tag{3}$$

2c) For $\alpha = -1$ – i.e. when the electron is in the valence band and has a negative kinetic energy – compare the direction of the wavector to the direction of the propagation of the wave (i.e. to the velocity). Any comment ?

2d) The probability density of the state $|\psi\rangle$ is $|\psi(\vec{r}, t)|^2$ and the associated (average) probability current is called $\vec{j}(\vec{r}, t)$. The average current for Dirac spinors is defined as $\vec{j} = \psi^\dagger \hat{\vec{\sigma}} \psi$. For an eigenstate $|\vec{k}, \alpha\rangle$, show that the average current is equal to the average velocity.

3) **General conservation laws.** For a potential barrier defined by $V(x, y) = V(x)$, beyond the energy conservation, exhibit two other conserved quantities.

2 Potential step (np junction)



Let us first consider a square (sharp) potential step of height V_0 on which an electron of energy $E = k_F > 0$ is incident (see the figure) Here $V(\boldsymbol{r}) = 0$ if $x < 0$ (zone 1) and $V(\boldsymbol{r}) = V_0 > 0$ if $x > 0$ (zone 2). The electron

is incident with an energy $E > 0$, which is below the step height V_0, and its momentum $\boldsymbol{k}$ makes an angle ϕ with the normal $\tan\phi = k_y/k_x$. The different wavectors are written as $\vec{k}^{(j)} = (k_x^{(j)}, k_y^{(j)}) = |\vec{k}^{(j)}|(\cos\theta_j, \sin\theta_j)$, where $E_{\mathrm{kin},j} = \alpha_j|\vec{k}^{(j)}|$ with $j = \{\underline{\mathrm{i}}\mathrm{ncident}, \underline{\mathrm{r}}\mathrm{eflected}, \underline{\mathrm{t}}\mathrm{ransmitted}\}$.

4a) Use the conservation of the wavevector projection along y to relate θ_r, θ_t to $\theta_i = \phi$, E and V_0. Show that we obtain the equivalent of the Snell-Descartes law $n_1 \sin\theta_1 = n_2 \sin\theta_2$ for an electron in graphene and show that the "optical index" n is proportional to the kinetic energy $E - V_0$ where $\theta_1 = \phi$ and $\theta_2 = \theta_t - \pi$. Discuss the case of negative optical index (Cheianov, Falko and Altshuler, Science 315, p 1252 (2007)).

4b) Show that total reflection is possible if $E > V_0/2$ and compute the corresponding critical angle ϕ_c. For angles ϕ larger than ϕ_c, an evanescent wave is present in the step.

5) From the continuity of the (spinorial) wavefunction at the interface $x = 0$, obtain the reflection and transmission amplitude r and t. Infer the transmission probability $T \equiv 1-|r|^2$ and compare it to $|t|^2$. Comments ?

6) Use the current conservation equation $j_x = const$ to show that

$$\cos\phi - |r|^2\cos\phi = -|t|^2\cos\theta_t. \tag{4}$$

7) Show finally that

$$T = -\frac{\cos\phi\cos\theta_t}{\sin^2\left(\frac{\phi+\theta_t}{2}\right)} \text{ and } R = \frac{\cos^2\left(\frac{\phi-\theta_t}{2}\right)}{\sin^2\left(\frac{\phi+\theta_t}{2}\right)} \tag{5}$$

where the transmitted angle is :

$$\theta_t = \theta_2 + \pi = \arcsin\left(\frac{E}{V_0 - E}\sin\phi\right) + \pi \tag{6}$$

These equations are equivalent to the Fresnel formulae in optics.

8) Draw a polar plot of the transmission probability $T(\phi)$ for the potential step. What is the value of $T(0)$?

9) The previous result is quite general. To show it, we consider a massless Dirac electron, which is incident on an impurity whose potential is smooth on the lattice scale such that intervalley scattering is suppressed. The problem can be described within a single valley model. The impurity potential is therefore $\hat{V}_{\mathrm{imp}}(\vec{r}) \approx U(\vec{r})\hat{1}$. Using the first order Born approximation, the scattering probability is given by

$$P(\theta) \propto |\langle\vec{k'}, \alpha'|U(\vec{r})\hat{1}|\vec{k}, \alpha\rangle|^2 \tag{7}$$

where $|\vec{k}, \alpha\rangle$ and $|\vec{k'}, \alpha'\rangle$ are the initial and the final states respectively and θ is the angle between the final and initial wavevectors. Show that the scattering matrix element reads :

$$\langle\vec{k'}, \alpha'|U(\vec{r})\hat{1}|\vec{k}, \alpha\rangle = \frac{1 + e^{i\theta}}{2}\tilde{U}(\vec{k'} - \vec{k}) \tag{8}$$

where $\tilde{U}(\vec{q}) \equiv \int d^2r U(\vec{r})\exp(i\vec{q}\cdot\vec{r})$ is the Fourier transform of the potential $U(\vec{r})$. Deduce that the scattering probability reads :

$$P(\theta) \propto |\tilde{U}(\vec{q})|^2 \times \cos^2\frac{\theta}{2} = |\tilde{U}(\vec{q})|^2 \times \frac{1 + \cos\theta}{2} \tag{9}$$

Backscattering corresponds to $\theta = \pi$ which implies $P(\pi) = 0$. Provide an intuitive explanation of this absence of backscattering

3 conclusion

You can find the detailed correction and discussion of the Klein tunneling in the pedagogical review paper by P. E. Allais and J.-N. Fuchs, Eur. Phys. J. B 83, 301-317 (2011). Experiments with graphene has been realized in N. Stander, B. Huard and D. Goldhaber-Gordon, Phys. Rev. Lett. **102**, 026807 (2009) and A.F. Young and P. Kim, Nat. Phys. **5**, 222 (2009).

Tutorial 1 : Klein tunneling in graphene

I 1) We consider the 2D massless Dirac Hamiltonian $H = v_F \vec{p}\cdot\vec{\sigma} + V(r)\mathbb{1}$

We set $\hbar = v_F = 1$ and also take $V(r) = V_0 = \text{const}$

In position space $-i\,\vec{\sigma}\cdot\vec{\nabla}\,\Psi(r) = E\,\Psi(r)$

where $\Psi(r)^T = (\Psi_A(r), \Psi_B(r))$ is a spinor

$\{A, B\}$ labels sublattices $\Rightarrow$ "pseudo-spin"

We are looking for plane waves: $\Psi(r) = \frac{e^{i\vec{k}\vec{r}}}{\sqrt{2}\,N}\begin{pmatrix} u \\ v \end{pmatrix}$ ← normalization

Dirac eq. $\begin{pmatrix} V_0 & k_x - ik_y \\ k_x + ik_y & V_0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = E\begin{pmatrix} u \\ v \end{pmatrix}$

two eigenvalues: $E_\pm(k) = V_0 \pm k = V_0 + \alpha k$

Here $k = |\vec{k}|$ | $\alpha = 1 \Rightarrow$ conduct° band | $\alpha = -1 \Rightarrow$ valence band

eigenvectors: Indeed $\begin{cases} u = 1 \\ v = \alpha e^{i\theta_k} \end{cases}$ with $\theta_k = \tan^{-1}\left(\frac{k_y}{k_x}\right)$

is an eigenvector.

We assume the area of the graphene sheet is $\mathcal{A} = 1 \Rightarrow N = 1$

2) a) $\vec{v} = \frac{d\vec{r}}{dt} \Rightarrow \vec{v} = \frac{1}{i}[\vec{r}, \hat{H}] = \frac{1}{i}[\vec{r}, \vec{p}\cdot\vec{\sigma}] = \vec{\sigma}$

b) $v^\dagger = \langle k\alpha | \sigma^\dagger | k\alpha \rangle = \frac{1}{2}\begin{pmatrix} 1 & \alpha e^{-i\theta_k} \end{pmatrix}\sigma^\dagger\begin{pmatrix} 1 \\ \alpha e^{i\theta_k} \end{pmatrix}$

$\Rightarrow v^x = \alpha \cos\theta_k = \alpha\frac{k^x}{k}$

Similarly $v^y = \alpha\frac{k^y}{k}$

$\Rightarrow \boxed{\vec{v} = \alpha\frac{\vec{k}}{k}}$

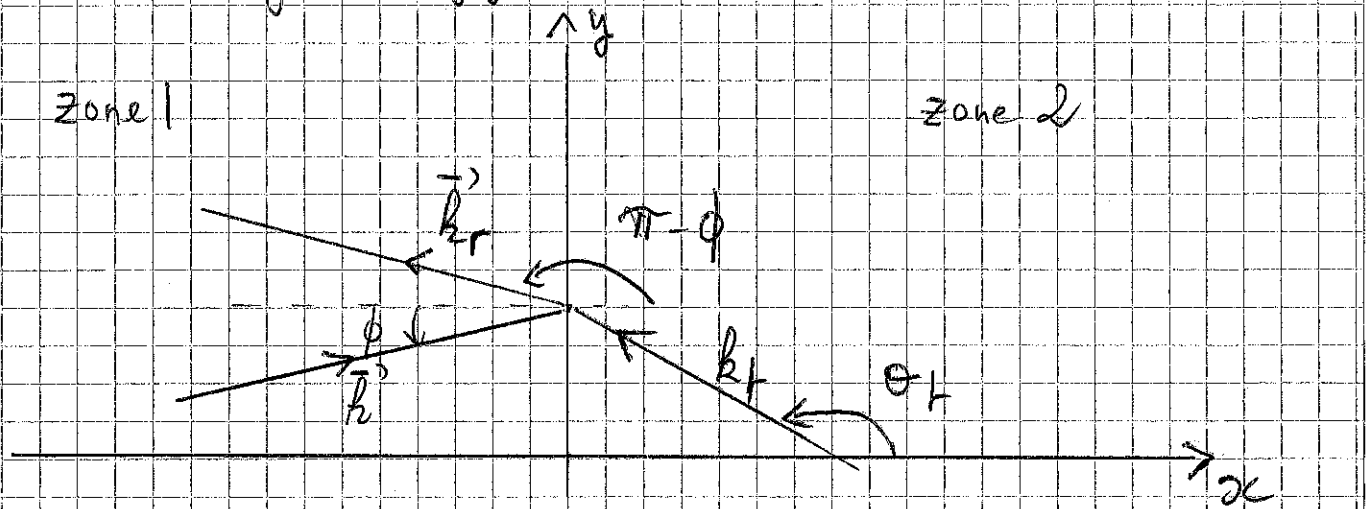
c) For $\alpha = -1$ $\vec{v} = -\vec{k}$ This means that the direction of propagation is opposite to the momentum direction
This is quite non-intuitive!

d) Average current $\vec{j} = \psi^\dagger \vec{\sigma} \psi$
This ensures a covariant definition of the current:
Moreover $\partial_\mu j^\mu + \frac{\partial \rho}{\partial t} = 0$ is verified!
With our definition $\vec{j} \equiv \langle k\alpha | \vec{\sigma} | k\alpha \rangle = \vec{v}$
Average current = Average velocity for states $|k\alpha\rangle$

3) $V(x,y) = V(x)$. We assume the barrier to be smooth at the lattice scale → no intervalley scattering is possible by momentum conservation
- k_y is conserved by translation invariance in the y direction
- $\frac{\partial \rho}{\partial t} = 0$ (no charge dynamics) $\Rightarrow j(x,y) = j(x)$
$\vec{\nabla} \cdot \vec{j} = 0 \Rightarrow \underline{j^x = \text{const}} \Rightarrow$ conserved

Obviously energy is also conserved.

II)



$V(x) = 0$ if $x < 0$
$V(x) = V_0$ if $x \geq 0$
$\Big\}$ → sharp potential at scale $\lambda_F \equiv k_F^{-1}$

$E_{inc} = k_F > 0$

We assume $k_F < V_0$ $(E_{inc} < V_0)$

Remark on question 3)

$\vec{j} = \psi^\dagger \vec{\alpha} \psi$ is the average current.

Translation invariance along the y direction imposes waves of the form $\psi(\vec{r}) = \frac{e^{ik_y y}}{\sqrt{N}} \begin{pmatrix} u_i(x) \\ v_i(x) \end{pmatrix}$

Therefore $\vec{j} = \vec{j}(x)$ → problem becomes separable in space

$\vec{\nabla} \cdot \vec{j} = 0 \Rightarrow j^x = \text{const}$

We are in the linear approximation

4a) Therefore $k^j = (k_x^j, k_y^j) = |k^j|(\cos\theta_j, \sin\theta_j)$

and $E_{kin}^j = \alpha_j |k^j|$ with $j = \{$incident, reflected, transmitted$\}$

For the incident and reflected $\alpha_j = 1$ $(E > 0)$

$\theta_i = \phi$; $\theta_r = \pi - \phi$

For the transmitted $\alpha_j = -1$ $\left(E = \underset{\text{here}}{V_0} < 0\right)$

Conservation of k_y : $k_y^i = k_y^r \Rightarrow \sin\theta_i = \sin\theta_r$

$\theta_r = \pi - \theta_i = \pi - \phi$

$k_y^i = k_y^t \rightarrow E\sin\phi = -(E - V_0)\sin\theta_t$

$$\sin\theta_t = \frac{E}{V_0 - E}\sin\phi$$

$$\theta_t = \arcsin\left(\frac{E\sin\phi}{V_0 - E}\right) \text{ or } \pi - \arcsin(\ )$$

This is useful to introduce $\begin{cases} \theta_1 \equiv \phi \\ \theta_2 = \theta_t - \pi \end{cases} \Rightarrow |\theta_{1,2}| < \pi/2$

$$\frac{E}{\underbrace{n_1}}\sin\theta_1 = \frac{(E - V_0)}{\underbrace{n_2 < 0}}\sin\theta_2$$

We have an analogy with Snell-Descartes laws but with negative index ! The negative index can be related to the fact that k_t and k_t' are a consequence of the spinorial nature of the wave function

In Optics, materials with negative index are called meta materials

4b) We have the equation $\sin\theta_t = \frac{E}{V_0 - E}\sin\phi$

This eq^n has solution if $\left|\frac{E\sin\phi}{V_0 - E}\right| > 1$

this determines ϕ_c / $\sin\phi_c = \frac{V_0 - E}{E}$

Such ϕ_c exists only if $E > \frac{V_0}{2}$ $\rightarrow$ total reflexion

Therefore when $E > \frac{V_0}{2}$, there exists an angle beyond which for $\phi > \phi_c$ the reflection is total.

If this condition is not satisfied, one can show that there will be evanescent modes.

5) Continuity of the wave function

$$\psi_{1(x)} = \frac{1}{\sqrt{2}} e^{ik_y y} \left[e^{ik_x x} \begin{pmatrix} 1 \\ +e^{i\phi} \end{pmatrix} + r e^{-ik_x x} \begin{pmatrix} 1 \\ e^{i(\pi-\phi)} \end{pmatrix} \right]$$

$$\psi_2^{(t)} = \frac{1}{\sqrt{2}} e^{ik_y y} \left[e^{ik'_x x} \begin{pmatrix} 1 \\ -e^{i\theta_t} \end{pmatrix} \right]$$

$$\psi_1 = \psi_2 \quad \text{in } x=0$$

$$\Rightarrow \begin{cases} 1 + r = t \\ e^{i\phi} - r e^{i\phi} = -t e^{i\theta_t} \end{cases}$$

this gives $r = \dfrac{e^{i\theta_t} + e^{i\phi}}{e^{-i\phi} - e^{i\theta_t}}$; $t = \dfrac{e^{i\phi} + e^{-i\phi}}{e^{-i\phi} - e^{i\theta_t}}$

6) Conservation of current

$$j_x^{(i)} = \psi^\dagger \sigma^x \psi = \frac{1}{2} \begin{pmatrix} 1 & \alpha e^{-i\theta_i} \end{pmatrix} \sigma^x \begin{pmatrix} 1 \\ \alpha e^{i\theta_i} \end{pmatrix}$$

$$= \alpha \cos(\theta_i)$$

The conservation of current reads

$$j_x^i + j_x^r = j_x^t$$

$$\Leftrightarrow \alpha \cos\phi - |r|^2 \cos\phi = |t|^2 \cos\theta_t$$

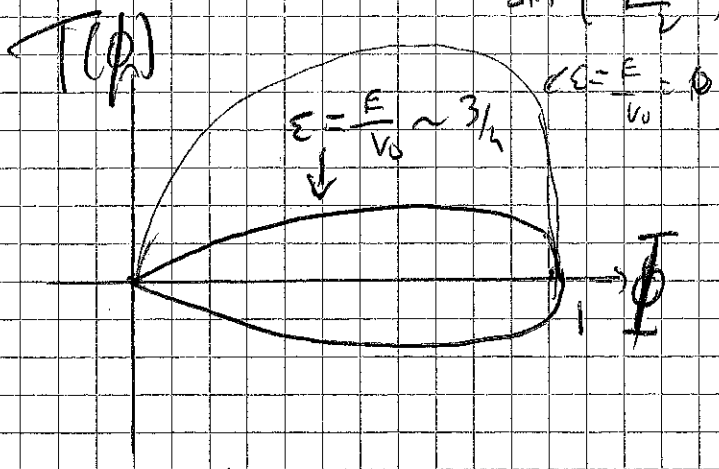
$$1 = |r|^2 + |t|^2 \frac{\cos\theta_t}{\cos\phi}$$

$$= R + T$$

Therefore by identification $\boxed{T = |t|^2 \frac{\cos\theta_t}{\cos\phi}}$ $\quad \left(\triangle\ T \neq |t|^2 \right)$

7) $$T = -\frac{\not{4}\cos^{\not 2}\phi}{|e^{-i\phi} - e^{i\theta_L}|^2}\,\frac{\cos\theta_L}{\cos\phi} = -\frac{\cos\phi\cos\theta_L}{\sin^2\left(\frac{\phi+\theta_L}{2}\right)}$$

Similarly $\Rightarrow$ $$R = \frac{\cos^2\left(\frac{\phi-\theta_L}{2}\right)}{\sin^2\left(\frac{\phi+\theta_L}{2}\right)}$$

8) 

$T(0) = 1$

perfect transmission

9) We consider an impurity $V_{imp}(\vec{r}) = U(\vec{r})$

$$P(\theta) \propto |\langle k' s' | U(r) | k s \rangle|^2$$

The collision is elastic $\Rightarrow$ $k = k'$ and $s = s'$

Only the angle can vary

With loss of generality, we can assume $\phi_k = 0$; $\phi_{k'} = \theta$

$$\langle k' s' | U(r) | k s \rangle = \frac{1+e^{i\theta}}{2}\,\underbrace{\tilde{U}(\vec{k}'-\vec{k})}_{\text{Fourier transform of } U(r)}$$

$$P(\theta) \propto \left|\frac{1+e^{i\theta}}{2}\right|^2 \propto \frac{(2+2\cos\theta)}{4} = \frac{1+\cos\theta}{2}$$

Therefore $P(\pi) = 0$ $\Rightarrow$ this is independent of $U(r)$ but only related to the spinor wave funct° of the Dirac equation!

As we have seen in the main lecture, backscattering implies $\vec{k}' = -\vec{k}$ but the electron has to reverse $\sigma \to -\sigma$ (sublattice)

This is not possible if the impurity is smooth on the lattice scale

M2 ICFP 2016/2017

Graphene, Dirac fermions and topological matter

by Pascal Simon (pascal.simon@u-psud.fr)

TD No 2 : Berry and Zak phases

1 A two-level system

We consider a simple two-level system in a normalzied magnetic field magnetic field. The Hamiltonian simply reads

$$\hat{H}(\vec{\xi}) = \vec{\xi}\cdot\hat{\vec{\sigma}} = (\sin\theta\cos\varphi\hat{\sigma}_x + \sin\theta\sin\varphi\hat{\sigma}_y + \cos\theta\hat{\sigma}_z), \tag{1}$$

where $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ denote the Pauli matrices, $\vec{\xi} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ with θ, φ are the two spherical angles.

1) The two eigenenergies are $E_\pm = \pm 1$. Calculate their corresponding eigenvectors $|\psi_\pm(\theta,\varphi)\rangle$.

2) For the two eigenvectors, express the Berry connection $\vec{\chi}_\pm(\vec{\xi}) = i\langle\psi_\pm|\vec{\nabla}_{\vec{\xi}}|\psi_\pm\rangle$.

3) Deduce the Berry curvature $\Omega_\pm(\theta,\varphi)$

4) Calculate the first Chern number $C_1^\pm$. Check that $C_1^+ + C_1^- = 0$.

2 The Zak phase of the dimerized chain

We consider a dimerized chain, the so-called Su-Schrieffer-Heeger model of polymer chain (see FIGURE (1)).

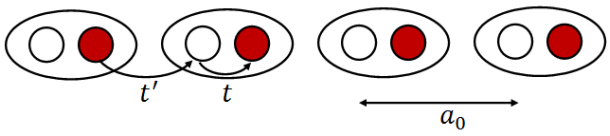


FIGURE 1 – A dimerized chain of atoms

This chain is described by a tight-binding Hamiltonian with two different hoping amplitudes t and t' for two adjacent sites. We have two different sorts of atoms a and b on which electrons can hop. We denote by m the m^{th} dimer of the chain. The Hamiltonian can be written as

$$\hat{H} = -\sum_{m=1}^{M}\left[t\hat{b}_m^\dagger\hat{a}_m + t'\hat{a}_{m+1}^\dagger\hat{b}_m + \text{h.c.}\right] \tag{2}$$

where $\hat{a}_n^\dagger$ and $\hat{b}_n^\dagger$ define creation operators of the atom a and b on the n^{th} dimer .

1) Before diagonalizing the Hamiltonian, we want to derive a few simple properties for this system. We first consider our one-dimensional model with open boundary conditions. What happens at the boundaries of the chain for the two limiting cases $t = 1, t' = 0$ and $t = 0, t' = 1$?

2) We now consider periodic boundary conditions. In order to diagonalize this Hamiltonian, we first introduce the vectors

$$\hat{\psi_k}^\dagger = (\hat{\psi}_{Ak}^\dagger\ ,\quad \hat{\psi}_{Bk}^\dagger) = \frac{1}{\sqrt{M}}\sum_{m=1}^{M} e^{ia_0mk}(\hat{a}_m^\dagger\ ,\quad \hat{b}_m^\dagger),$$

Show that we can write H under the following form

$$\hat{H} = \sum_{k=2\pi n/a_0} \hat{\psi}_k^\dagger\hat{\mathcal{H}}^B(k)\hat{\psi}_k. \tag{3}$$

with

$$\hat{\mathcal{H}}^B(\vec{k}) = -t \begin{pmatrix} 0 & \rho(\vec{k}) \\ \rho^*(\vec{k}) & 0 \end{pmatrix},$$

with $\rho(k)$ a function to be determined.

3) show that $\hat{\mathcal{H}}^B(k)$ can be written as

$$\hat{\mathcal{H}}^B(\vec{k}) = -t\vec{d}(\vec{k}) \cdot \vec{\sigma},$$

where $\vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \end{pmatrix}$, and $\vec{d}(\vec{k})$ is a 2-dimensional vector to be determined.

4) Diagonalize the Hamiltonian and find the dispersion relation of the two bands.

5) We define the phase $\phi(\vec{k})$ by $\rho(\vec{k}) = |\rho(\vec{k})|e^{-i\Phi(\vec{k})}$. Calculate $\phi(\vec{k})$. $\rho(k)$ is thus a complez number defined by its modulus and its phase. Using a polar representation, plot $\rho(k)$ for $t' > t$ and $t' < t$ (this is equivalent to plot the extremity of the vector $\vec{d}(\vec{k})$. What can you already infer from this ? What happens at $t' = t$?

6) Show that the eigenvectors $|u_{k,\pm}\rangle$ can be written in the following form

$$|u_{k,\pm}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi(k)} \\ \pm 1 \end{pmatrix}.$$

7) Determine the Zak phase defined as

$$Z_\alpha = \oint dk \, \langle u_{k,\alpha} | i\partial_k u_{k\alpha} \rangle, \tag{4}$$

where $\alpha = \pm 1$.

Calculate the Zak phase in the two cases $t' > t$ and $t' < t$. What are the differences between these two cases ? Similarly to the Zak phase, one often defines the winding number which reads here $\nu = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \frac{d}{dk} \ln(\rho(k)) = Z/\pi$. In the present example $\nu = 0, 1$. Could you establish a bulk/boundary correspondence between what happens at the edges of the chain (for open boundary conditions) and the bulk topological invaraint ν ?

8) Can you find some 1D models where $\nu > 1$?

9) Take parallel copies of the SSH chain and couple them without breaking chiral symmetry (it means here they all start on the left side with white points for example). What will happen with the edge states ?

M2 ICFP 2015/2016

Dirac matter and topology in many particle systems

by Pascal Simon (pascal.simon@u-psud.fr)

Correction of the TD No 2 : Berry phases

1 A two-level system

The Hamiltonian simply reads

$$\hat{H}(\vec{\xi}) = \vec{\xi}\cdot\hat{\vec{\sigma}} = (\sin\theta\cos\varphi\sigma_x + \sin\theta\sin\varphi\sigma_y + \cos\theta\sigma_z), \tag{1}$$

1) In matrix form,

$$H = \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix},$$

Let us focus on the ground state.

The ground state is associated with the eigenenergy $E_{-1} = -1$. The eigenvector can be written as :

$$|\psi_{-1}(\theta,\varphi)\rangle = \begin{pmatrix} \sin\frac{\theta}{2}e^{-i\varphi} \\ -\cos\frac{\theta}{2} \end{pmatrix}.$$

To show it, just use trigonometric formulas.

Similarly, you can check that the eigenvector associated with the exited state reads :

$$|\psi_{1}(\theta,\varphi)\rangle = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\varphi} \\ \sin\frac{\theta}{2} \end{pmatrix}.$$

2) Two options : The simplest ones is to assume that $\varphi \in [0, 2\pi]$ and $\theta \in [0, \pi]$ and use cartesian coordinates for these two variables.

The other option is to use spherical coordinates and write the gradient and curvature in spherical coordinates. I will choose the first one which is simpler. But you can check that both give the same result.

The Berry connection for the ground state writes as :

$$\chi_\theta^{(-1)} = i\langle\psi_{-1}|\partial_\theta\psi_{-1}\rangle = 0 \tag{2}$$

$$\chi_\varphi^{(-1)} = i\langle\psi_{-1}|\partial_\varphi\psi_{-1}\rangle = \sin^2\frac{\theta}{2} = \frac{1-\cos\theta}{2} \tag{3}$$

Within our gauge choice, the connection is exactly zero at the north pole for the ground state. One can repeat these calculations for the first (and only) exited state and just notice that the other eigenstate is obtained by $\theta \to \theta + \pi/2$.

3) One can therefore immediately obtain the Berry curvature :

$$\Omega^{(-1)} = \partial_\theta\chi_\varphi^{(-1)} - \partial_\varphi\chi_\theta^{(-1)} = \frac{\sin\theta}{2}. \tag{4}$$

Notice that the Berry curvature is gauge invariant while the Berry connection is not. The curvature cancels for $\theta = 0$ and $\theta = \pi$. Notice that the Berry connection cancels at the north pole. This corresponds to a singularity. We can move the position of this singularity BUT not remove it. The algebra is the same as for Dirac's theory of the magnetic monopole : the degeneracy at the origin is the monopole, and the singularity is the "Dirac string"

4) The domain of variation of the variables θ, φ is a rectangle. This is closed surface which has the same topology as the torus. The first Chern number associated with the ground state is then obtained by integration of the Berry curvature up to a factor 2π :

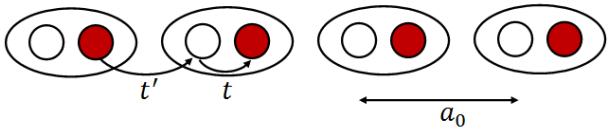
$$\frac{1}{2\pi}\int d\theta d\varphi \frac{1}{2}\sin\theta = 1 = C_1^{(-1)}.$$

The fact that C_1 is an integer comes from the following general homotopy argument : The Hamiltonian defines a map from a sphere S^2 toward a sphere S^2. The Chern number is therefore classified according to $\Pi_2(S^2) = \mathbb{Z}$. This implies that the ground state of this Hamiltonian is very robust toward continuous deformations.

The same type of work can be done for the excited state associated with the eigenvalue $E_{+1} = 1$. One can explictly check that $C_1^{\psi_1} = -1$, which implies that $\sum_{n=-1,1} C_1^{(n)} = 0$, as it should be.

2 The Zak phase of a dimerized chain

We consider a dimerized chain as depicted in (see FIGURE (1)).



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The Hamiltonian reads

$$\hat{H} = -\sum_{m=1}^{M} \left[t\hat{b}_m^\dagger \hat{a}_m + t'\hat{a}_{m+1}^\dagger \hat{b}_m + \text{h.c.} \right]. \tag{5}$$

1) For $t = 1$ and $t' = 0$, we obtained a set of decoupled dimers. However, in the other limit $t' = 1$ and $t = 0$, we notice that a_0 and b_M disappear from the Hamiltonian. They therefore correspond to decoupled zero energy states localized at the boundaries of the chain. They will the role of edge states. This first consideration suggests that these cases may correspond to two representative points in the phase diagram of two topological distinct phases.

2) Introducing

$$\hat{\psi_k}^\dagger = \begin{pmatrix} \hat{\psi}_{Ak}^\dagger & \hat{\psi}_{Bk}^\dagger \end{pmatrix} = \frac{1}{\sqrt{M}} \sum_{m=1}^{M} e^{ia_0 mk} \begin{pmatrix} \hat{a}_m^\dagger & \hat{b}_m^\dagger \end{pmatrix},$$

and

$$\hat{\mathcal{H}}^B(\vec{k}) = -t \begin{pmatrix} 0 & \rho(\vec{k}) \\ \rho^*(\vec{k}) & 0 \end{pmatrix},$$

with $\rho(k) = 1 + \frac{t'}{t} e^{-ika_0}$, the Hamiltonian takes the following form :

$$\hat{H} = \sum_{k=2\pi n/a_0} \hat{\psi}_{k,n}^\dagger \hat{\mathcal{H}}^B(k) \hat{\psi}_{k,n}. \tag{6}$$

3) The Hamiltonian $\hat{\mathcal{H}}^B(\vec{k})$ can be also written as

$$\hat{\mathcal{H}}^B(\vec{k}) = -t\vec{g}(\vec{k}) \cdot \vec{\sigma},$$

with $\vec{g}(\vec{k}) = \left(1 + \frac{t'}{t}\cos ka_0, \frac{t'}{t}\sin ka_0\right)$.

4) The diagonalization of the Hamiltonian is straightforward (as usual square the Hamiltonian) and we obtain two bands with a dispersion relation

$$\varepsilon_\pm(\vec{k}) = \pm t|g(\vec{k})| = \pm\sqrt{t^2 + t'^2 + 2tt'\cos ka_0}.$$

5) We define the phase $\phi(\vec{k})$ by $\rho(\vec{k}) = |\rho(\vec{k})|e^{-i\Phi(\vec{k})}$. The phase thus reads

$$\phi(\vec{k}) = \arctan\left[\frac{t\sin ka_0}{t + t'\cos(ka_0)}\right].$$

One can use a polar representation to plot $\rho(\vec{k})$. This is also obvious to notice that the extremity of the vector $\vec{d}(\vec{k})$ actually describe a circle of radius t'/t ansd centered around the point $(1, 0)$. Therefore when $t' < t$ this circle never encircles the origin while for $t' > t$ it does. At the particular point $t' = t$, the circle touches the origin. This point also corresponds to the clsoing of the gap. We will see that we can interprete this point as a topological transition.

6) One can explicitely check that the eigenfunctions $|u_{k,\pm}\rangle$ defined in the text are indeed eigenvectors (the calculations are straightforward).

7) The Zak phase is defined as

$$Z_\alpha = \oint dk \, \langle u_{k,\alpha} | i\partial_k u_{k\alpha} \rangle = \frac{1}{2} \oint dk \frac{d\phi}{dk} = \frac{\Delta\phi}{2}. \tag{7}$$

When $t' < t$, $Z = 0$, while for $t' > t$, $Z = \pi$. The Zak phase is some kind of equivalent of the Chern number but in one dimension. This is a topological invariant. Similarly to the Zak phase, one often defines the winding number which reads here $\nu = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \frac{d}{dk} \ln(\rho(k)) = Z/\pi$.

When $Z = \pi$ ($\nu = 1$), the phase is topologically non-trivial. This implies teh existence of edge states (bound states) which do not disperse when the system has open boundary conditions. They correspond to almost unpaired electrons as we have seen in 1). We can actually go beyond question 1) and find the spectrum for open boundary condition whatever t, t'. We will find that for $t' > t$, the bound states are exponentially localized with a localization length $\xi = a_0 / \ln(t'/t)$.

These two phases are separated by the point $t'/t = 1$ which correspondS to a topological transition where the band gap closes.

At $k = 0$, $\hat{\mathcal{H}}^B(0) = -(t' + t)\sigma_x$,with eigenvalues $\pm(t' + t)$. One can therefore label each band by a parity index. At $k = \pi$, $\hat{\mathcal{H}}^B(\pi) = -(t - t')\sigma_x$, with eigenvalues $\pm(t - t')$.

Our topological transition is therefore characterized by a band inversion.

To summarize, this very simple example has already all key features which we will meet later when we will introduce the topological insulators.

8) It would be interesting to extend the previous model taking into account next to nearest neighbour t'' and look at the Zak phase (or equivalently here the winding number) in the plane $(t'/t, t''/t)$. Some higher winding number $\nu = \pm 2$ are possible.

9) We take similar chains and form a 2D lattice by weakly coupling them in the y direcion. Our localized bound states can start dispersing along the y direction. We form this way a (weak) topological insulator with dispersive edge state.

M2 ICFP 2016/2017

Graphene, Dirac fermions and topological matter

by Pascal Simon (pascal.simon@u-psud.fr)

TD No 3 : Topological properties of a 2-band model in two dimensions

1 A 2-band tight-binding model Hamiltonian

We consider a two-dimension (2D) model hamiltonian whose kernel reads

$$h(\vec{k}) = \Delta(\sin(k_x)\sigma_x + \sin(k_y)\sigma_y) - (2t(\cos(k_x) + \cos(k_y)) + M)\sigma_z \quad (1)$$

where the $\vec{\sigma}$ describe the Pauli matrices. If not specified, we consider periodic boundary conditions.

1) In real space (on a square lattice), could you tell what could this Hamiltonian correspond to ?

2) Compare the form of this Hamiltonian to a spin 1/2 in a magnetic field. Find the eigenvalues of this Hamiltonian. Notice that $h(\vec{k}) = \vec{g}(\vec{k}) \cdot \sigma$.

3) Depending on t, M, Δ, find the points in the Brillouin zone where the system becomes gapless.

4) Find the eigenfunctions of this hamiltonian.

5) When the system is gapped, we may introduce $\vec{d}(\vec{k}) = \frac{\vec{g}(\vec{k})}{|\vec{g}(\vec{k})|}$ whihc lives on the unit sphere. Discuss the surface described by $\vec{d}(\vec{k})$ when $\vec{k}$ runs over the first Brillouin zone. Hint : You should distinguish the cases $M < -4t$, $-4t < M < 0$, $0 < M < 4t$, $M > 4t$.

6) When it is possible, calculate the Berry connection, the Berry curvature and the Chern number for both bands.

7) We now consider this model on a strip parallel to the x-axis (therefore we have periodic boundary conditions in that direction) of finite size L in the y direction (say $y \in [-L/2, L/2]$. Perform numerically an exact diagonalization of this model in the different cases mentioned previously. Conclusion ?

8) More advanced : assuming $L >> a$, where a is the lattice spacing, could you find an approximate expression of the edge states (when they exist) which are localized near $y = \pm L/2$. Hint : consider an half-place, say y<0, where we define this hamiltonian.

M2 ICFP 2015/2016

Dirac matter and topology in many particle systems

by Pascal Simon (pascal.simon@u-psud.fr)

TD No 3 : Topological properties of a 2-band model in two dimensions

1 A 2-band tight-binding model Hamiltonian

We consider a two-dimension (2D) model hamiltonian whose kernel reads

$$h(\vec{k}) = \sum_{k_x,k_y} \Delta(\sin(k_x)\sigma_x + \sin(k_y)\sigma_y) - (2t(\cos(k_x)+\cos(k_y)) + M)\sigma_z \quad (1)$$

where the $\vec{\sigma}$ describe the Pauli matrices. If not specified, we consider periodic boundary conditions.
Assume $t > 0$, $\Delta > 0$ real.

1) We consider a square lattice with two sorts of fermion per unit cell, say a and b. The term $2t(\cos(k_x) + \cos(k_y))$ correspond to the standard dispersion relation of fermions (belonging to the same specie) with a nearest neighbor hopping parameter t. M can be regarded as a chemical potential. However, notice that we have two sorts of fermions here but with some inverted band index ; $t- > -t$; $M- > -M$. Concerning the first term, this corresponds to a complex nearest neighbour hopping term $i\Delta$ between fermion a and fermion b. Therfore this term corresponds to some chirality. Note that the total flux per plaquette is zero. This model has some clear analogy with the Haldane model and contains similar ingredients.

2) This Hamiltonian has the similar form as a spin $1/2$ in a magnetic field. We have $h(\vec{k}) = \vec{g}(\vec{k}) \cdot \sigma$, with

$$\vec{g}(\vec{k}) = (\Delta \sin k_x, \Delta \sin k_y, -2t(\cos(k_x)+\cos(k_y)) - M).$$

The spectrum is thus trivially obtained by $\epsilon(k) = \pm|\vec{g}(\vec{k})|$.

We have therefore two bands labeled by the index $\pm$ and the gap between the two bands is $G = 2\min(|\vec{g}(\vec{k})|)$. As long as the gap $G > 0$ the bands never cross each other.

3) The spectrum becomes gapless if $|\vec{g}(\vec{k})| = 0$. This implies

$$\Delta^2[\sin^2 k_x + \sin^2 k_y] + [2t(\cos(k_x)+\cos(k_y)) + M]^2 = 0$$

We thus see that we have a few special points in the Brillouin zone, namely :
$\vec{k} = (0,0), \vec{k} = (\pi,\pi), \vec{k} = (0,\pi), \vec{k} = (\pi,0)$.
At these four points,

$$\vec{g}(\vec{k}=(0,0)) = (0,0,-4t-M)\ ,\ \vec{g}(\vec{k}=(\pi,\pi)) = (0,0,4t+M)\ ,\ \vec{g}(\vec{k}=(0,\pi)) = \vec{g}(\vec{k}=(\pi,0)) = (0,0,M).$$

Therefore, the spectrum can become gapless when $M = -4t, M = 0, M = 4t$. We should thus divide the analysis of the Hamiltonian in the four intervals $M < -4t$, $-4t < M < 0$, $0 < M < 4t$, $M > 4t$.

4) We already met in the main lecture different parametrization of the eigenvectors for a general 2-band model. Let us focus first on the lowest band denoted as ϵ_-. The eigenvector can be parametrized as

$$u_-^{(1)}(k) = \frac{1}{\mathcal{N}_-^{(1)}}(g_z - g, g_x + ig_y), \quad (2)$$

where $g = \sqrt{g_x^2 + g_y^2 + g_z^2}$. The factor $\mathcal{N}_-$ is a normalization factor. Notice that this eigenvector is defined up to a global phase (i.e. up to a gauge choice). For example, we can multiply the vector $u_-^{(1)}(k)$ by an appropriate phase in order to obtain for example

$$u_-^{(2)}(k) = \frac{1}{\mathcal{N}_-^{(2)}}(-g_x + ig_y, g_z + g,) \quad (3)$$

Since the hamiltonian has the same form as a spin $1/2$ in a magnetic field, there is another more convenient representation for these eigenvectors namely the Bloch sphere. When $g(k) \neq 0$ we may thus introduce the following parametrization :

$$\cos(\theta) = \frac{g_z}{g} \quad ; \quad e^{i\phi} = \frac{g_x + ig_y}{\sqrt{g_x^2 + g_y^2}} \tag{4}$$

where $\theta \in [0, \pi[$, $\phi \in [0, 2\pi[$. Note that the phase ϕ is not well-defined at the poles as expected. The eigenvectors read within this representation :

$$u_-(k) = e^{i\alpha(\theta,\phi)} \left(e^{-i\phi/2} \sin(\theta/2), -e^{i\phi/2} \cos(\theta/2) \right),$$

where $\alpha(\theta, \phi)$ is an arbitrary phase. Fixing this phase corresponds to fixing the gauge. Similarly, we get for $u_+(k)$:

$$u_+(k) = e^{i\beta(\theta,\phi)} \left(e^{-i\phi/2} \cos(\theta/2), e^{i\phi/2} \sin(\theta/2) \right).$$

The eigenvector $u_+(k)$ can be readily obtained from the eigenvector $u_-(k)$ by changing $\vec{g} \to -\vec{g}$ *i.e.* $\theta \to -\theta$.

To show the equivalence between both representation, just inject for example the spherical parametrization in Eq. (4) into Eq. (2) or Eq. (3).

5) When the system is gapped, we introduce $\vec{d}(\vec{k}) = \frac{\vec{g}(\vec{k})}{|\vec{g}(\vec{k})|}$ which lives on the unit sphere. As suggested by the text, let us consider separately the four intervals.

1. Case $M < -4t$. We see that $cos(\theta) > 0$. This means that area swept by the vector $\vec{d}(k)$ belongs to the northern hemisphere of the Bloch sphere. As we have seen in the main lecture, we can always choose a gauge such that the north pole is well defined (chose for example $\alpha = -\phi/2$). In this case, the eigenvectors are well-behaved over the whole Brillouin zone and we expect this phase to be topologically trivial.
2. Case $-4t < M < 0$. In this regime, $cos(\theta)$ changes signs. More specifically, at the Γ point, $k_x = k_y = 0$, we reach the south pole ($\theta = 0$) while at the other special points $(0, \pi), (\pi, 0), (\pi, \pi)$, we reach the north pole ($\theta = \pi$). We can convince ourselves that we span the whole Bloch sphere including both north and south pole. Therefore we cannot find a choice of gauge where our eigenvectors are well behaved for the whole Brillouin zone. We expect this phase to be topological as it will be confirmed by the calculation of the Chern number. If we want our wave vectors to be well behaved everywhere, we need to separate the Brillouin zone into two parts. We draw a small circle around the origin. Inside this small circle, which we will call region $D^{(1)}$, we use the wave vector $u^{(1)}$ and outside this circle, we use for example $u^{(2)}$. This amounts to define two different choices of the gauge. The wavefunctions for these two regions are connected by a gauge transformation which wikll leave to a non-trivial Berry curvature as we will see.

   The special point $M = -4t$ corresponds to a closure of the gap at $(k_x, k_y) = (0, 0)$. This corresponds to a single Dirac point where the system is a semi metal. This value corresponds to a topological transition where the two bands are talking to each other (and somehow change their Chern number).
3. Case $0 < M < 4t$. In this regime, we encounter the same problems as in the case $-4t < M < 0$. At $k_x = k_y = \pi$, we reach the north pole while for the other three special points we reach the south pole. The discussion is therefore exactly similar as in the previsou one and we expect this pahse to be topological too.

   The special point $M = 4t$ corresponds to a closure of the gap at $(k_x, k_y) = (\pi, \pi)$.
4. Case $M > 4t$. This case is similar to the case $M < -4t$ except that now $\cos(\theta) > 0$. In that case, the vector $\vec{d}(k)$ belongs to the southern hemisphere of the Bloch sphere. Again we can find a gauge such that the eigenvectors are all well behaved. This is this a trivail insulating phase.

6) Let us now concretize the previous reasoning by computing the Berry connection, the Berry curvature and Chern numbers in the previous intervals. We will work only with the lower band and thus the eigenvector $u_-(k)$. There are many ways to perform these calculations.

1. Case $M < -4t$. Here we can use a gauge such that the north pole is well defined (chose for example $\alpha = -\phi/2$). The eigenvector reads :

$$u_-(k) = \left(e^{-i\phi} \sin(\theta/2), -\cos(\theta/2) \right),$$

The singularity has been pushed to the south pole which is never reached. Therefore, we can use our results for the spin $1/2$ in a magnetic field. The Berry connection is defined on the Bloch sphere and parametrized by the unit vectors $\vec{e}_\theta, \vec{e}_\phi$.

$$\vec{A}_{(-)} = (A^\theta_{(-)}, A^\phi_{(-)}) = (0, (1-\cos(\theta))/2).$$

The Berry curvature is radial, therefore orthogonal to $\vec{e}_\theta$ and $\vec{e}_\phi$ and reads

$$\vec{\Omega}_{(-)} = \frac{\sin\theta}{2}\vec{e}_r.$$

The Chern number is defined by

$$C^{(-)} = \frac{1}{2\pi}\oint_{\partial BZ}\vec{A}_{(-)}\cdot\vec{dk} = \frac{1}{2\pi}\iint_{BZ}\Omega_{(-)}d^2k$$

Since the Chern number is an integer, we can convince ourselves that this corresponds to the number of time the sphere is wrapped. Here no singularity is meet and this integral is thus zero. This corresponds to a trivial phase.

2. Case $-4t < M < 0$. In this regime, $\cos(\theta)$ changes sign and the whole sphere is spanned. Therefore we cannot escape the singularity. There are many strategies. We need two well defined wavefunctions to describe the whole BZ. First, we draw a small circle around the origin of the BZ. Inside this small circle, which we will call region $D^{(1)}$, we use the following eigenfunction $u^{(1)}_-(k) = \big(\sin(\theta/2), -e^{i\phi}\cos(\theta/2)\big)$. and outside (say area $D^{(2)}$), we use $u^{(2)}_-(k) = \big(e^{-i\phi}\sin(\theta/2), -\cos(\theta/2)\big)$.
Clearly $u^{(2)}_-(k) = e^{-i\phi(k)}u^{(1)}_-(k)$. Therefore the Berry connection

$$\vec{A}^{(2)}_{(-)} = \vec{A}^{(1)}_{(-)} + \nabla_k\phi(k).$$

Therefore, we get

$$\iint_{BZ}\Omega_{(-)}d^2k = \iint_{D^1}\nabla\times\vec{A}^{(1)}_{(-)} + \iint_{D^2}\nabla\times\vec{A}^{(2)}_{(-)} \tag{5}$$

$$= \oint_{\partial D^1}\vec{A}^{(1)}_{(-)}\vec{dk} + \oint_{\partial D^2}\vec{A}^{(2)}_{(-)}\vec{dk} = \oint_{\partial D^1}\vec{A}^{(1)}_{(-)}\vec{dk} - \oint_{\partial D^1}\vec{A}^{(2)}_{(-)}\vec{dk} \tag{6}$$

$$= -\oint_{\partial D^1}\nabla_k\phi(k)\vec{dk} = \phi(0) - \phi(2\pi) = 2\pi. \tag{7}$$

Indeed, in our case the phase ϕ is defined

$$e^{i\phi(k)} = \frac{g_x + ig_y}{|g_x + ig_y|} \approx \frac{k_x + ik_y}{|k_x + ik_y|} = e^{i\psi},$$

where we use the fact that $D^{(1)}$ is around the north pole and we introduce $k_x + ik_y = e^{i\psi}$. Therefore where we run over $D^{(1)}$, the angular variable ψ, goes from 0 to 2π and so does $\phi(k)$.
Thus

$$C^{(-)} = 1.$$

We can convince also ourselve that $C^{(+)} = -1$.

3. Case $0 < M < 4t$. In this regime, we encounter the same problems as in previous the case $-4t < M < 0$. We can proceed similarly and find $C^{(-)} = -1$.
4. Case $M > 4t$. No singularity is reached so $C = 0$.

Let me also use another straighforward approach which use the fact that the Hamiltonian $h(\vec{k})$ and $\tilde{h}(\vec{d}) = \vec{d}\cdot\vec{\sigma}$ have the same topological properties provided $h(\vec{k})$ is gapped. We already studied in the tutorial 2 the properties of $\tilde{h}(\vec{d})$. The Berry connection is defined by

$$\vec{A}_-(\vec{d}) = i\langle u_-|\nabla_{\vec{d}}|u_-\rangle$$

where $\nabla_{\vec{d}}$ simply means the vector $(\nabla_{d_x}, \nabla_{d_y}, \nabla_{d_z})$. This implies $\vec{A}_-(\vec{d}) = i\langle u_-|\vec{\sigma}|u_-\rangle$. This quantity is basis dependent. We may instead compute the Berry curvature and use Berry's general expression which is gauge independent. This is given in the main lecture where we wrote

$$\vec{B}^{(n)} = -Im\left(\sum_{k\neq n} \frac{\langle n|\nabla_{\vec{\xi}}|k\rangle \times \langle k|\nabla_{\vec{\xi}}|n\rangle}{(E_n - E_k)^2}\right)$$

where $\vec{B}^{(n)}$ is the Berry curvature associated with level n and here $\vec{\xi} \equiv \vec{d}$. Since we only have two levels, this is straighforward. If we chose our quantization axis (z axis) always parallel to $\vec{d}$, the eigenvectors become $|u_-^{\vec{d}}\rangle = (0,1)$ and $|u_+^{\vec{d}}\rangle = (1,0)$ like a spin $1/2$. We immediately find

$$\vec{B}^{(n)} = -\frac{\vec{d}}{2d^3}$$

which is an expression we already met. This corresponds to the field of a monopole at the center. Since $d = 1$ by construction, The Chern number is just $C = \frac{1}{4\pi}\iint \vec{d}\cdot\vec{dS}$. When $\vec{d}$ wraps the whole Bloch sphere, we will find $C = \pm 1$.

7) We now consider this model on a strip parallel to the x-axis (therefore we have periodic boundary conditions in that direction) of finite size L in the y direction (say $y \in [-L/2, L/2]$. Perform numerically an exact diagonalization of this model in the different cases mentioned previously.

The goal of this numerical exercice is to show the presence of edge states in the topological phases which crosses the gap.

8) More advanced : assuming $L >> a$, where a is the lattice spacing, could you find an approximate expression of the edge states (when they exist) which are localized near $y = \pm L/2$. Hint : consider an half-place, say y<0, where we define this hamiltonian.

We will see in the next chapter how to find an approximate (low energy) form for the edge states.

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Graphene, Dirac fermions and topological matter

by Pascal Simon (pascal.simon@u-psud.fr)

TD No 4 : The Kitaev model and Majorana fermions

There is currently much excitement in parts of the condensed matter community because of a potential observability of Majorana fermions in solid state systems. Majorana fermions are linear combinations of particle and antiparticle states (in condensed matter : particles and holes) such that the Majorana particle is its own antiparticle. In the second quantized language, the Majorana operators c are thus hermitian, $c^\dagger = c$ (hence they are often called "real" fermions). While such a fermion was over decades just a sometimes convenient theoretical trick for representing fermions, the mere possibility of actually observing such a state is already intriguing. In addition, however, there are by now proposals that build on Majorana fermions for the so-called topological quantum computation, which is a further driving force for many physicists.

In this exercise set, you will start from a simple spin-chain model. By a Jordan-Wigner (JW) transformation you will map it onto a fermionic system, which has Majorana edge states. Based on this insight, you are encouraged to speculate about what conditions must be fulfilled for a true electron system to exhibit similar physics.

1 Spin chain and sketch of the phase diagram

Consider a one-dimensional system of spins $S = 1/2$ described by the Hamiltonian

$$H = \sum_i \left[J\sigma_i^x \sigma_{i+1}^x - h\sigma_i^z \right], \tag{1}$$

where i runs over the lattice sites and $\sigma_i^{x,y,z}$ are the Pauli matrices for the spin operators (the true spins are given by $S_i^{x,y,z} = \frac{\hbar}{2}\sigma_i^{x,y,z}$, but for simplicity we use the Pauli matrices with eigenvalues ± 1 here). Nearest neighbor spins interact by an antiferromagnetic exchange coupling $J > 0$, and h is a uniform external field in the z direction.

1) Determine the ground state spin configuration in the limits $J \gg |h|$ and $J \ll |h|$, and then give an argument at which ratio $J/|h|$ the transition from one to the other phase occurs.

2) The Jordan Wigner transformation is the mapping of the spin chain onto a system of spinless fermions. It is given by

$$\sigma_i^z = 2a_i^\dagger a_i - 1, \qquad \sigma_i^x = (a_i^\dagger + a_i)\prod_{j<i}\sigma_j^z, \qquad \sigma_i^y = -i(a_i^\dagger - a_i)\prod_{j<i}\sigma_j^z. \tag{2}$$

Show that these fermion operators a_i obey the anticommutation relations $\{a_i, a_j\} = 0$ and $\{a_i, a_j^\dagger\} = \delta_{ij}$.

3) Show then that the Hamiltonian can be written as

$$H = \sum_i \left[-J(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + J(a_i a_{i+1} - a_i^\dagger a_{i+1}^\dagger) - 2h a_i^\dagger a_i \right], \tag{3}$$

and give an interpretation of the different terms.

2 Spectrum for an infinite chain

4) Assume an infinite chain with lattice constant a. Show that the Hamiltonian can then be written in the form

$$\begin{aligned} H &= \sum_p \left\{ -2[h + J\cos(ap)]a_p^\dagger a_p - J(e^{iap}a_p^\dagger a_{-p}^\dagger + e^{-iap}a_{-p}a_p) \right\} \\ &= \sum (a_p^\dagger, a_{-p}) \begin{pmatrix} -[h + J\cos(ap)] & -Je^{iap} \\ -Je^{-iap} & +[h + J\cos(ap)] \end{pmatrix} \begin{pmatrix} a_p \\ a_{-p}^\dagger \end{pmatrix}, \\ &= \frac{1}{2}\sum_p (a_p^\dagger, a_{-p}) \begin{pmatrix} -2[h + J\cos(ap)] & -2iJ\sin(ap) \\ 2iJ\sin(ap) & +2[h + J\cos(ap)] \end{pmatrix} \begin{pmatrix} a_p \\ a_{-p}^\dagger \end{pmatrix}. \end{aligned} \tag{4}$$

The main interest of such representation is to treat on equal footing particle and hole excitations. Such a Hamiltonian is particle-hole symmetric.

5) The diagonalization of such a Hamiltonian is known as a Bogoliubov transformation. For now, however, we are only interested in the spectrum. Calculate it (eigenvalues of the 2×2 matrix in Eq (4)) and show that there is a gap given by $\Delta = \min\{|J+h|, |J-h|\}$ such that all eigenvalues ϵ_p fulfill $\epsilon_p > \Delta$ or $\epsilon_p < -\Delta$.

3 Majorana fermions

Note that σ_i^x and σ_i^y depend on the hermitian combinations $a_i^\dagger + a_i$ and $-i(a_i^\dagger - a_i)$. These are the combinations we can use to define Majorana fermions,

$$c_i^1 = a_i^\dagger + a_i, \qquad c_i^2 = -i(a_i^\dagger - a_i). \tag{5}$$

6) Show that $\{c_i^a, c_j^b\} = \delta_{ab}\delta_{ij}$ and that the Hamiltonian becomes

$$H = -i \sum_i \left[J c_i^2 c_{i+1}^1 - \frac{h}{2} c_i^2 c_i^1 \right] + \text{const.} \tag{6}$$

7) For a chain of finite length, $i = 1, \ldots, N$, with open boundary conditions, most of the eigenstates have energies $\epsilon_n > \Delta$ or $\epsilon_n < -\Delta$ (with Δ given above), but there are in addition precisely 2 states of energies $\epsilon \approx 0$, one located near $i = 1$ and one near $i = N$.

Consider the special case $h = 0$ and show that it is indeed the case. Can you relate this feature to the SSH model we treated in TD 2. What can you infer by analogy ?

8) For simplicity, we consider here a semi-infinite system ($N \to \infty$), where only one bound state remains that has exactly $\epsilon = 0$. Show then that the bound state is of the form $|b_1\rangle = A(c_1^1 + \lambda c_2^1 + \lambda^2 c_3^1 + \ldots)|\rangle$. Show that it is a Majorana fermion, determine λ, and give the conditions necessary for the existence of the normalization constant A (i.e., such that the bound state can exist).

9)For finite length N, estimate then the energy splitting between the bound states on both ends (remember the splitting between bonding and antibonding states in the H^2 molecule). In the limit $\lambda \to 0$, to which state does the bound state at $i = 1$ correspond ?

4 Majorana fermions with electrons

10) Reconsider now Eq. (4) and assume that the a_p describe real electrons. Speculate what type of interaction, band structure, etc. is necessary to obtain such a Hamiltonian.

Hint : Expressions of the form $a_p a_{-p}$ appear whenever superconductivity is involved, and they represent 2 electrons that are bound together in a Cooper pair. For conventional superconductors, the Cooper pairs are in a spin-singlet state and so the operators are complemented by spin indices $\sigma = \uparrow, \downarrow$ as $a_{p\uparrow} a_{-p\downarrow}$. What does this imply for the $a_{p\sigma}^\dagger a_{p\sigma}$ terms of the kinetic energy ?

M2 ICFP 2015/2016

Dirac matter and topology in many particle systems

by Pascal Simon (pascal.simon@u-psud.fr)

Correction TD4 : the Kitaev model and Majorana fermions

1 Spin chain and sketch of the phase diagram

1) The Hamiltonian of the spin chain is defined by

$$H = \sum_i \left[J\sigma_i^x \sigma_{i+1}^x - h\sigma_i^z \right], \tag{1}$$

If $J \ll |h|$, we have a ferromagnet with all spins aligned in the z direction. Therefore the system has a gap. While for $J \gg |h|$, we expect an antiferromagnet (AF) which is gapless. We thus expect a quantum phase transition when $J \sim h$ with a closure of the gap spectrum from the ferromagnet to the AF. This is exactly what happens.

2) The Jordan-Wigner transformation is defined by :

$$\sigma_i^z = 2a_i^\dagger a_i - 1, \qquad \sigma_i^x = (a_i^\dagger + a_i)\prod_{j<i}\sigma_j^z, \qquad \sigma_i^y = -i(a_i^\dagger - a_i)\prod_{j<i}\sigma_j^z. \tag{2}$$

One can inverse these relations and show

$$a_i = (\prod_{j<i}\sigma_i^z)\sigma_i^+ \qquad a_i^\dagger = (\prod_{j<i}\sigma_i^z)\sigma_i^-, \tag{3}$$

where $\sigma_i^\pm = (\sigma_i^x \pm i\sigma_i^y)/2$.

By help of these fermion operators a_i and $a_i^\dagger$, we can check that they indeed obey the anticommutation relations $\{a_i, a_j\} = 0$ and $\{a_i, a_j^\dagger\} = \delta_{ij}$ using standard algebra of the Pauli matrices.

3) Using the following identities :

$$a_i^\dagger a_i = \frac{1}{2}(\sigma_i^z + 1), \tag{4}$$

$$(a_i^\dagger - a_i)(a_{i+1}^\dagger + a_{i+1}) = i\sigma_i^y\sigma_{i+1}^x\sigma_i^z = -\sigma_i^x\sigma_{i+1}^x, \tag{5}$$

$$(a_i^\dagger + a_i)(a_{i+1}^\dagger - a_{i+1}) = i\sigma_i^x\sigma_{i+1}^y\sigma_i^z = \sigma_i^y\sigma_{i+1}^y. \tag{6}$$

we immediatly find that the Hamiltonian can be written as

$$H = \sum_i \left[-J(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) - J(a_i a_{i+1} - a_i^\dagger a_{i+1}^\dagger) - 2ha_i^\dagger a_i \right]. \tag{7}$$

The first line corresponds to a standard hopping term, the second line to some pairing term between nearest neighbours while the last term corresponds to a chemical potential.

2 Spectrum for an infinite chain

4) We consider an infinite chain with lattice constant a. Using translation invariance, we can go in Fourier space and write the hamiltonian as

$$\begin{aligned} H &= \sum_p \left\{ -2[h + J\cos(ap)]a_p^\dagger a_p + J(e^{iap}a_p^\dagger a_{-p}^\dagger + e^{-iap}a_{-p}a_p) \right\} \\ &= \frac{1}{2}\sum_p (a_p^\dagger, a_{-p}) \begin{pmatrix} -2[h + J\cos(ap)] & 2iJ\sin(ap) \\ -2iJ\sin(ap) & +2[h + J\cos(ap)] \end{pmatrix} \begin{pmatrix} a_p \\ a_{-p}^\dagger \end{pmatrix}. \end{aligned} \tag{8}$$

Note that the kernel of this Hamiltonian reads $\mathcal{H}(k) = \sigma_2 h_2(k) + \sigma_3 h_3(k)$ with $h_3(k) = h + J\cos(ap)$, $h_2(k) = -J\sin(ap)$. We already met a similar problem when dealing with the dimerized chain or SSH chain. When the system is gapped, we can define the vector $\hat{h} = (h_2, h_3)/|h|$ which defines a map between the torus T^1 (a circle) to another circle. The Jacobian of such mapping defines a topological invariant which is an integer (see TD 2).

5) The diagonalization of such Hamiltonian is straightforward and we obtain the spectrum :

$$E_\pm = \pm\sqrt{[h + J\cos(ap)]^2 + J^2\sin^2(ap)}. \tag{9}$$

The spectrum is generically gapped and the gap is $\Delta = \min(|h + J|, |h - J|)$. Therefore the system becomes gapless for $h = \pm J$.

3 Majorana fermions

6) We define Majorana fermions as

$$c_i^1 = a_i^\dagger + a_i, \qquad c_i^2 = -i(a_i^\dagger - a_i). \tag{10}$$

Using the fermionic anticommutation relations, it is immediate to show that $\{c_i^a, c_j^b\} = \delta_{ab}\delta_{ij}$.
Using the definition of the Majorana fermion operators, we can rewrite the Hamiltonian as

$$H = -i\sum_i \left[J c_i^2 c_{i+1}^1 - \frac{h}{2} c_i^2 c_i^1 \right] + \text{const.} \tag{11}$$

7) We consider now a finite size chain with N sites labeled by, $i = 1, \ldots, N$. Note first that for $h = 0$, the two Majorana fermion operators c_1^1 and c_2^N decouple from the Hamiltonian and thus correspond to zero energy states localized at the two extremities of the chain.

Most of the eigenstates have energies $\epsilon_n > \Delta$ or $\epsilon_n < -\Delta$ where $\Delta = |J|$ is the gap. They correspond to quasi-particles which are high energy excitations (not in the gap). We are interested in low energy excitations within the gap near $\epsilon \approx 0$.

For simplicity, we consider here a semi-infinite system ($N \to \infty$), where only one bound state remains that has exactly $\epsilon = 0$.

We use the fact that the matrix can be written in the following form :
$|b_1\rangle = A(c_1^1 + \lambda c_2^1 + \lambda^2 c_3^1 + \ldots)|\rangle$.
to be done

4 Majorana fermions with electrons

8) Reconsider now Eq. (8) and assume that the a_p describe real electrons. Speculate what type of interaction, band structure, etc. is necessary to obtain such a Hamiltonian.