LCM Phase Transition in Different Disorder Distributions

Michael Alexander Kurniawan[1] and Ady Stern[2]

[1]*Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay Road, Kowloon, Hong Kong*

[2]*Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel*

(Dated: August 17, 2023)

Abstract

This is a constantly updated note for the LCM project. Stay tune for more!

I. WHAT IS THE CHERN NUMBER ACTUALLY?

Note: Most of the content of this section stems from Niu, 2010 incredible review paper!

A. Berry Phase

Let us start from the discovery of Berry phase. Consider a Hamiltonian that could be described by a number of parameters that depend on time

$$H = H(\mathbf{R}), \quad \mathbf{R} = \mathbf{R}(t) \tag{1}$$

Now, we consider that the Hamiltonian changes very slowly with time in which a more pedantic way to say it is that $\mathbf{R}(t)$ moves slowly along a path $\mathcal{C}$ in the parameter space. This adiabatic evolution (or approximation) ables us to write down an **instantaneous** orthonormal basis from the eigenstates of $H(\mathbf{R})$ at a certain value of $\mathbf{R}$. In other words,

$$H(\mathbf{R})|n(\mathbf{R})\rangle = \epsilon_n(\mathbf{R})|n(\mathbf{R})\rangle \tag{2}$$

Notice, how peculiar this approximation is! In a general case, we can't actually have these eigenstates when the Hamiltonian is time-dependent. This is because there is no stationary states! Or to be more specific, when the Hamiltonian is time-dependent, we could not perform separation of variables between position and time that we usually do to obtain the eigenstates or stationary states. However, in the adiabatic case, since the $H(\mathbf{R})$ changes very very slowly in time, we could approximate that it is actually kinda constant in time, and thus have these eigenstates we define on Eq. (2).

After we have this,we could write a state as

$$|\psi_n(t)\rangle = e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int_0^t dt' \epsilon_n(\mathbf{R}(t'))} |n(\mathbf{R}(t))\rangle \tag{3}$$

Here we can see that there are two phase factors. The second exponential is known as the dynamical phase factor, but what interests us is the first phase term. Putting Eq. (3) to the Schroedinger equation, we found that γ_n could actually be written down as

$$\gamma_n = \int_{\mathcal{C}} d\mathbf{R} \mathcal{A}_n(\mathbf{R}) \quad \text{where} \quad \mathcal{A}_n(\mathbf{R}) = i\langle n(\mathbf{R})| \frac{\partial}{\partial \mathbf{R}} |n(\mathbf{R})\rangle \tag{4}$$

This new quantity $\mathcal{A}_n$ we introduce here is what we call as the **Berry connection**. But notice that $\mathcal{A}_n$ is gauge-dependent! Why? Because

$$\int_{\mathcal{C}} d\mathbf{R} \frac{\partial}{\partial \mathbf{R}} \xi(\mathbf{R}) = \xi(\mathbf{R}(0)) - \xi(\mathbf{R}(t)) \tag{5}$$

and we could derive that:

$$|n(\mathbf{R})\rangle \longrightarrow |n(\mathbf{R})\rangle = e^{i\xi(\mathbf{R})}|n(\mathbf{R})\rangle \tag{6}$$

$$\mathcal{A}_n(\mathbf{R}) \longrightarrow \mathcal{A'}_n(\mathbf{R}) = \mathcal{A}_n(\mathbf{R}) - \frac{\partial}{\partial \mathbf{R}}\xi(\mathbf{R}) \tag{7}$$

Now this is the crazy part, it took around 60 years to finally a guy by the name of Michael Berry consider the cyclic evolution of the system along a closed parameter path $mathcalC$ with $\mathbf{R}(T) = \mathbf{R}(0)$. What this means is that:

$$\xi(\mathbf{R}(0) - \xi(\mathbf{R}(t)) = 2\pi m \tag{8}$$

where m here must be an integer. This consequence mean that we could not always set γ_n to be zero and thus γ_n is gauge invariant! With the above in mind, we define the following

$$\gamma_n = \oint_{\mathcal{C}} d\mathbf{R} \cdot \mathcal{A}_n(\mathbf{R}) \tag{9}$$

which is the renowned **Berry phase**, hidden in plain sight for over 60 years. Notice that the Berry phase only depends on the geometric aspect of the closed path and is independent of how $\mathbf{R}(t)$ actually changes in time. This means that the explicit time dependence is thus not essential in the description of the Berry phase. Amazing!

B. Berry Curvature

You must have seen in electrodynamics that you could rewrite Maxwell's equation in tensor notation. Here, in analogy to that, we also rewrite the above results to

$$\Omega^n_{\mu\nu}(\mathbf{R}) = \frac{\partial}{\partial R^\mu}\mathcal{A}^n_\nu(\mathbf{R}) - \frac{\partial}{\partial R^\mu}\mathcal{A}^n_\nu(\mathbf{R}) \tag{10}$$

$$= i[\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} | \frac{\partial n(\mathbf{R})}{\partial \mathbf{R}^\nu}\rangle - (\nu \longleftrightarrow \mu)] \tag{11}$$

But in the 3D parameter space $\mathbf{R}$, the Berry curvature could be written as

$$\Omega_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathcal{A}_n(\mathbf{R}) \tag{12}$$

$$\gamma_n = \int_S d\mathbf{S} \cdot \Omega_n(\mathbf{R}) \tag{13}$$

This form equation for Berry curvature gives a better intuition on what it is actually: It is the magnetic field in the parameter space!

C. Adiabatic Transport and Electric Polarization

If a potential varies on a lattice varies slowly in time and it is periodical, then the particle transport (which is basically a current) in a period can be expressed as a Berry phase and it is an integer.

Some points that is important (not ordered yet):

1. The Chern number counts the net number of monopoles enclosed by the surface
2. For c_n to be nonzero is that a certain degeneracy point must occur on the parameter space of q, R_1, R_2. If you have three components of R, then the particle transport would also be affected!

D. Summary

To put it short, the Chern number in a nutshell is the Berry curvature being integrated over a closed surface such as a torus or a sphere. This integrated quantity is found to be quantized as integers in which we call it as the Chern number.

II. OUR HAMILTONIAN MODEL

We implement the following Hamiltonian model in the **momentum space**

$$H(\mathbf{k}) = d_z(\mathbf{k})\sigma_z \otimes I_2 + d_x(\mathbf{k})\sigma_x \otimes I_2 + d_y(\mathbf{k})\sigma_y \otimes I_2 \tag{14}$$

where σ_i are pauli matrices and the coefficients in front of them are defined as

$$d_z = m + t_1 \sin^2(k_x/2) + t_1 \sin^2(k_y/2) \tag{15}$$

$$d_x = t_2 \sin k_x \tag{16}$$

$$d_y = t_2 \sin k_y \tag{17}$$

Hence, in matrix form, the Hamiltonian in momentum space would be

$$H = \sum_k \mathbf{c}_\mathbf{k}^\dagger \begin{pmatrix} d_z & 0 & d_x - id_y & 0 \\ 0 & d_z & 0 & d_x - id_y \\ d_x + id_y & 0 & -d_z & 0 \\ 0 & d_x + id_y & 0 & -d_z \end{pmatrix} \mathbf{c}_\mathbf{k} \tag{18}$$

where

$$\mathbf{c}_{\mathbf{k}}^{\dagger} = \begin{pmatrix} c_{\mathbf{k},a}^{\dagger} & c_{\mathbf{k},b}^{\dagger} & c_{\mathbf{k},c}^{\dagger} & c_{\mathbf{k},d}^{\dagger} \end{pmatrix} \tag{19}$$

in which $a, b, c,$ and d denotes the 4 orbitals that we have. However, since we would like to calculate the Local Chern Marker (LCM), we would need to transform the above momentum space Hamiltonian into the real space. Using the fact that,

$$c_{\mathbf{k},\alpha} = \frac{1}{N} \sum_{x,y} c_{xy,\alpha} e^{-ik_x x} e^{-ik_y y} \tag{20}$$

where α denotes the different orbitals, and the relation that

$$\frac{1}{N} \sum_{k_x,k_y} e^{-ik_x(x-x')} e^{-ik_y(y-y')} = \delta_{xx'}\delta_{yy'} \tag{21}$$

we would then get the following **real space** Hamiltonian

$$H_0 = \sum_{\mathbf{R}} [\sum_{s=a,b} (m + t_1) c_{\mathbf{R},s}^{\dagger} c_{\mathbf{R},s} + \sum_{p=c,d} (-m - t_1) c_{\mathbf{R},p}^{\dagger} c_{\mathbf{R},p}] \tag{22}$$

$$H_1 = \sum_{R} \sum_{\mu=\pm x,\pm y} \sum_{s=a,b;p=c,d} (\frac{-t_1}{4} c_{\mathbf{R}+\mathbf{l}_\mu,s}^{\dagger} c_{\mathbf{R},s} + \frac{t_1}{4} c_{\mathbf{R}+\mathbf{l}_\mu,p}^{\dagger} c_{\mathbf{R},p} + e^{i\theta_\mu} \frac{t_2}{2} c_{\mathbf{R}+\mathbf{l}_\mu,s}^{\dagger} c_{\mathbf{R},p} + e^{-i\theta_\mu} \frac{t_2}{2} c_{\mathbf{R}+\mathbf{l}_\mu,(s;p)}^{\dagger} c_{\mathbf{R},(p;s)}) \tag{23}$$

$$H = H_0 + H_1 \tag{24}$$

Some notations definition:

1. Here s indicates the orbital a and b while p indicates the orbital c and d.
2. $\mathbf{R}$ indicates the coordinate to one of the sites, in which $\mathbf{R} = (x, y)$.
3. θ_μ is the angle between the y-axis and the direction of the hopping $\mathbf{l}_\mu$ as also seen in Fig.(1).Since we only consider the nearest neighbour hopping then the value of θ_μ would be $0, \pm\pi/2, \pi$ only.
4. $\frac{t_1}{4}$ indicates the hopping between the s-orbitals while $\frac{-t_1}{4}$ indicates the hopping between the p-orbitals.
5. $\frac{t_2}{2}$ indicates the hopping between s and p orbitals and vice versa.
6. m indicates the "mass" of the orbital
7. H is the total real space Hamiltonian

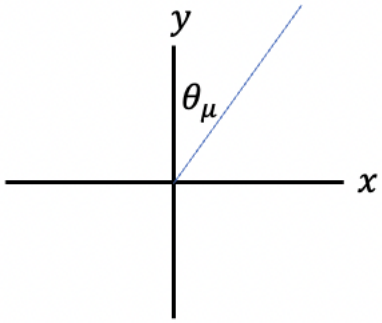

FIG. 1: Definition of θ_μ sketched in the Cartesian coordinate in which the blue line indicates the direction l_μ is pointing at

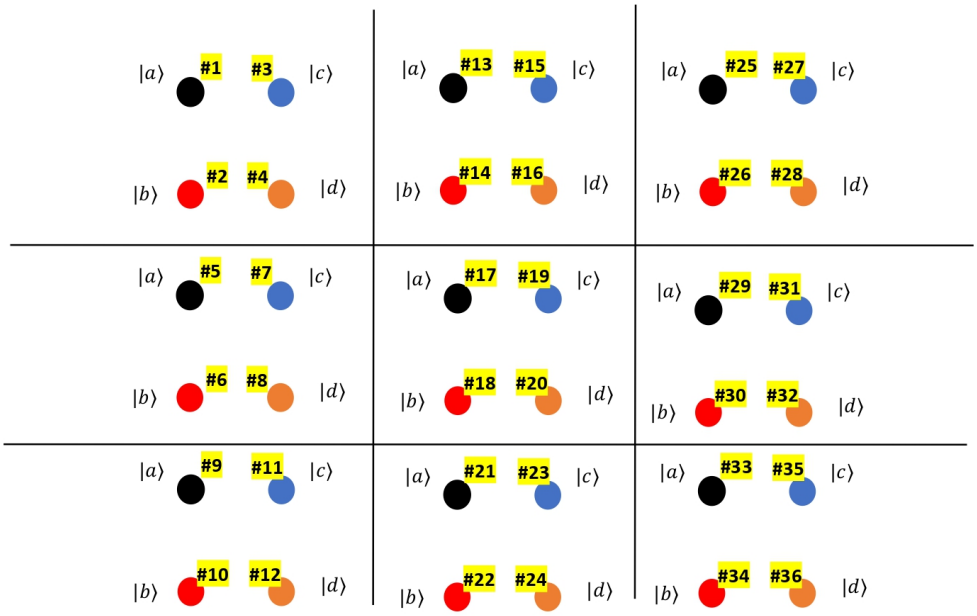

FIG. 2: An illustration of how our model looks model in real space. Here $|a\rangle, |b\rangle, |c\rangle,$ and $|d\rangle$ denote the 4 orbitals for each site that we have

III. DISPERTION RELATION

From the above Bloch Hamiltonian we obtain the following dispertion relation

$$E_k = \pm\sqrt{d_x^2 + d_y^2 + d_z^2} \tag{25}$$

Let's do this one by one

$$d_z^2 = m^2 + t_1^2 \sin^4(k_x/2) + t_1^2 \sin^4(k_y/2) + 2mt_1 \sin^2(k_x/2) + 2mt_1 \sin^2(k_y/2) + t_1^2 \sin^2(k_x/2)\sin^2(k_y/2) \tag{26}$$

$$d_x^2 = t_2^2 \sin^2 k_x \tag{27}$$

$$d_y^2 = t_2^2 \sin^2 k_y \tag{28}$$

IV. LCM CALCULATION

This section shows how to calculate the LCM analytically (if possible) and numerically. I believe the first paper to introduce the idea of LCM is from Resta, et. al, 2011.

V. CALCULATING LOCALIZATION LENGTH IN 2D LATTICE

So we start by a weird problem already: we have a 2D system, how do we calculate the localization since transfer matrices could only be calculated in 1D chain? This problem is answered in Sarma's paper where we transform the problem into a quasi-1D problem which means that the system is approximately 1D but not actually 1D (weird right, but thats the creative part!). This happens for example if you see a cylinder with much much longer axial length compared to the radius, and if you see this very long radius from far away, what you see is just a 1D strip.

We define the quasi-1D localization length as $\rho_q 1D$ while also defining the dimensionless quasi-1D localization length as $\Lambda = \rho_q 1D/L$. By scaling analysis (haven't understood what this is) we then could get the localization of the original 2D shape system.

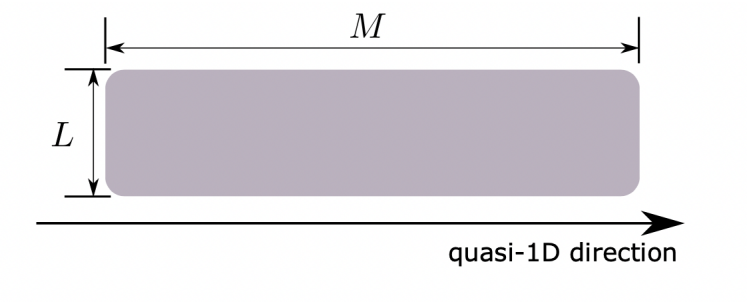

FIG. 3: Illustration of quasi-1D direction taken from F. J. Wang, et. al paper