Lecture 12 Basics of quantum geometry and topology

Literature: R. Resta, The insulating state of matter: a geometrical theory, The European Physical Journal B 79, 121 (2011); B.A. Bernevig and T.L. Hughes, Topological Insulators and Topological Superconductors, Princeton University Press (2013) (available as an electronic book at Aalto library https://aalto.finna.fi/Record/alli.775616).

Learning goals

- To know what are Berry connection, Berry phase, Berry curvature, Chern number and quantum metric, and how they are connected with each other.
- To have some idea about the importance of these concepts in physics.

A key question in quantum physics is how to classify, in a conceptually elegant and efficient way, the various states of matter that have been observed in nature, and which nowadays can be created by artificial quantum systems and simulators. The band structure theory for electrons in solids has been quite powerful in this: we know that electrons in periodic potentials (i.e., lattices, formed for example by the crystal of nuclei) may have a band structure. If the Fermi level of the system is within the band gap, we have an *insulator*. If the band-gap is small, the system is *semiconducting*. If the Fermi level is in the conduction band, we have a *metal*. However, there are also concepts like the *Mott insulator* that you have learned in this course: there the insulating behaviour is not explained by the simple band theory, but requires taking into account the strong interactions (correlations) in the system. Another example of an insulator not explained by band theory is the *Anderson insulator*, where disorder felt by the electrons is the underlying cause of non-conductance of current. In recent years, the concept of a *topological insulator* has become extremely important. There the insulating behaviour results from quantum geometric and topological properties of the system. An interesting feature of topological insulators is that, even when the bulk material is insulating, there can be transport (current) on the surface of the material. This current is robust against perturbations (such as scattering from a material defect) due to the topological properties. In practice, for instance, backscattering of electrons from a defect can be forbidden due to topological properties.

In recent times, it has become more and more clear that a key underlying concept for classifying different states of matter are the localization properties of wavefunctions that describe the system. The eigenfunctions of a periodic system are the Bloch functions (as discussed for instance in Lecture 9), parametrized by the lattice wavevector (also called crystal quasimomentum) $\mathbf{k}$ which is a good quantum number in a perfectly periodic system:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \tag{26.18}$$

where $u_{\mathbf{k}}(\mathbf{r})$ is periodic with the lattice period. One can transform the Bloch functions to define so-called Wannier functions

$$w_{\mathbf{R}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in BZ} e^{-i\mathbf{k}\cdot\mathbf{R}} \psi_{\mathbf{k}}(\mathbf{r}), \tag{26.19}$$

where N is the number of lattice sites, the $\mathbf{k}$ summation is over the first Brillouin zone (BZ), and $\mathbf{R}$ a vector of the Bravais lattice (that is, the position of one lattice site; since in an infinite lattice they are all equal, it does not matter which one we choose). The Wannier function characterizes how the particle (e.g., electron) is spread around the position $\mathbf{R}$ (a useful discussion on Wannier functions can be found for instance in Marzari *et al.*, Rev. Mod. Phys. 84, 1419 (2012)). Whether the Wannier functions are delocalized, or localized over some finite range of lattice sites, whether they overlap, etc. has turned out to be a crucial feature determining the state of the system. It is easy to understand that totally localized and disconnected Wannier functions lead to an insulating state while completely delocalized functions help carry current. Localized but overlapping functions are an interesting intermediate case. The story of course becomes more complicated when the particles interact with each other.

The properties of Wannier functions naturally depend on the Bloch function. The key properties turn out to be those related to the quantum geometry and topology of the system. The basic concepts of quantum geometry and topology, such as Berry phase, Berry connection, Berry curvature, Chern number and quantum metric have become important basic building blocks of modern quantum physics. In this lecture, you will learn these basic concepts. But we will not have time to discuss in detail how properties of quantum states and phases can be explained using them. You can read about the topic independently. Or, perhaps, you will learn about it in your own future research!

26.7 Geometry in quantum mechanics: phase and distance

Let us consider quantum states that are eigenstates of the Schrödinger equation

$$H(\mathbf{k})|\Psi(\mathbf{k})\rangle = E_{\mathbf{k}}|\Psi(\mathbf{k})\rangle. \tag{26.20}$$

Here $\mathbf{k}$ is a parameter (real number); for instance in a lattice system it could be the lattice wavevector, but the discussion here is completely general and it can be something else. The set of wavevectors $|\Psi(\mathbf{k})\rangle$ that fulfil the equation (26.20) form a sub-manifold of the Hilbert space. In the lattice case they would be the Bloch functions of the different energy bands of the lattices. Interesting quantum geometrical or topological effects usually require a multi-band (multi-component) system, where the bands (components) can come for instance from lattice geometry, effective finite lattice unit cell size (caused, e.g., by an effective or real magnetic field), or existence of two spin components and spin-orbit coupling.

In classical physics, the definition of distance between two points is quite straightforward: draw the shortest possible line between them and measure it. Of course, this is more tricky if the geometry is non-trivial: for instance, on the surface of a sphere the distance between two points is defined differently, as function of the coordinates, than on a flat surface. Curved space-time geometries appear also in the context of general relativity. The quantity that takes into account the geometry of the system in defining the distance is called **metric**.

Now, we may ask whether it is possible to define the distance between quantum states on a given manifold (for instance the sub-manifold defined by Equation (26.20)). We use the Bures distance (there are other definitions too, for instance the standard definition of distance in a Hilbert space has a factor of two difference to the Bures distance):

$$D_{12} = \sqrt{1 - |\langle\Psi(\mathbf{k}_1)|\Psi(\mathbf{k}_2)\rangle|^2}. \tag{26.21}$$

As one can easily see, the distance is zero for equal states, and one for orthogonal ones. Since the definition contains square of the inner product, we obviously loose any information related to phase of the inner product. Indeed one can define also the concept of phase difference:

$$e^{-i\Delta\varphi_{12}} = \frac{\langle\Psi(\mathbf{k}_1)|\Psi(\mathbf{k}_2)\rangle}{|\langle\Psi(\mathbf{k}_1)|\Psi(\mathbf{k}_2\rangle|} \tag{26.22}$$

$$\Delta\varphi_{12} = -Im\log\langle\Psi(\mathbf{k}_1)|\Psi(\mathbf{k}_2)\rangle. \tag{26.23}$$

You have probably learned in earlier quantum mechanics courses that one can always add an arbitrary phase factor to a quantum state and it does not change any observable quantity. In another language, multiplying a quantum state by an arbitrary phase factor is a so-called gauge transformation, and the overall phase of the wavefunction is a gauge-dependent quantity. Gauge-dependent quantities are not physical properties of the system, in the sense that they cannot be observed. The phase difference defined above is gauge-dependent, and therefore does not as such have a physical meaning. This relation holds also the other way round: if one can show that some quantity is gauge independent, it is physically meaningful and can (at least in principle) be measured. The Bures distance is an example of such gauge-independent, measurable quantity.

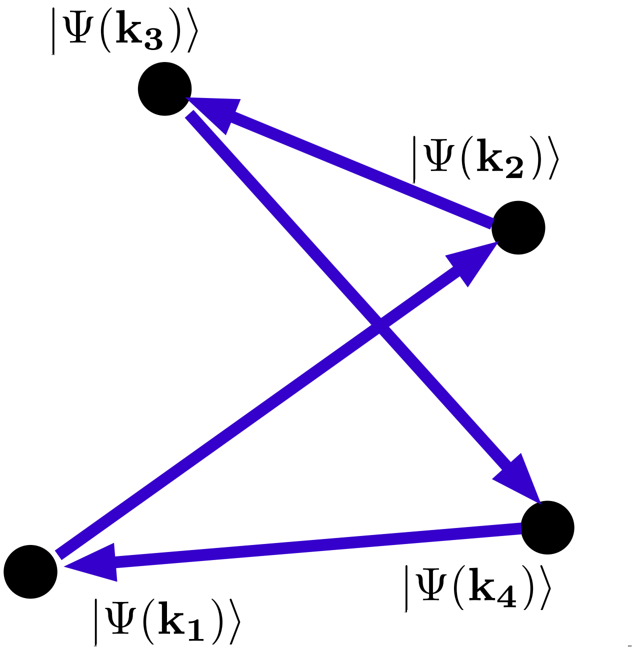

Figure 20: A closed path that connects four states in the **k** space.

So why are we still interested in the phase difference? Well, let us see what we get if we try to measure the total phase difference when we make a closed loop between a set of states, see Figure 20, that is, calculate the phase difference between states 1 and 2, then 2 and 3, 3 and 4, and finally between 4 and 1, and sum them. The total phase difference becomes

$$\begin{aligned}\gamma &= \Delta\varphi_{12} + \Delta\varphi_{23} + \Delta\varphi_{34} + \Delta\varphi_{41} \qquad (26.24)\\ &= -Im\log\langle\Psi(\mathbf{k}_1)|\Psi(\mathbf{k}_2)\rangle\langle\Psi(\mathbf{k}_2)|\Psi(\mathbf{k}_3)\rangle\langle\Psi(\mathbf{k}_3)|\Psi(\mathbf{k}_4)\rangle\langle\Psi(\mathbf{k}_4)|\Psi(\mathbf{k}_1)\rangle.\end{aligned}$$

Now all gauge-arbitrary phases cancel. Example: if for instance $|\Psi(\mathbf{k}_1)\rangle = |1\rangle + e^{i\phi}|2\rangle$ where $|1\rangle$, $|2\rangle$ are some orthogonal basis states, then the state $e^{i\theta}|\Psi(\mathbf{k}_1)\rangle = e^{i\theta}(|1\rangle + e^{i\phi}|2\rangle)$ is a physically equivalent state and the gauge-arbitrary phase θ cancels away. However, the phase ϕ is physically meaningful and affects the value of the inner products with $|\Psi(\mathbf{k}_2)\rangle$ and $|\Psi(\mathbf{k}_4)\rangle$, if those states contain $|2\rangle$.

As a gauge invariant quantity, the total phase difference (26.24) is potentially an observable quantity! Let us now consider, instead of four states, a smooth curve in the parameter space $\mathbf{k}$, and discretize it. The phase difference between two points in the curve separated by a small distance $\mathbf{\Delta k}$ is

$$
\begin{aligned}
e^{-i\Delta\varphi} &= \frac{\langle \Psi(\mathbf{k})|\Psi(\mathbf{k}+\mathbf{\Delta k})\rangle}{|\langle \Psi(\mathbf{k})|\Psi(\mathbf{k}+\mathbf{\Delta k}\rangle|} && (26.25)\\
\Delta\varphi &= -Im \log\langle \Psi(\mathbf{k})|\Psi(\mathbf{k}+\mathbf{\Delta k})\rangle. && (26.26)
\end{aligned}
$$

If the phase varies in a differentiable way, then (take a Taylor series of the above and keep terms up to the order Δk)

$$
i\Delta\varphi \simeq \langle \Psi(\mathbf{k})|\nabla_{\mathbf{k}}\Psi(\mathbf{k})\rangle \cdot \Delta\mathbf{k}. \tag{26.27}
$$

If the set of points in the path becomes dense, that is, $\mathbf{\Delta k}$ is infinitesimally small, we can write the discrete sum of distances from point 1 to point M as an integral over the corresponding smooth curve C from 1 to M:

$$
\gamma = \sum_{s=1}^{M} \Delta\varphi_{s,s+1} \longrightarrow \gamma = \int_C \mathcal{A}\cdot d\mathbf{k}. \tag{26.28}
$$

Here the vector $\mathcal{A}$ is called the **Berry connection**:

$$
\mathcal{A} = i\langle \Psi(\mathbf{k})|\nabla_{\mathbf{k}}\Psi(\mathbf{k})\rangle. \tag{26.29}
$$

The state vectors are assumed to be normalized at any $\mathbf{k}$ which means that the Berry connection is real (just take the derivative, using the chain rule, of both sides of $\langle\Psi|\Psi\rangle^2 = 1$). Therefore one can also write

$$
\mathcal{A} = -Im\langle \Psi(\mathbf{k})|\nabla_{\mathbf{k}}\Psi(\mathbf{k})\rangle. \tag{26.30}
$$

The integral γ is called the **Berry phase**. It has already been observed in numerous physical systems and has become an important concept of modern quantum (and classical optical) physics.

26.7.1 Berry curvature

If the curl of the Berry connection is well-defined on a surface Σ whose boundary is the curve C (notation $C = \partial\Sigma$), then one can use Stokes theorem to write the Berry phase in an alternative way

$$
\gamma = \int_{\partial\Sigma} \mathcal{A}\cdot d\mathbf{k} = \int_{\Sigma} \mathbf{\Omega}\cdot\mathbf{n}d\sigma. \tag{26.31}
$$

Stokes theorem transforms a line integral to an integral over an area, with the integrand replaced by its curl. Here $\mathbf{n}$ is a vector normal to the surface that is integrated over. The quantity $\mathbf{\Omega}$ is the **Berry curvature**

$$
\begin{aligned}
\mathbf{\Omega} &= \nabla_{\mathbf{k}} \times \mathcal{A} && (26.32)\\
&= -Im\langle \nabla_{\mathbf{k}}\Psi(\mathbf{k})| \times |\nabla_{\mathbf{k}}\Psi(\mathbf{k})\rangle && (26.33)\\
&= i\langle \nabla_{\mathbf{k}}\Psi(\mathbf{k})| \times |\nabla_{\mathbf{k}}\Psi(\mathbf{k})\rangle. && (26.34)
\end{aligned}
$$

In dimensions other than three the Berry curvature can be written component-wise ((α, β) denote Cartesian coordinates and $\partial_\alpha \equiv \partial/\partial k_\alpha$) as

$$\Omega_{\alpha\beta}(\mathbf{k}) = -2Im\langle\partial_\alpha\Psi(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle. \tag{26.35}$$

The Berry curvature is a gauge-invariant quantity, and naturally then also the Berry phase calculated from it. Indeed, both can (and have been) observed. The Berry connection and Berry curvature play a similar role as the vector potential $\mathbf{A}$ and the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, respectively, in elementary magnetostatics. As you remember from earlier this course, the vector potential is gauge-dependent and one can choose the gauge (for instance the Coulomb gauge by $\nabla \cdot \mathbf{A} = 0$), while the magnetic field is a gauge-independent, physical quantity that can be measured.

26.7.2 Chern number

We discussed above the Berry phase defined for a certain path C, and via Stokes theorem, for a surface Σ that the path C is a boundary for. But one can define such a phase also for a closed surface Σ. Naturally, the path C is then vanishing. Think about a part of a sphere being the surface: that can be circulated by a finite path. But if the whole sphere is the surface, then the "path" is vanishing. It can be shown that the integral of the Berry curvature over such a closed surface is quantized:

$$\int_\Sigma \mathbf{\Omega} \cdot \mathbf{n} d\sigma = 2\pi C_1. \tag{26.36}$$

Here C_1 is an integer, called Chern number of the first class (or often just Chern number). The closed surface can be, for example, the first Brillouin zone in a lattice system. We will not go through the proof for Equation (26.36), but if you are interested, you can find it from Section 2.4 of the article by Resta mentioned in *Literature*, or Chapter 3.6 of Bernevig's book. The system is said to be topologically trivial if $C_1 = 0$, and topologically non-trivial if C_1 is some finite integer. It can be shown that in order to have non-zero Chern number, the Berry connection must have singularities somewhere on the surface (i.e. somewhere in the Brillouin zone in a lattice system).

The Chern number is a **topological invariant**. It stays invariant between two topological spaces that are connected by a homeomorphism. Sounds abstract, but just go to https://en.wikipedia.org/wiki/Homeomorphism to see a movie about how a coffee cup transforms continuously to a donut which shows that they are homeomorphic. The topological invariant in that case is the number of holes in the object. Of course in quantum physics things are more abstract: we are now talking about topological properties and invariants of the eigenstates of a certain system. Analogously to the number of holes in a cup and a donut, the topological invariant of a quantum system does not necessarily change due to small changes in the system Hamiltonian. The fact that the topological invariant is insensitive to small changes and perturbations can potentially be used, for instance for robust quantum computing, or protected uni-directional currents. See Figure (21) for illustration of this point. In the previous section we discussed the analogue between Berry curvature and the magnetic field. Within this analogy, a non-zero Chern number corresponds to having a magnetic monopole. This gives some intuition to why the Chern number must be quantized and it why it is a topological invariant.

A famous example of the significance of the Chern number is the quantum Hall effect. There the conductance of the system is quantized, that is, it changes

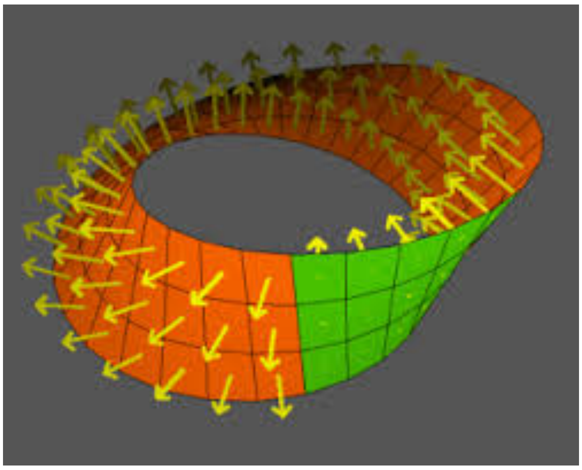

Figure 21: Arrows on a Möbius stripe. The existence of the twist in the Möbius stripe means that the arrows change direction when you go around the loop. The change of the direction cannot be eliminated just by deformations of the stripe, without cutting it. Analogously, certain properties of quantum states are robust to small perturbations, when those properties are caused by the quantum geometry and topology related to the system's eigenstates. Image from plus.maths.org.

in steps when a magnetic field that penetrates the sample is changed, see Figure (22). It was shown in 1982 by Thouless, Kohmoto, Nightingale and den Nijs that the conductance is given by the Chern number and thereby topological properties of the system are the origin of the quantum Hall effect. Thouless got the Nobel prize 2016 for this and his other theoretical work on topological physics. There are also other types of topological invariants than the Chern number. Topological quantum physics has become an extremely important and fast growing field of research, inspired by the experimental observation of topological insulators and by the concept of a topological superconductor.

26.7.3 Quantum metric

Based on the definition of the Bures distance, Equation (26.21), one can calculate the infinitesimal distance. Start from

$$D_{12}^2 = 1 - |\langle \Psi(\mathbf{k}) | \Psi(\mathbf{k} + d\mathbf{k}) \rangle|^2 \tag{26.37}$$

and use the Taylor expansion to second order

$$|\Psi(\mathbf{k} + d\mathbf{k})\rangle \simeq |\Psi(\mathbf{k})\rangle + \sum_\alpha |\partial_\alpha \Psi(\mathbf{k})\rangle dk_\alpha + \frac{1}{2} \sum_{\alpha,\beta} |\partial_\beta \partial_\alpha \Psi(\mathbf{k})\rangle dk_\alpha dk_\beta. \tag{26.38}$$

In the calculation it is good to remember which quantity is imaginary, and separate the real and imaginary parts. Higher than second order terms are neglected. The result becomes

$$D_{\mathbf{k},\mathbf{k}+d\mathbf{k}}^2 = \sum_{\alpha,\beta=1}^{d} g_{\alpha\beta}(\mathbf{k}) dk_\alpha dk_\beta, \tag{26.39}$$

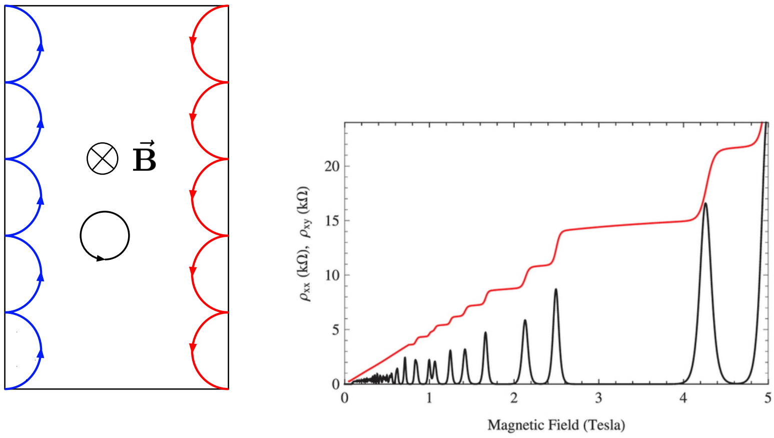

Figure 22: Quantum Hall effect. Magnetic field penetrates the sample and quantized conductance as function of the magnetic field emerges. Image on the right from Research Gate.

where we have the **quantum metric** tensor (this tensor is also called the Fubini-Study metric)

$$g_{\alpha\beta}(\mathbf{k}) = Re\left(\langle\partial_\alpha\Psi(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle - \langle\partial_\alpha\Psi(\mathbf{k})|\Psi(\mathbf{k})\rangle\langle\Psi(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle\right). \tag{26.40}$$

One can express it also using the projector $Q(\mathbf{k}) = 1 - |\Psi(\mathbf{k})\rangle\langle\Psi(\mathbf{k})|$

$$g_{\alpha\beta}(\mathbf{k}) = Re\langle\partial_\alpha\Psi(\mathbf{k})|Q(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle. \tag{26.41}$$

Now let us recall the definition of the Berry curvature:

$$\Omega_{\alpha\beta}(\mathbf{k}) = -2Im\langle\partial_\alpha\Psi(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle. \tag{26.42}$$

We can insert the projector $Q(\mathbf{k})$ into this definition, because as said above, $\langle\partial_\alpha\Psi(\mathbf{k})|\Psi(\mathbf{k})\rangle$ is imaginary, and thus the product $\langle\partial_\alpha\Psi(\mathbf{k})|\Psi(\mathbf{k})\rangle\langle\Psi(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle$ real. We have

$$\Omega_{\alpha\beta}(\mathbf{k}) = -2Im\langle\partial_\alpha\Psi(\mathbf{k})|Q(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle. \tag{26.43}$$

We see that (apart from the factor of two difference which is trivial) the quantum metric and the Berry curvature are the real and imaginary parts of the same quantity. This quantity is called **quantum geometric tensor**:

$$\eta_{\alpha\beta} = \langle\partial_\alpha\Psi(\mathbf{k})|Q(\mathbf{k})|\partial_\beta\Psi(\mathbf{k})\rangle. \tag{26.44}$$

In summary, the quantum geometric tensor has a real part, the symmetric tensor called quantum metric describing the amplitude distance between quantum states, and an imaginary part, the antisymmetric tensor called Berry curvature which is related to the phase distance between two states. The quantum metric, Berry curvature and the quantum geometric tensor are all gauge-invariant, measurable quantities.

The Berry phase has been observed in a multitude of systems, and also Berry curvature has been measured. The first direct measurements of the quantum metric were published in 2019, and it is a concept whose significance in physics is emerging right now. It has been predicted to appear in a few contexts, one of them is superconductivity. The Quantum Dynamics group at Aalto University has shown that the quantum metric of the system affects superfluidity and superconductivity. In particular, its non-zero value guarantees that supercurrent exists even in a situation where the group velocities of non-interacting electrons are zero (so called flat energy bands). The quantum metric is part of the quantum geometric tensor, which contains the Berry curvature and thereby relates to topological invariants like the Chern number; therefore the findings of the Quantum Dynamics group have made a new connection between quantum geometry, topology and superfluid transport (supercurrents).

Finally, let us come back to where this lecture started. It was mentioned that localization properties of the Wannier functions are crucial in describing properties of quantum phases of matter. As you have learned above, the quantum metric and Berry curvature depend on derivatives of the eigenfunctions, in a lattice system this would mean derivatives of the Bloch functions. Via this, there is a connection between the localization properties of Wannier functions (which are combinations of Bloch functions) and quantum geometry.

The understanding of all the consequences of quantum geometry, especially in interacting many-body systems, is only in the beginning.