Zak phase and electric polarization

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We shall look at the electric polarization for 1D crystal from the view point of Berry phase. We find that the electric polarization not only reflects the *local* charge density ρ but also the *global* topology of the band which encoded in the phase of the Bloch wave functions and thus in the Berry connection. Here, the *Zak phase*, which is basically the Berry phase obtained by integrating the Berry connection across the Brillouin zone, plays an important role. The Zak phase turns out to be taken only two values (modulo 2π), 0 or π, when the crystal has the spatial symmetry of inversion.

I. ELECTRIC POLARIZATION [1, 2]

A. Statement of the problem

Electric dipole moment of an macroscopic object should be a vector with the dimension *charge* × *distance*. Thus, it is tempting to think that the electric polarization (electric dipole moment per volume) can be defined by the average of the charge density $\rho(\boldsymbol{r})$ times the position $\boldsymbol{r}$ over the volume, that is

$$\boldsymbol{P} = \frac{1}{V_{\text{cell}}} \int \boldsymbol{r}\rho(\boldsymbol{r})dV. \tag{1}$$

Quantum mechanically, this formula invovles the *position operator* $\boldsymbol{r}$, which is ill-behaved in the cell-periodic crystaline material where the electric states are descrived by Bloch functions with quantum number $\boldsymbol{k}$. Moreover, the definition is equivocal in a sense that the value $\boldsymbol{P}$ in Eq. (1) would change depending on how we define the unit cell. We thus need to seek an alternative formula for the electric polarization.

B. Seeking an alternative expression

The key is to find the relationship between the electric polarization and the current. Let us find it from the simple argument. The total charge in a dielectric sample is zero when the sample is electrically neutral. Thus, the volume integral of the macroscopically averaged charge density ρ is zero, that is,

$$\int_{\mathcal{V}} \rho dV = 0. \tag{2}$$

This suggests [3] that ρ can be given by

$$\rho = -\nabla \cdot \boldsymbol{P}, \tag{3}$$

where $\boldsymbol{P}$ is a vector quantity called the *electric polarization*, which has only nonzero vector inside the sample. We can see why this is true by

$$\begin{aligned} \int_{\mathcal{V}} \rho dV &= -\int_{\mathcal{V}} (\nabla \cdot \boldsymbol{P})\, dV \\ &= -\int_{\mathcal{A}} \boldsymbol{P} dS = 0 \end{aligned} \tag{4}$$

where the integration volume $\mathcal{V}$ in the first line covers the entire smaple and the integration area $\mathcal{A}$ is the surface enclosing the volume $\mathcal{V}$, which means the area $\mathcal{A}$ is not touching the sample and the last equality results.

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On the other hand, the continuity equation tells us

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0. \tag{5}$$

From Eqs. (3) and (5), we have

$$\nabla \cdot \left(\frac{\partial \boldsymbol{P}}{\partial t} - \boldsymbol{j} \right) = 0. \tag{6}$$

Apart from the divergent-free terms (the so-called *magnetization current*) the chnage of the electric polarization can thus be given by

$$\Delta \boldsymbol{P} = \boldsymbol{P}(T) - \boldsymbol{P}(0) = \int_0^T \boldsymbol{j} dt, \tag{7}$$

where the problematic position operator $\boldsymbol{r}$ is absent!

In 1993, King-Smith and Vanderbilt suggested [4] that the polarization current $\boldsymbol{j}$ appears in Eq. (7) is nothing but the Berry-curvature induced adiabatic current we have derived in the context of the *Thouless pumping* [5]. Let us see this in more detail in the next section.

II. ZAK PHASE AND THE MODERN THEORY OF ELECTRIC POLARIZATION [2, 6]

What King-Smith and Vanderbilt discovered [4] is the overlooked link between the band topology of dielectrics and their electric polarization. The important message here is that the electric polarization not only reflects the *local* charge density ρ but also the *global* topology of the band which encoded in the phase of the Bloch wave functions and thus in the Berry connection.

For the 1D crystal, the Berry-curvature induced adiabatic current can be given by

$$j(t) = e \sum_n \int_{\text{BZ}} \frac{dk}{2\pi} \Omega_{k,n}(t), \tag{8}$$

where $\Omega_{k,n}$ is the Berry curvature. The chnage of the electric polarization can thus be rewritten as

$$\begin{aligned} \Delta \boldsymbol{P} &= e \sum_n \int_0^T dt \int_{\text{BZ}} \frac{dk}{2\pi} \Omega_{k,n}(t) \\ &= e \sum_n \int_0^1 d\lambda \int_{\text{BZ}} \frac{dk}{2\pi} \Omega_{k,n}(\lambda), \end{aligned} \tag{9}$$

where, in the second equation, we explicitly introduced a normalized adiabatic parameter $\lambda(t)$ with $\lambda(0) = 0$ and $\lambda(T) = 1$. We can thus recognize that the electric polarization is proportional to the Berry phase for which the parameter space is spaned by λ and k, as for the Thouless pumping, and is not a torus but a cylinder.

Using the Berry connections the Berry curvature $\Omega_{k,n}(\lambda)$ is rewritten as

$$\begin{aligned} \Omega_{k,n}(\lambda) &= \begin{bmatrix} \frac{\partial}{\partial k} \\ \frac{\partial}{\partial \lambda} \end{bmatrix} \times \begin{bmatrix} A_k^{(n)} \\ A_\lambda^{(n)} \end{bmatrix} \\ &= \frac{\partial A_\lambda^{(n)}}{\partial k} - \frac{\partial A_k^{(n)}}{\partial \lambda} \\ &= i \left(\frac{\partial}{\partial k} \left\langle u_{k,n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{k,n}(\lambda) \right\rangle - \frac{\partial}{\partial \lambda} \left\langle u_{k,n}(\lambda) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(\lambda) \right\rangle \right). \end{aligned} \tag{10}$$

Then, the change of the polarization as the control parameter λ changes from 0 to 1 is given by the line integral

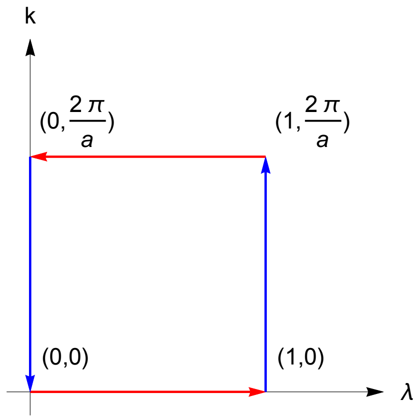

FIG. 1: Path $\mathcal{C}$ is starting from $(0,0) \to (1,0) \to (1,\frac{2\pi}{a}) \to (0,\frac{2\pi}{a}) \to (0,0)$ in λ-k space.

along the path $\mathcal{C}$ shown in Fig. 1:

$$
\begin{aligned}
\Delta \boldsymbol{P} &= \frac{e}{2\pi}\sum_n \int_0^1 d\lambda \int_0^{\frac{2\pi}{a}} dk \left(\frac{\partial A_\lambda^{(n)}}{\partial k} - \frac{\partial A_k^{(n)}}{\partial \lambda} \right) \\
&= i\frac{e}{2\pi}\sum_n \left(\int_0^1 d\lambda \underbrace{\int_0^{\frac{2\pi}{a}} dk \frac{\partial}{\partial k}\left\langle u_{k,n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{k,n}(\lambda) \right\rangle}_{\left\langle u_{\frac{2\pi}{a},n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{\frac{2\pi}{a},n}(\lambda) \right\rangle - \left\langle u_{0,n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{0,n}(\lambda) \right\rangle} - \int_0^{\frac{2\pi}{a}} dk \underbrace{\int_0^1 d\lambda \frac{\partial}{\partial \lambda}\left\langle u_{k,n}(\lambda) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(\lambda) \right\rangle}_{\left\langle u_{k,n}(1) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(1) \right\rangle - \left\langle u_{k,n}(0) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(0) \right\rangle} \right) \\
&= -i\frac{e}{2\pi}\sum_n \left(\int_0^1 d\lambda \left\langle u_{0,n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{0,n}(\lambda) \right\rangle + \int_0^{\frac{2\pi}{a}} dk \left\langle u_{k,n}(1) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(1) \right\rangle \right. \\
&\qquad \left. + \int_1^0 d\lambda \left\langle u_{\frac{2\pi}{a},n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{\frac{2\pi}{a},n}(\lambda) \right\rangle + \int_{\frac{2\pi}{a}}^0 dk \left\langle u_{k,n}(0) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(0) \right\rangle \right). \qquad (11)
\end{aligned}
$$

Now, we exploit the so-called *periodic gauge* (as opposed to the parallel transport gauge encountered last lecture), which can be specified by the boundary condition, $\left|\psi_{\frac{2\pi}{a},n}(\lambda)\right\rangle = |\psi_{0,n}(\lambda)\rangle$ for the Bloch function, or,

$$
\left|u_{\frac{2\pi}{a},n}(\lambda)\right\rangle = e^{-i\frac{2\pi}{a}x}\,|u_{0,n}(\lambda)\rangle \qquad (12)
$$

for the cell-periodic Bloch function, to obtain

$$
\begin{aligned}
\Delta \boldsymbol{P} &= -i\frac{e}{2\pi}\sum_n \left(\int_0^1 d\lambda \left\langle u_{0,n}(\lambda) \middle| \frac{\partial}{\partial \lambda} \middle| u_{0,n}(\lambda) \right\rangle + \int_0^{\frac{2\pi}{a}} dk \left\langle u_{k,n}(1) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(1) \right\rangle \right. \\
&\qquad \left. + \int_1^0 d\lambda \left\langle u_{0,n}(\lambda) e^{i\frac{2\pi}{a}x} \middle| \frac{\partial}{\partial \lambda} \middle| e^{-i\frac{2\pi}{a}x} u_{0,n}(\lambda) \right\rangle + \int_{\frac{2\pi}{a}}^0 dk \left\langle u_{k,n}(0) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(0) \right\rangle \right) \\
&= -i\frac{e}{2\pi}\sum_n \left(\int_0^{\frac{2\pi}{a}} dk \left\langle u_{k,n}(1) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(1) \right\rangle + \int_{\frac{2\pi}{a}}^0 dk \left\langle u_{k,n}(0) \middle| \frac{\partial}{\partial k} \middle| u_{k,n}(0) \right\rangle \right). \qquad (13)
\end{aligned}
$$

The important point here is that with the periodic gauge the line integral of the Berry connection along the lower red line in Fig. 1 cancels out the one along the upper red line in Fig. 1. Thus we arrive at the so-called *modern theory of* *electric polarization* [2, 6]:

$$\begin{aligned}\Delta\boldsymbol{P} &\equiv \boldsymbol{P}(1)-\boldsymbol{P}(0)\\ &= -\frac{e}{2\pi}\sum_n\left\{\underbrace{\int_0^{\frac{2\pi}{a}} dk\left(i\left\langle u_{k,n}(1)\left|\frac{\partial}{\partial k}\right|u_{k,n}(1)\right\rangle\right)}_{\phi_n(1)}-\sum_n\underbrace{\int_{\frac{2\pi}{a}}^{0} dk\left(i\left\langle u_{k,n}(0)\left|\frac{\partial}{\partial k}\right|u_{k,n}(0)\right\rangle\right)}_{\phi_n(0)}\right\}. \qquad (14)\end{aligned}$$

This means that the electric polarization can be obtained by integrating the Berry connection over the Brillouin zone, which is called the *Zak phase* [7],

$$\phi_n(\lambda)=\int_0^{\frac{2\pi}{a}} dk\left(i\left\langle u_{k,n}(\lambda)\left|\frac{\partial}{\partial k}\right|u_{k,n}(\lambda)\right\rangle\right). \qquad (15)$$

Roughly speaking we can consider the operator $i\frac{\partial}{\partial k}$ as a kind of position operator x. In fact the Zak phase $\phi_n(\lambda)$ is related to the so-called *Wannier centor* $\bar{x}_n$ as

$$\bar{x}_n(\lambda)=\frac{a}{2\pi}\phi_n(\lambda)=\frac{a}{2\pi}\int_0^{\frac{2\pi}{a}} dk\left(i\left\langle u_{k,n}(\lambda)\left|\frac{\partial}{\partial k}\right|u_{k,n}(\lambda)\right\rangle\right). \qquad (16)$$

The electric polarization can thus be given by marvelously simple form with the Zak phases $\phi_n(\lambda)$ for the filled band n:

$$\begin{aligned}\boldsymbol{P}(\lambda) &= -\frac{e}{2\pi}\sum_n\phi_n(\lambda) \qquad (17)\\ &= -\frac{e}{a}\sum_n\bar{x}_n(\lambda). \qquad (18)\end{aligned}$$

Indeed, the final expression is what we expect from the naive guess, $P=\frac{ex}{a}$ in 1D, or,$\boldsymbol{P}=\frac{e\boldsymbol{r}}{V_{\rm cell}}$ in 3D, as in Eq. (1).

III. SYMMETRY AND ZAK PHASE [2, 6]

When the parameter λ goes circle like $0\to1\to0$ we find that the situation is the one encountered when analyzing the Thouless pumping. The relation between the Zak phase $\phi_n(\lambda)$ and the number of charges transported by the n-th band per one-cycle c_n is

$$c_n=\frac{1}{2\pi}\left(\phi_n(0=0\to1\to0)-\phi_n(0)\right). \qquad (19)$$

Since $c_n=Z$ where Z is any integer we can conclude that the Zak phase $\phi_n(\lambda)$ is only defined up to modulo 2π. This in turn means the electric polarization $\boldsymbol{P}(\lambda)$ is also defined up to modulo e, that is,

$$\boldsymbol{P}(\lambda)=-e\left(\sum_n\frac{\phi_n(\lambda)}{2\pi}+Z\right). \qquad (20)$$

Now suppose that the 1D crystal that we have been interested in has the spatial symmetry of inversion. The symmetry constrains the topology of the Bloch wave function and thus constrains the Zak phase. Let us see this interesting phenomenon. For simplicity, we consider one band problem. Under the spatial inversion, the electric polarization changes its sign, that is,

$$P\to -P. \qquad (21)$$

However, these two polarization has to have the same physical contents to assume the spatial symmetry of inversion. This is possible either when $P=0$ or when $P=-P+e$. These cases corresponds to $\phi=0$ or $\phi=\pi$, respectively. We thus find that the Zak phase for the 1D crystal with the spatial symmetry of inversion only takes 0 or π. Moreover, the electric polarization is either $P=0$ or $P=\frac{e}{2}$.

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