BERRY PHASES AND WYCKOFF POSITIONS FOR ENERGY BANDS IN SOLIDS*†

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As was shown by Berry [1] the wave function of a time dependent physical system acquires a geometric phase under an adiabatic and cyclic variation. Soon after its discovery, Berry's phase was measured in numerous experiments in different fields of physics [2]. Two ingredients appear in the definition of Berry's phase: adiabaticity and the existence of a parameter space. Thus, in the elementary example of a spin 1/2 particle in a magnetic field $\vec{B}$, one has the following situation: adiabaticity is satisfied when the period T of the $\vec{B}$-rotation is much larger than the period τ of the Zeeman splitting $\tau = \frac{2\pi}{\omega}$ ($h\omega$ is the Zeeman splitting); the parameter space is given by the direction angles of the field $\vec{B}$. In the band structure of solids, adiabaticity is satisfied, when the time dependent perturbation is slow, e.g., when the frequencies corresponding to the relevant energy gaps are much larger than the frequencies in the Fourier transform of the perturbation. Since in solids, the energy bands form a piecewise continuous spectrum, the $\vec{k}$-vector in the Brillouin zone can serve as the parameter space for the definition of Berry's phase [3]. In a periodic solid, $\vec{k}$ is a conserved quantity, and the Bloch function $\psi_{nk}(\vec{r})$ is specified by a band index n and $\vec{k}$. By applying a perturbation one can make $\vec{k}$ vary on a closed path in the Brillouin zone, and $\psi_{nk}(\vec{r})$ will acquire a Berry phase. The latter can assume in general a value between 0 and 2π. However, when the solid possesses some symmetry, Berry's phases can become quantized and they assume discrete values when $\vec{k}$ varies along vectors of the reciprocal lattice $\vec{K}$ [3]

On the other hand, it is well known that energy bands can be generated by using Wannier functions which are defined with respect to discrete centers in the Bravais lattice. These discrete centers are called Wyckoff positions and they are the symmetry centers in the unit cell of the Bravais lattice [4]. The Wyckoff positions are used for labeling band representations of space groups [5,6]. In this talk we show how the Wyckoff positions are connected to Berry phases for energy bands in solids. The discussion is restricted to simple energy bands (in a simple energy band one Bloch function corresponds to each k-vector in the Brillouin zone).

Let G_w be an isotropy group of the Wyckoff position $\vec{w}$. An element $(\gamma/\vec{t})$ of G_w when applied to $\vec{w}$ gives

$$(\gamma/\vec{t})\,\vec{w} = \gamma\vec{w} + t \tag{1}$$

We define a Bravais lattice vector $\vec{R}_w^{(\gamma/t)}$ in such a way that

$$\left(\gamma/\vec{t} - \vec{R}_w^{(\gamma/t)}\right)\vec{w} = \vec{w}\ ,\ \vec{R}_w^{(\gamma/t)} = \gamma\vec{w} + \vec{t} - \vec{w} \tag{2}$$

In the case of a simple band, we have for any element of G_w the following relation [5]

$$(\gamma/\vec{t})\, e^{i\vec{k}\cdot\vec{R}}\, U_n\left(\gamma^{-1}\vec{k}, \vec{q}\right) = D^{(j)}(\gamma)\, U_n\left(\gamma^{-1}k, \vec{q}\right) \tag{3}$$

where $U_n(\vec{k}, \vec{q})$ is the periodic part of the Bloch function $\psi_{nk}(\vec{r})$, $D^{(j)}(\gamma)$ is a one-dimensional representation of the point group of G_w, and where the subscript and superscript of $\vec{R}$ were deleted for simplifying notations.

Berry's phase in solids, for an energy band n and a $\vec{K}$-vector of the reciprocal lattice, is defined in the following way [3]

$$\beta_n(\vec{k}) = \int_{\vec{K}} \vec{X}_{nn}(\vec{k}) \cdot d\vec{k} \tag{4}$$

where the integration is along the $\vec{K}$-vector, and where

$$\vec{X}_{nn}(\vec{k}) = i\,\Omega \int_{u.c.} U_n^*(\vec{k},\vec{q})\,\frac{\partial}{\partial \vec{k}}\,U_n(\vec{k},\vec{q})\,d\vec{q} \tag{5}$$

In Eq. (5), Ω is the volume of the unit cell of the reciprocal lattice, and where the integration is over the unit cell in the Bravais lattice. From Eqs. (3) and (5) we find

$$\vec{X}(k) = -\vec{R} + \frac{\partial \vec{k}'}{\partial \vec{k}}\,\vec{X}(\vec{k}') \tag{6}$$

where $\vec{k}' = \gamma^{-1}\vec{k}$, and where the second term is a diadic product. This means that the i-component of both sides of Eq. (6) can be written as follows

$$X_i(\vec{k}) = -R_i + \frac{\partial \vec{k}'}{\partial k_i} \cdot \vec{X}(\vec{k}') \tag{6a}$$

where now the re is a scalar product on the right-hand side. By using the definition of Berry's phase [Eq. (4)], we find

$$\beta_n(\vec{k}) - \beta_n(\gamma^{-1}\vec{k}) = -\vec{R} \cdot \vec{K} \tag{7}$$

This is the main result of the talk: Eq. (7) gives a connection between Berry's phase on the $\vec{K}$-vector path in the energy band n, and the Bravais lattice vector $\vec{R}$ which according to Eq. (2) can be used for determining the Wyckoff position $\vec{w}$.

As an example, let us consider the space group F222 (#22). The Wyckoff positions corresponding to maximal isotropy groups [3] are as follows [4] (U^x, U^y, U^z are rotations by π around the x, y, and z-axes correspondingly)

$$\begin{aligned}
&\vec{a} = (0, 0, 0);\ G_a:\ E, U^x, U^y, U^z \\
&\vec{b} = \left(0, 0, \frac{c}{2}\right);\ G_b:\ E, (U^x/00c), (U^y/00c), U^z \\
&\vec{c} = \left(\frac{a}{4}, \frac{b}{4}, \frac{c}{4}\right);\ G_c:\ E, \left(U^x/0\,\frac{b}{2}\,\frac{c}{2}\right), \left(U^y/\frac{a}{2}\,0\,\frac{c}{2}\right), \left(U^z/\frac{a}{2}\,\frac{b}{2}\,0\right) \\
&\vec{d} = \left(\frac{a}{4}, \frac{b}{4}, \frac{3c}{4}\right);\ G_d:\ E, \left(U^x/0\,\frac{b}{2}\,\frac{3c}{2}\right), \left(U^y/\frac{a}{2}\,0\,\frac{3c}{2}\right), \left(U^z/\frac{a}{2}\,\frac{b}{2}\,0\right)
\end{aligned} \tag{8}$$

The F222-space group is face-centered orthorhombic with unit vectors of the Bravais lattice

$$\vec{a}_1 = (0, \frac{b}{2}, \frac{c}{2}),\ \vec{a}_2 = (\frac{a}{2}, 0, \frac{c}{2}),\ \vec{a}_3 = (\frac{a}{2}, \frac{b}{2}, 0) \tag{9}$$

and unit vectors of the reciprocal lattice

$$\vec{K}_1 = (-\frac{2\pi}{a}, \frac{2\pi}{b}, \frac{2\pi}{c}),\ \vec{K}_2 = (\frac{2\pi}{a}, -\frac{2\pi}{b}, \frac{2\pi}{c}),\ \vec{K}_3 = (\frac{2\pi}{a}, \frac{2\pi}{b}, -\frac{2\pi}{c}) \tag{10}$$

The band representations for the Wyckoff positions in Eq. (8), all correspond to simple energy bands. Let us apply Eq. (7) to the Wyckoff positions $\vec{a}$ and $\vec{b}$ in Eq. (8). For $\vec{a}$, the $\vec{R}$-vectors [Eq. (2)] are zero for all the symmetry elements. Correspondingly, from Eq. (7), one finds

$$\beta_n^{(a)}(\vec{K}) = \beta_n^{(d)}(\vec{K}) = \beta_n^{(a)}(\vec{K}) = 0 \tag{11}$$

For the $\vec{b}$-Wyckoff position $\vec{R}_b$ is zero for U^z and is -(00c) for U^z and U^y. Formula (7) gives a set of equations for determining the Berry phases of the energy bands that are built on the Wyckoff position $\vec{b}$. We have $\alpha^{-1} = U^x$ or U^y in [Eq. (7)]

$$\begin{aligned} &U^x\,\vec{K}_1 = -(\vec{K}_1 + \vec{K}_2 + \vec{K}_3),\ U^x\,\vec{K}_2 = \vec{K}_3,\ U^x\,\vec{K}_3 = \vec{K}_2 \\ &U^y\,\vec{K}_1 = \vec{K}_3,\ U^y\,\vec{K}_2 = -(\vec{K}_1 + \vec{K}_2 + \vec{K}_3),\ U^y\,\vec{K}_3 = \vec{K}_1 \end{aligned} \tag{12}$$

By using the fact that $\beta_n(-\vec{K}) = -\beta_n(\vec{K})$ we find the following set of equations (we use Eqs. (7), (12) and the value of the $\vec{R}_b$ vector for U^x and U^y [$\vec{R}_b = -(0,0,c)$])

$$2\beta_n^{(b)}(\vec{K}_1) + \beta_n^{(b)}(\vec{K}_2) + \beta_n^{(b)}(\vec{K}_3) = 2\pi$$

$$\beta_n^{(b)}(\vec{K}_2) - \beta_n^{(b)}(\vec{K}_3) = 2\pi$$

$$\beta_n^{(b)}(\vec{K}_1) - \beta_n^{(b)}(\vec{K}_3) = 2\pi$$

The solution of these equations is as follows

$$\beta_n(\vec{K}_1) = \beta_n(\vec{K}_2) = -\beta_n(\vec{K}_3) = \pi \tag{13}$$

In a similar way, one finds the following Berry phases for the Wyckoff positions c and d. We have

$$\begin{aligned} \beta_n^{(c)}(\vec{K}_1) = \beta_n^{(c)}(\vec{K}_2) = \beta_n^{(c)}(\vec{K}_3) = \frac{\pi}{2} \\ \beta_n^{(d)}(\vec{K}_1) = \beta_n^{(d)}(\vec{K}_2) = \beta_n^{(d)}(\vec{K}_3) = -\frac{\pi}{2} \end{aligned} \tag{14}$$

Let us remark that the choice of the group F22 was not accidental. In fact, there is a very special reason for choosing this group, and it is as follows. In one-dimensional crystals, it was proven many years ago [7] that there is a one-to-one correspondence between the Wyckoff positions (these are 0 and a/2, where a is the lattice constant) and the symmetries of the Bloch functions in the Brillouin zone. It turns out that such a one-to-one correspondence is, in general, correct also for simple bands in three-dimensional solids. There are, however, exceptions, and one of them is the F222-group. Thus, it was recently found [6] that the a, b, and c, d Wyckoff positions, in pairs, lead to identical symmetries of Bloch functions in the Brillouin zone. These pairs of Wyckoff positions constitute therefore an example, when Wannier functions around different symmetry centers in the unit cell of the Baravais lattice, lead to identical symmetries for their Bloch functions. It was recently shown [8] that despite of them having identical symmetries, the Bloch functions $\psi_k^{(a)}$ and $\psi_k^{(b)}$ for bands of the type a and b (belonging to Wyckoff positions a and b) cannot be connected by a continuous k-dependent phase factor when the crystal becomes infinite. A similar situation prevails for the Wyckoff positions c and d. What this means is that topologically the bands of type a and b are different (also c

and d). In this talk we show that the bands, a and b (also c and d) have also different Berry phases [Eqs. (11), (13), and (14)].

The discussion in this talk was restricted to simple bands. The latter correspond to a single Wyckoff position. In general, for composite energy bands, there is a star of Wyckoff positions that appear in their definition via band representations [5]. Little is known about the topology of composite bands, and it should be of much interest to connect their Wyckoff positions and Berry phases.

References

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