Berry's Phase for Energy Bands in Solids

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Berry's phase is defined for the dynamics of electrons in periodic solids and an explicit formula is derived for it. Because of the special torus topology of the Brillouin zone a nonzero Berry phase is shown to exist in a one-dimensional parameter space. Symmetry of the Bloch functions in the Brillouin zone leads to the quantization of Berry's phase. A connection is established between the latter and the Wyckoff positions in the crystal in the framework of band representations of space groups. Berry's phase can therefore be used for labeling energy bands in solids.

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The concept of Berry's phase[1] has recently caused a great deal of interest in a variety of fields in physics. Thus, in the last two years experiments have been carried out for measuring this phase in neutron spin rotation,[2] in nuclear quadrupole resonance,[3] in rotation of polarized light,[4] in fractional quantization of orbital quasirotation of molecules,[5] and in electronic states of Jahn-Teller systems.[6] In addition, a considerable number of theoretical papers have been published dealing with both quantum[7] and classical[8] aspects of the problem. It seems, however, that one important and natural system for the appearance of Berry's phase was left out. We have in mind the motion of an electron in a periodic solid. That such a system should be of interest can be seen in the following way.

In solids the energy spectrum has a band structure, e.g., it is piecewise continuous. The energy in each continuous piece depends on the Bloch quasimomentum $\mathbf{k}$, which varies in the Brillouin zone. What is most characteristic for the concept of Berry's phase is the existence of a continuous parameter space in which the state of the system can travel on a closed path. Such a parameter space exists naturally in the band structure of solids. This parameter space is the Brillouin zone which is a torus, and in which the Bloch $\mathbf{k}$ vector is used for describing an energy band.[9] In a periodic solid $\mathbf{k}$ is a conserved quantity and the Bloch function $\psi_{nk}(\mathbf{r})$ is specified by a band index n and $\mathbf{k}$. If by applying a perturbation to the solid one can make $\mathbf{k}$ vary on a closed path in the Brillouin zone, then $\psi_{nk}(\mathbf{r})$ should, in general, pick up a Berry phase. Since the Brillouin zone is a torus, one can vary $\mathbf{k}$ in a given direction and when the edge of the zone is reached the path closes automatically. This is best seen in a one-dimensional solid where the Brillouin zone is the interval $[-\pi/a,\pi/a]$ with the end points $-\pi/a$ and π/a identified (a is the lattice constant). In the particular case of a one-dimensional crystal, when k is made to vary in the whole Brillouin zone, the Bloch functions $\psi_{nk}(x)$ correspond to the whole energy band. One should therefore expect that when k sweeps the interval $[-\pi/a,\pi/a]$, the Bloch function $\psi_{nk}(x)$ will pick up a Berry phase. This is a very amazing situation because in a one-dimensional crystal $\psi_{nk}(x)$ can be chosen to be periodic in k with the period $2\pi/a$ of the reciprocal lattice. Nevertheless, because of the torus topology of the Brillouin zone a Berry phase is picked up when k is forced to vary by an external perturbation through the entire zone. In solids the continuous parameter space is therefore already built in as a part of the unperturbed problem. What the perturbation does is that it makes k vary in this parameter space (the Brillouin zone). It should be pointed out that in all the above-mentioned physical systems for the observation of the Berry phase the parameter space is multidimensional.[1–8] Because of this very unique situation in the Bloch dynamics of solids, we shall concentrate in what follows on one-dimensional crystals. Keeping in mind that an entire energy band corresponds to the variation of k in the Brillouin zone $[-\pi/a,\pi/a]$, one is to expect that the Berry phase which is picked up by $\psi_{nk}(x)$ in such a variation process should have to do with some characteristic feature of the energy band as a whole entity. Such a characteristic feature is known to exist in the framework of band representations of space groups[10] and it is described by the band-center operator.[11] The eigenvalues of the latter correspond to the Wyckoff positions in the solid. A connection should therefore be anticipated between the Berry phase and the band center in the dynamics of electrons in solids. This is shown in what follows.

In this Letter I derive a formula for the Berry phase for an electron in a periodic potential (one dimension) in the presence of an externally applied time-dependent vector potential $A(t)$. The formula turns out to coincide with the expression for the band center in the framework of the band representations of space groups.[10,11] When the linear chain has no symmetry, the Berry phase can assume any value. However, when inversion symmetry is present, Berry's phase becomes quantized, and it can assume only the values 0 and π (modulo 2π). For three-dimensional solids, the Brillouin zone is a three-dimensional torus and one expects to obtain a nonvanishing

Berry phase for any closed path in the Brillouin zone. When symmetry is present one can make **k** vary through the entire Brillouin zone in a given symmetry direction. As a consequence of symmetry in the Brillouin zone (parameter space) Berry's phase turns out to be quantized and it assumes well defined discrete values that correspond to the Wyckoff positions in the crystal.[12] Our conclusion is that Berry's phase can therefore be utilized for specifying entire bands in solids, in very much the same way as the band center is used in the framework of band representations of space groups.

Consider a Bloch electron in one dimension under the influence of a time-dependent vector potential $A(t)$. The Schrödinger equation for this problem is

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{1}{2m}\left(p-\frac{e}{c}A(t)\right)^2+V(x)\right]\psi, \quad (1)$$

where $V(x+a)=V(x)$. At this stage there is no need to specify the source of the potential $A(t)$. However, the assumption will be made that $A(t)$ is time dependent only and that the variation of $A(t)$ with time is adiabatic [the frequencies corresponding to the relevant gaps in the energy spectrum of the solid are much larger than the frequencies in the Fourier expansion of $A(t)$]. Having defined the problem, one could directly use Berry's closed formula[1] for the dynamics of electrons in solids. However, it is instructive to rederive it again because, unlike in Ref. 1, the spectrum of Eq. (1) is bandlike (quasicontinuum), and the parameter space is one dimensional. Following the adiabatic approximation one is to solve the equation

$$\left[\frac{1}{2m}\left(p-\frac{e}{c}A(t)\right)^2+V(x)\right]\psi_{nt}(x)=\epsilon_n(t)\psi_{nt}(x), \quad (2)$$

where n labels the energy band and $\epsilon_n(t)$ is the energy function (its meaning is given below). Equations (1) and (2) are well known in the literature of a Bloch electron in an electric field,[13,14] and one can seek a solution of Eq. (2) in the form

$$\psi_{nt}(x)=\exp(ikx)u_{nk(t)}(x), \quad (3)$$

where k is the quasimomentum [in $\exp(ikx)$ it is time independent, while in the function u, $k(t)=k-(e/c\hbar)\times A(t)$] and $u_{nk}(x)$ is the periodic part of the Bloch function. It satisfies the equation

$$\left[\frac{1}{2m}\left(p+\hbar k-\frac{e}{c}A(t)\right)^2+V(x)\right]u_{nk(t)}=\epsilon_n(k(t))u_{nk(t)}, \quad (4)$$

where k in the Hamiltonian is time independent, and where $\epsilon_n(t)$ of Eq. (2) is now written as $\epsilon_n(k(t))$ [$\epsilon_n(k)$ is the energy spectrum for the band n]. With these notations, it now follows that the solution of Eq. (1) can be given the adiabatic form[1,13]

$$\psi(x,t)=\exp\left[i\gamma_n(t)-\frac{i}{\hbar}\int_0^t\epsilon_n(k(t'))dt'\right]\psi_{nt}, \quad (5)$$

where $\gamma_n(t)$ is a time-dependent phase for the energy band n. By substituting this solution into Schrödinger's equation [Eq. (1)] and by using Eqs. (2) and (4), one finds [$u_{nk}(x)$ is normalized as $(2\pi/a)\int_0^a|u_{nk}(x)|^2dx=1$] for Berry's phase γ_n the expression

$$\left[\dot{\gamma}_n(t)=i\int_0^a u^*_{nk(t)}(x)\frac{\partial}{\partial t}u_{nk(t)}(x)dx\right],$$

$$\gamma_n=\int_{-\pi/a}^{\pi/a}X_{nn}(k)dk, \quad (6)$$

where the quantity $X_{nn}(k)$ is widely used in the band theory of solids and is given by[11,14]

$$X_{nn}(k)=\frac{2\pi}{a}\int_0^a u^*_{nk}(x)i\frac{\partial u_{nk}(x)}{\partial k}dx. \quad (7)$$

It is clear that the result for γ_n [Eq. (6)] is obtained when k is made to vary over the whole Brillouin zone $[-\pi/a,\pi/a]$ by the external perturbation $A(t)$. Here the following remark is appropriate. Originally, Berry's phase was defined for a system with a cyclic Hamiltonian $H(t+T)=H(t)$, where T is the period of the cycle. Our Hamiltonian does not satisfy this cyclic condition. However, for k to vary over the Brillouin zone, $A(t)$ has to change by $2\pi/a$ [see Eq. (4)]. In the Bloch problem such a change of k in Eq. (4) should be considered cyclic because this is a gauge change which is compensated by the fact that $u_{nk+2\pi/a}(x)=\exp(-i2\pi x/a)u_{nk}(x)$. The Bloch problem is therefore a generalization of the Berry phase to a noncyclic change of the Hamiltonian, up to a gauge transformation. We would like to point out that the result for Berry's phase [relation (6)] is gauge invariant. As an example, consider the constant electric field E, when $A=-cE$. Then by a gauge transformation $\exp[-(1/\hbar)eExt]$, the Hamiltonian in Eq. (1) will become $(1/2m)p^2+V(x)-eEx$. A corresponding change will appear in Eq. (4). We can still seek the solution in the form of Eqs. (3) and (5) but now k is time dependent in $\exp(ikx)$ of Eq. (3). By using the acceleration theorem $\hbar\dot{k}=-eE$ one recovers the result (6) for Berry's phase. Formula (6) coincides in form with the original expression of Berry.[1] The novel feature of this formula is in the fact that we have here, for the first time, the appearance of Berry's phase for a one-dimensional parameter space in a purely quantum-mechanical system (the Bloch problem has no analog for a particle in classical mechanics). It will soon be shown that γ_n is, in general, nonzero.

By using the periodicity properties of $u_{nk}(x)$ it follows that $X_{nn}(k)$ [Eq. (7)] is periodic in k with the period $2\pi/a$ (the constant of the reciprocal lattice). It also follows from Eq. (7) that $X_{nn}(k)$ is phase dependent;

e.g., when $u_{nk} \rightarrow \bar{u}_{nk} = \exp(i\phi)u_{nk}$, $X_{nn}(k) \rightarrow \bar{X}_{nn}(k) = X_{nn}(k) - \partial\phi/\partial k$. Since the general form for ϕ is $mka + \alpha(k)$, where m is an integer and $\alpha(k)$ is a periodic function, the phase γ_n in Eq. (6) changes by $-2\pi m$ under such a general phase transformation. This means that $\exp(i\gamma_n)$ [in Eq. (5) for the wave function] is invariant under any phase transformation and it is therefore a well defined quantity for each energy band.

By using the Wannier function $a_n(x)$ for the band n, an alternative expression can be derived for γ_n. Thus, with the help of the relation between $u_{nk}(x)$ and $a_n(x)$, which is[15]

$$\exp(ikx)u_{nk}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \sum_m \exp(ikma)a_n(x - ma) , \quad (8)$$

γ_n assumes the form [Eqs. (6)–(8)]

$$\gamma_n = \int_{-\pi/a}^{\pi/a} X_{nn}(k)dk = \left(\frac{a}{2\pi}\right)^{-1} \int_{-\infty}^{\infty} x\,|a_n(x)|^2 dx . \quad (9)$$

Formula (9) gives Berry's phase for the nth energy band expressed either via the Bloch function $u_{nk}(x)$ or the Wannier function $a_n(x)$ of this particular band.

Let us now connect the result in Eq. (9) to the band center[11] and the Wyckoff position[12] of the energy band. In Ref. 11 the band center for the energy band n was defined by the following formula [Eq. (5) of Ref. 11]:

$$q_n = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} X_{nn}(k)dk = \int_{-\infty}^{\infty} x\,|a_n(x)|^2 dx . \quad (10)$$

By comparing q_n with γ_n we see that the following connection holds:

$$\gamma_n = (2\pi/a)q_n . \quad (11)$$

When there is no symmetry in the one-dimensional chain, q_n as well as γ_n can assume any value as a function of the band index n. However, when inversion symmetry is present, it follows from the symmetry of the Wannier functions[11] that q_n can assume two values only, $q_n = 0$ or $a/2$. This follows from the following argument. When the crystal possesses inversion symmetry, the phase of the Bloch function can always be chosen in such a way as to make the Wannier function even or odd around either of the two centers[16] $x = 0$ or $a/2$. Thus, assume that $a_n(-x) = \pm a_n(x)$, it then follows that $q_n = 0$ [see Eq. (10)]. In the other case, when $a_n(-x + a) = \pm a_n(x)$ (inversion around $a/2$), then it follows from Eq. (10) that $q_n = a/2$. 0 and $a/2$ are also the Wyckoff positions of the one-dimensional crystal. From Eq. (11) it follows that Berry's phase for a one-dimensional crystal with inversion symmetry can be 0 or π only. Equation (11) establishes therefore a connection between Berry's phase, the band center, and the Wyckoff position.

Having established the connection between Berry's phase and the label of an energy band as a whole entity, let us now come back to the question of the specification of the vector potential $A(t)$ in Schrödinger's equation [Eq. (1)]. It was required that $A(t)$ changes adiabatically and that it makes k vary over the entire Brillouin zone. This requirement is not very restrictive and is practically met by any homogeneous external electric field E whose frequency is much smaller than the relevant band gaps.[17] Such an electric field is derived from the following vector potential: $A(t) = -c\int_0^t E(t')\times dt'$. The variation of k with time is then given by the relation[9] $\hbar\dot{k} = -eE(t)$ which holds also for a time-dependent adiabatically varying electric field. A particular case is the constant electric field which has been widely investigated in connection with the Wannier-Stark ladder problem.[18] It is of interest to point out that the Wannier-Stark spectrum contains the band center q_n [Eq. (10)] explicitly.[16] Since γ_n is connected to q_n, this establishes a connection of Berry's phase to the well known Wannier-Stark ladder problem in solids.[19] Bearing in mind that different energy bands, say n and n', have, in general, different γ's (when symmetry is present γ assumes the values 0 and π only), electrons in these two bands will pick up different Berry phases in the presence of an electric field. In principle, any interference experiment with electrons from two such energy bands should enable one to measure the phase difference between γ_n and $\gamma_{n'}$. This is so very much in principle, because one has to make sure that the phase is fully controlled by the electric field and that scattering by imperfections can be neglected. As is well known this is not a simple problem.[18]

The generalization of the results to three-dimensional crystals is straightforward conceptually, but technically the problem becomes much more involved because of the energy-band topology in three dimensions.[10,20] No attempt will be made here to go into any details, but one should point out that the Berry's phase in the framework of energy bands in three-dimensional crystals is a very exciting and rich subject. In particular, the whole band-labeling problem will assume the geometrical form of topological invariants.

In conclusion, we have shown how to define Berry's phase in the dynamics of electrons in solids. There are a number of unique features that appear in this problem. First, the parameter space is furnished by the system itself, namely, the Brillouin zone of the solid. This is unlike the other physical examples of the appearance of Berry's phase[1-8] where the parameter space is introduced externally, e.g., the parameters of the magnetic field,[2,3] the optical fiber parameters,[4] etc. In the case of the solid the parameter space (the Brillouin zone) exists naturally and what the external field does is to change the Bloch quasimomentum $\mathbf{k}$ inside this space. Second, the Brillouin zone is a torus and this is why even in a one-dimensional parameter space a nonvanishing Berry phase can appear. Third, the Bloch states possess symmetry properties in the Brillouin zone (parameter space), and, as a consequence of this symmetry, Berry's phase

becomes quantized. Finally, we would like to comment on the possible significance of Berry's phase in solids. We have already mentioned the Stark ladder where Berry's phase γ_n appears explicitly in the energy spectrum. Thus, when $\gamma_n=\pi$, $q_n=a/2$ [see Eq. (11)] and the Wannier-Stark ladders is half integer. This is reminiscent of the influence of Berry's phase on the molecular spectrum, where it leads to fractional quantization of the angular momentum.[5] In three-dimensional crystals, because of the torus topology of the Brillouin zone, there are, in general, nonvanishing Berry phases along any path that covers a vector of the reciprocal lattice. This by itself contains a very rich structure of Berry phases which should lead to a better understanding of the topology of energy bands. In addition, one can also define Berry's phase on closed circuits in the Brillouin zone. As will be shown in a separate publication[21] if a perturbation in the solid makes $\mathbf{k}$ vary on a closed orbit (the impurity problem or the dynamics in a magnetic field), then the Berry phase assumes the form

$$\gamma_n(C)=\oint_C \mathbf{X}_{nn}(\mathbf{k})\cdot d\mathbf{k}\,, \tag{12}$$

where C is the path of integration and $\mathbf{X}_{nn}(\mathbf{k})$ is a three-dimensional generalization of Eq. (7). As was proven by Berry,[1] $\gamma_n(C)$ is nonvanishing when the integration path lies in the vicinity of a point of degeneracy. This is very often the case in the valence and conduction bands of semiconductors.[22] We expect therefore Berry's topological phase to play an important role in the whole dynamics of Bloch electrons in solids.

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