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Berry's phase for an electron in a periodic potential without inversion symmetry

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Abstract. Berry's phase is calculated for an electron in a simple one-dimensional solid. The model used is a generalized Kronig-Penney potential, parameterized so that it may or may not have inversion symmetry. It is shown that the Berry's phase as a function of an asymmetry parameter evolves from a linear to a non-linear form as inversion symmetry is broken. The functional form of the Berry's phase is seen to be band-dependent in a simple way, suggesting that it can be used to identify the band in question.

PACS. 03.65.Vf Phases: geometric; dynamic or topological – 71.20.-b Electron density of states and band structure of crystalline solids – 71.15.-m Methods of electronic structure calculations

Berry's phase (BP) plays an important role in a variety of seemingly dissimilar areas of physics [1–3] including optics [4], molecular physics [5], and spin-wave dynamics in crystals [6,7]. An understanding of the BP was crucial in developing a complete theory of electric polarization in dielectrics [8,9], and it has been shown that the presence of a BP modifies the semiclassical equations of motion for Bloch electrons [10]. The connection between Thomas precession and the spin-orbit interaction is best understood as a manifestation of the BP [11]. Even the Aharonov-Bohm effect [12] — a phenomenon that has been understood for over forty years — receives its most elegant treatment when considered in the light of BP theory. Hence the search continues for physical systems in which the existence of a BP significantly alters the (traditional) physics in question or clarifies its interpretation. Such research is of course helped by investigations into existence criteria [13], in an effort to understand the kind of systems in which a BP is likely to be manifest.

Typically the BP is defined as a phase shift in a system's state vector $|\psi(\xi)\rangle$ that appears after the system has traced a closed loop in the space of some parameter ξ. The key feature of this definition is that the BP does not depend upon the choice of phase of $|\psi(\xi)\rangle$ at each ξ value; it depends solely upon the geometry of the ξ–space and the path taken in that space, and is therefore potentially observable. This space often describes some parameters appearing in the Hamiltonian, but this is not required. For example, the Bloch wave function $\psi_{n\mathbf{k}}(\mathbf{x})$ describing an electron in a periodic potential is a function of the wave vector $\mathbf{k}$, which does not appear in the Hamiltonian. However, $\mathbf{k}$ is a parameter in the pseudo-Hamiltonian that appears in the Schrödinger-like equation for the periodic part of the Bloch function [14],

$$\tilde{H}_{\mathbf{k}} u_{n\mathbf{k}}(\mathbf{x}) = \left[\frac{-\hbar^2}{2m}(\nabla + i\mathbf{k})^2 + V(\mathbf{x})\right] u_{n\mathbf{k}}(\mathbf{x}) = \varepsilon_{n\mathbf{k}} u_{n\mathbf{k}}(\mathbf{x}), \quad (1)$$

where $u_{n\mathbf{k}}(\mathbf{x}) = \exp(-i\mathbf{k}\cdot\mathbf{x})\psi_{n\mathbf{k}}(\mathbf{x})$ is the periodic part of the Bloch function, and n is the band index. In this case the BP is calculated from the function $u_{n\mathbf{k}}(\mathbf{x})$ [15].

For an electron in a periodic one-dimensional solid, the situation is particularly simple. The parameter k is now a scalar, and a straightforward discretization of k-space [9] allows us to find the BP for band n as

$$\gamma_n = -\mathrm{Im}\ln\prod_{i=1}^{N-1}\Big\langle u(n,k_i) \mid u(n,k_{i+1})\Big\rangle, \quad (2)$$

where the space integral implied by the inner product is over the unit cell. The k's span the Brillouin zone (i.e. $k_1 = -\pi/\alpha$ and $k_N = +\pi/\alpha$, where α is the lattice constant), and therefore they go through a closed loop because of the torus topology of the Brillouin zone. When the periodic part of the Bloch function is normalized as $\Big\langle u(n,k) \mid u(n,k)\Big\rangle = \alpha/(2\pi)$ then the continuum limit of equation (2) gives [15]

$$\gamma_n = \frac{2\pi}{\alpha}\int_{B.Z.} i\left\langle u(n,k)\,\middle|\,\frac{\partial}{\partial k}u(n,k)\right\rangle dk. \quad (3)$$

Because k is made to vary across the Brillouin zone, a BP appears in the periodic part of the Bloch function.

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The value of the BP that appears depends upon the symmetry of the lattice in question; for models with inversion symmetry the BP is usually found to be either 0 or π [15]. (In the literature such BP values are often referred to as "trivial".) Note, however, that for Bloch systems obeying equation (1) the BP depends upon the choice of origin [16]. Thus seemingly non-trivial BP's can "unexpectedly" arise in inversion-symmetric models when the origin is not a center of inversion symmetry. In such cases (e.g. the model described below) the BP can still be classified as "trivial" because there is *some* choice of origin that produces a constant value for the BP.

Consider the well-known Kronig-Penney model [17] that is defined by the one-dimensional potential

$$V(x) = \sum_{m=-\infty}^{\infty} V_0 \delta(x - m\alpha), \tag{4}$$

with m running through the integers. V_0 is the strength of the delta functions. This model has an infinite number of points of inversion symmetry, and so is an inappropriate choice for a model designed to exhibit BP effects. Thus to force asymmetry we superimpose two potentials of the above form. For an electron in such a system the Schrödinger equation is

$$\left\{ \frac{-\hbar^2}{2M}\frac{d^2}{dx^2} + \sum_{m=-\infty}^{\infty} [V_1 \delta(x - m\alpha) + V_2 \delta(x - m\alpha - \beta)] \right\} \psi(x) = E\psi(x). \tag{5}$$

Again, m is an integer, α is the lattice constant (i.e. the distance between V_1 peaks), and β is the distance between a V_1 peak and the next V_2 peak to the right. We assume $V_1 > 0$ and $V_2 > 0$ so that there are no $E < 0$ solutions. It is clear that if $\alpha \neq 0$, $\beta \neq 0$, $\beta \neq \alpha$ and $\beta \neq \alpha/2$, then the model consists of a series of delta functions spaced such that *no* points of inversion symmetry exist. Models of this type have been studied before, but not in the context of the Berry's phase [18–20].

We rewrite equation (5) using dimensionless variables, including a coordinate,

$$y \equiv \frac{x}{\alpha}, \tag{6}$$

a "wave vector",

$$q \equiv \sqrt{\frac{2ME\alpha^2}{\hbar^2}}, \tag{7}$$

and "weight factors" that correspond to the strengths V_1 and V_2:

$$g_1 \equiv \frac{2MV_1\alpha}{\hbar^2}, g_2 \equiv \frac{2MV_2\alpha}{\hbar^2}. \tag{8}$$

(Since we have already assumed that V_1 and V_2 are positive, we have $g_1, g_2 > 0$.) We also define the relative position of the delta peaks as $\ell \equiv \beta/\alpha$; the lattice constant is then 1 and the V_2 peak is located at the position $y = \ell$. (See Fig 1.) Of course if $\ell = 0, \ell = 1/2$, or $\ell = 1$, then inversion symmetry is regained. If $g_1 = g_2$, then there is inversion symmetry no matter what ℓ is. The "asymmetry parameter" ℓ is therefore a measure of how far the model deviates from inversion symmetry.

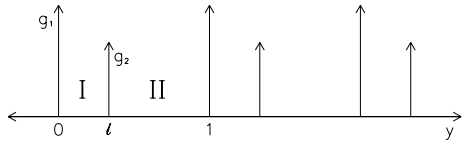

Fig. 1. Generalized Kronig-Penney potential: The dimensionless parameter ℓ determines the location of the g_2 peak within the unit cell, and divides the cell into two regions. Note that the heights of g_1 and g_2 in this figure are schematic only, and represent the "strength" of the delta peaks.

With these definitions, the final form of our Schrödinger equation is

$$\left\{ \frac{d^2}{dy^2} + q^2 - \sum_m [g_1 \delta(y - m) + g_2 \delta(y - m - \ell)] \right\} \psi(y) = 0. \tag{9}$$

In general, when $g_1 \neq 0, g_2 \neq 0$, we have solutions of the form

$$\psi(y) = \begin{cases} Ae^{iqy} + Be^{-iqy}, & 0 \leq y < \ell, \\ Ce^{iqy} + De^{-iqy}, & \ell \leq y < 1. \end{cases} \tag{10}$$

The coefficients A, B, C, and D can be found in several different ways [21]. Following the traditional approach, we join the solutions continuously at both $y = 0$ and $y = \ell$ and use the Bloch periodicity condition, which yields

$$A + B = e^{-ik}\left(Ce^{iq} + De^{-iq}\right), \tag{11}$$

$$Ae^{iq\ell} + Be^{-iq\ell} = Ce^{iq\ell} + De^{-iq\ell}. \tag{12}$$

Two other conditions are achieved by integrating the Schrödinger equation, equation (9), from $-\varepsilon$ to ε and then taking the limit as ε approaches zero:

$$iq\left(A - B - Ce^{i(q-k)} + De^{-i(q+k)}\right) = g_1\left(A + B\right), \tag{13}$$

$$iq\left(Ce^{iq\ell} - De^{-iq\ell} - Ae^{iq\ell} + Be^{-iq\ell}\right) = g_2\left(Ce^{iq\ell} + De^{-iq\ell}\right). \tag{14}$$

The requirement that the determinant of the coefficients of equations (11–14) vanishes yields the dispersion relation

$$\cos k = \cos q + \frac{(g_1 + g_2)}{2}\left(\frac{\sin q}{q}\right) - \frac{g_1 g_2}{2}\left(\frac{\sin q\ell}{q}\right)\left(\frac{\sin(q\ell - q)}{q}\right). \tag{15}$$

Figure 2 shows that this dispersion relation is qualitatively no different from that of the traditional Kronig-Penney model [17], and in fact the relations share some quantitative features as well. In both cases the bands alternate between two distinct types. Odd-indexed bands are concave up at the zone center and the values at the Brillouin

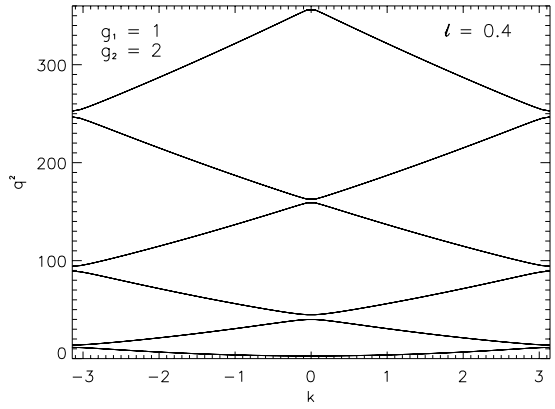

Fig. 2. The dispersion relation q^2 vs. k in the reduced-zone scheme for the first six bands. The qualitative features of the relation do not depend upon the values of g_1, g_2 or ℓ.

zone edge are "pinned", meaning that q (at $k = \pm\pi$) is an odd (fixed) multiple of π. Changing g_1 and/or g_2 does not affect these zone-edge q-values. Even-indexed bands are concave down at the zone center, and the q-values (at $k = 0$) are pinned at even multiples of π. In every case (n even or odd) the q-values are restricted to a particular range,

$$(n-1)\,\pi \leq q \leq n\pi, \tag{16}$$

which can be used to identify the band in question. For particular values of g_1 and g_2 the shape of the dispersion relation is extremely insensitive to the value of ℓ.

Returning to equations (11–14), we fix the phase by choosing $D = 1$; the other three coefficients are then found to be

$$A = \frac{Ce^{iq\ell} - Ce^{i(q-k)}e^{-iq\ell} + e^{-iq\ell} - e^{-i(q+k)}e^{-iq\ell}}{e^{iq\ell} - e^{-iq\ell}}, \tag{17}$$

$$B = \frac{-Ce^{iq\ell} + Ce^{i(q-k)}e^{iq\ell} - e^{-iq\ell} + e^{-i(q+k)}e^{iq\ell}}{e^{iq\ell} - e^{-iq\ell}}, \tag{18}$$

$$C = \frac{-e^{-iq\ell}e^{ik} + e^{-iq(\ell+1)} + \frac{g_1}{q}e^{-iq}\sin q\ell}{e^{iq\ell}e^{ik} - e^{iq(\ell+1)} - \frac{g_1}{q}e^{iq}\sin q\ell}. \tag{19}$$

(Note that A, B, and C depend upon both g_1 and g_2 through the dispersion relation.) This result can be obtained by at least two different methods [21,22] and is consistent with previous results [18]. (If we had allowed either V_1 or V_2 to be negative, then E could be negative, and the trigonometric functions containing q's would be replaced by hyperbolic functions.)

In order to calculate the BP for this model system, we first explicitly construct the periodic part of the Bloch function, giving

$$u(y) = \begin{cases} Ae^{i(q-k)y} + Be^{-i(q+k)y}, & 0 \leq y < \ell, \\ Ce^{i(q-k)y} + e^{-i(q+k)y}, & \ell \leq y < 1, \end{cases} \tag{20}$$

where we have now suppressed the band index. Either equation (2) or (3) can be used to calculate the BP. For systems such as ours, equation (2) is the better choice, since it has the distinct advantage of *not* depending upon the normalization of u_k. This can be shown as follows. Each inner product in equation (2) is a complex number of the form

$$|\langle u_i \mid u_{i+1}\rangle| \exp\left(i\phi_{i,i+1}\right), \tag{21}$$

where the normalization information about u_k is contained within the modulus. (We have now written $u_i \equiv u\left(k_i\right)$ for brevity.) Equation (2) then becomes

$$\gamma = -\mathrm{Im}\ln\left(|\langle u_1 \mid u_2\rangle|\,|\langle u_2 \mid u_3\rangle|\cdots|\langle u_{N-1} \mid u_N\rangle| \prod_{i=1}^{N}\exp\left(i\phi_{i,i+1}\right)\right) \tag{22}$$

$$= -\mathrm{Im}\left[\ln\left(|\langle u_1 \mid u_2\rangle|\,|\langle u_2 \mid u_3\rangle|\cdots|\langle u_{N-1} \mid u_N\rangle|\right) + \ln\exp\left(i\sum_{i=1}^{N}\phi_{i,i+1}\right)\right] \tag{23}$$

$$= -\sum_{i=1}^{N}\phi_{i,i+1}, \tag{24}$$

independent of the normalization.

From the above analysis it is clear that equation (2) is equivalent to

$$\gamma = -\sum_i \arctan\left(\frac{\mathrm{Im}\,\langle u\left(k_i\right) \mid u\left(k_{i+1}\right)\rangle}{\mathrm{Re}\,\langle u\left(k_i\right) \mid u\left(k_{i+1}\right)\rangle}\right), \tag{25}$$

which is more suited for numerical calculations. The above inner product can be written explicitly as

$$\langle u\left(k_i\right) \mid u\left(k_{i+1}\right)\rangle = \int_0^{\ell} dy\, u_I^*\left(k_i\right) u_I\left(k_{i+1}\right) + \int_{\ell}^{1} dy\, u_{II}^*\left(k_i\right) u_{II}\left(k_{i+1}\right), \tag{26}$$

where the subscripts $I$and II refer to the regions $0 \leq y < \ell$ and $\ell \leq y < 1$, respectively. These integrals can be determined analytically, so that our numerical work is limited only to evaluation of the dispersion relation and the calculation of the arctangent function. Note that the discretization of k requires k_i and k_{i+1} to be sufficiently close; in our work it suffices to partition the BZ into 40 k-values in the interval $-\pi \leq k < \pi$, in the sense that including more k-values does not lead to any noticeable change in our results.

We now comment on the observation [15] that the BP is either 0 or π (modulo 2π) for models with inversion symmetry. This is actually true only when the origin of the model coincides with a center of inversion symmetry of the crystal. This can be seen from the following analysis. Traditional inversion symmetry arguments hinge upon the observation that the BP is related to the Wannier function [23] $w_n\left(y\right)$ for band n through the relation [15]

$$\gamma_n = 2\pi \int_{-\infty}^{\infty} dy\; y\;\left|w_n\left(y\right)\right|^2. \tag{27}$$

When there is a center of inversion symmetry at either $y = 0$ or $y = 1/2$ (for a unit cell of size 1), then the even/odd properties of Wannier functions [24–26] guarantee that the BP vanishes or equals a constant value [15]. However, if neither $y = 0$ or $y = 1/2$ is a center of inversion symmetry then the situation is more complicated. In our model, for example, with $g_1 = g_2$ and $\ell \neq 1/2$ there are centers of inversion symmetry at $\ell/2$ and $\ell/2 + 1/2$. If the Wannier function is centered at $\ell/2$, then one can write

$$\gamma_n = 2\pi \int_{-\infty}^{\infty} dy \left(\frac{\ell}{2} + \left[y - \frac{\ell}{2} \right] \right) |w_n(y)|^2 = \pi\ell, \qquad (28)$$

because of the normalization and symmetry properties of the Wannier function. In the second case, with the Wannier function centered at $\ell/2 + 1/2$, a similar calculation gives $\gamma_n = \pi(1 + \ell)$. This shows that the BP, instead of being constant, acquires a linear dependence on the parameter ℓ. This dependence of the BP on the choice of origin for Bloch electrons was pointed out in reference [16] and is analogous to the origin dependence of angular momentum, for example.

Such origin-dependence is also seen in the theory of polarization of dielectrics [8], in which the polarization $\mathbf{P}^{(\lambda)}$ (as a function of a parameter λ) has the "Berry's phase" form

$$\mathbf{P}^{(\lambda)} \propto \sum_{bands} \int d\mathbf{r}\, \mathbf{r} \left| W_n^{(\lambda)}(\mathbf{r}) \right|^2, \qquad (29)$$

which has the same integral as equation (27). As in our equation (27), $\mathbf{P}^{(\lambda)}$ depends on the choice of origin, but the quantity $\Delta\mathbf{P} = \mathbf{P}^{(\lambda_2)} - \mathbf{P}^{(\lambda_1)}$ is origin-independent. The origin dependence of γ_n in our system is completely analogous to this $\mathbf{P}^{(\lambda)}$ situation. The Berry's phase itself is not observable because of its origin dependence, but changes in it are observable and are useful characterizations of system properties.

Using the approach described above, we have calculated the BP for different bands and for different values of g_1 and g_2. Our main goal has been to observe how the BP changes with differing ℓ values since this parameter controls how far the model is from inversion symmetry when $g_1 \neq g_2$. We first note that when either g_1 or g_2 is equal to zero (for any band n) we get anticipated values for the BP. Specifically, when $g_2 = 0$, the BP is just the constant π, as one would expect—the origin (upon which the g_1 peak sits) then corresponds to a center of inversion symmetry. For the other "trivial" case (when $g_1 = 0$) the BP is seen to vary linearly from π to 2π as ℓ varies from 0 to 1. This is because there are centers of inversion symmetry at ℓ and $\ell + 1/2$, but not at the origin.

Things become more interesting when both g_1 and g_2 are non-zero. In particular, as g_1 and g_2 approach each other we see a non-linear (non-trivial) relationship evolving continuously into a linear one. Figures 3 and 4 show typical cases: we have plotted γ (the BP) as a function of the parameter ℓ, for the bands $n = 1$ and $n = 7$. Here g_1 is fixed at a value of 5 while g_2 varies from 0 up to 5. The BP is seen to go from a constant π at $g_2 = 0$, through a variety of vaguely sinusoidal forms until finally reaching the limiting case of two linear functions at $g_2 = 5$: one running from 0 to π, the other from π to 2π. The straight lines have slope π, in agreement with equation (28). Note that the function jumps back and forth between one line, $\gamma = \pi\ell$, and another line, $\gamma = \pi(1 + \ell)$, corresponding to shifts in the location of the Wannier function (either $y = \ell/2$ or $y = \ell/2 + 1/2$). It is thus possible to determine the location of the Wannier function by determining the BP.

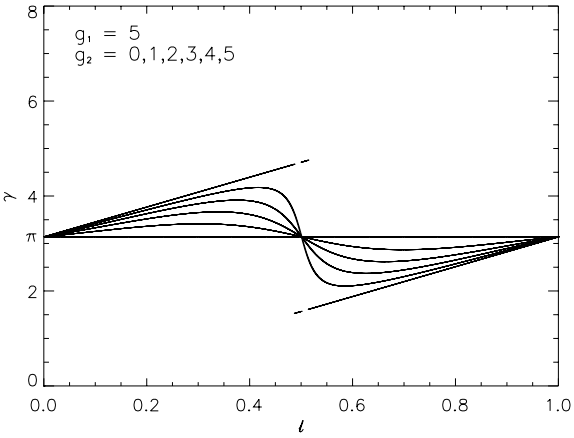

Fig. 3. Berry's phase γ vs. ℓ for fixed g_1 and variable g_2, in the first band ($n = 1$). The $g_2 = 0$ case is the straight line at $\gamma = \pi$; the $g_2 = 5$ case is the pair of lines with slope π. The gaps in these lines near $\ell = 1/2$ are real features of the graph, and indicate jumps in the location of the Wannier function.

These observations are representative of our data in general. In all cases the evolution of the functions is continuous, and the centers of inversion symmetry for various g values determine the limiting cases. In addition, $\ell = 1/2$ always gives a BP value of 0 or π.

We note that in Figures 3 and 4 the number of local minima of the functions (i.e. 1 or 7) is exactly the band number. Indeed, this relation holds for any band we choose. Figure 5 shows an $n = 32$ case very close to inversion symmetry ($g_1 \gg g_2$) with a function correspondingly very close to π; the patient observer will note that there are exactly 32 local minima within the interior of the interval $0 < \ell < 1$. In fact for every case we examined through $n = 80$ (we examined at least one-half of the cases) the number of minima was precisely n. We therefore have a simple way of identifying the band index: in this model, at least, the BP as a function of ℓ produces a unique signature, and determining n is as simple as counting minima on a graph. This observation is an example of the fact that bands can be specified by a label associated with the BP [15,16,27].

It is possible that these ideas can be verified experimentally. Consider a quasi-one-dimensional crystal with two atoms (or molecular units) per unit cell. In addition an electric field is applied to drive k across the Brillouin zone, and a measurement of the BP is made. Next

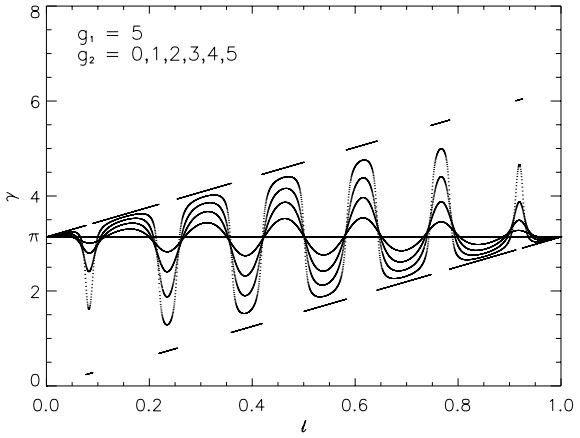

Fig. 4. γ vs. ℓ for fixed g_1 and variable g_2, in the 7th band ($n = 7$).

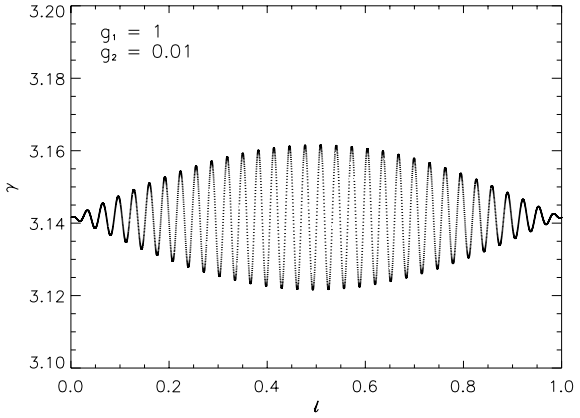

Fig. 5. γ vs. ℓ for a model close to being inversion symmetric ($g_1 \gg g_2$) in the 32nd band ($n = 32$). Note that there are 32 local minima within the interval $0 < \ell < 1$.

we imagine a uniaxial stress is also applied (along the quasi-1D direction), so that the value of ℓ changes. We imagine that the cell may change non-uniformly, due to steric or other reasons, if the macroscopic crystal deforms uniformly. (Recall that ℓ is the ratio of two lengths.) In three dimensions this effect occurs in crystals with the zinc-blende structure when stressed along the (111) direction [28]. If the BP remains constant or changes linearly with ℓ, then the crystal has inversion symmetry for the range of stress applied. If the BP changes nonlinearly, then the crystal does not have inversion symmetry.

In conclusion, we have examined how the Berry's phase depends upon inversion symmetry (or lack thereof) in a simple one-dimensional solid. There are simpler models that exhibit a BP [29,30], but these models depend upon parameters whose physical interpretation is unspecified. In our case the parameter is the Bloch wave vector k, which has experimental relevance. We have shown that the BP can be considered "trivial" for models with inversion symmetry, but only in the sense that the BP is a constant *for some choice of origin*. In general, if the origin does not correspond to a center of inversion symmetry of the crystal, the BP depends linearly upon the asymmetry parameter. We have also shown that the functional form of the BP changes continuously (with differing g values) between limiting values, and that each band can be identified by a "signature" function. These functions possess a number of local minima exactly equal to the band number. We conclude that the BP's functional dependence upon an asymmetry parameter can be used to identify an energy band, and perhaps the BP itself can be used as a "measure" of how far a crystal is from true inversion symmetry.

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