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5 Reformulation in terms of Wannier functions 9 h 29 29/9

An alternative, and in many ways more intuitive, way of thinking about the Berry-phase expression for the

5. Phát biểu lại (xây dựng lại công thức hoặc lý thuyết) theo các hàm Wannier

Trong số nhiều phương pháp dễ hiểu hơn, chúng ta hãy tìm hiểu phương pháp xét biểu thức pha Berry của độ

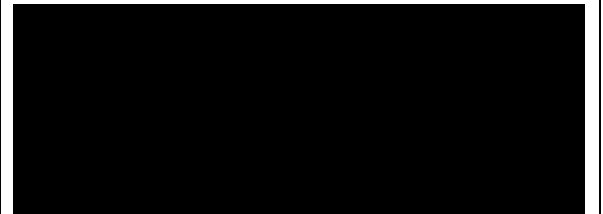
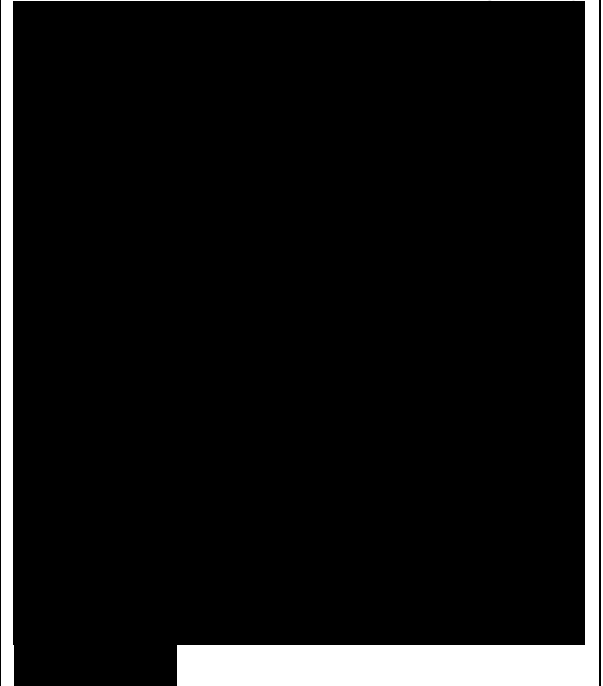
electronic polarization, Eq. (30), is in terms of Wannier functions (WFs). The WFs are localized functions w_n labeled by band n and unit cell R , that are constructed by carrying out a unitary transformation of the Bloch states $|0nk\rangle$. Thus, WFs and Bloch functions can be regarded as two different orthonormal representations of the same occupied Hilbert space. The construction is carried out via a Fourier transform of the form (41)

where the Bloch states are normalized in one unit cell. There is again some “gauge freedom” in the choice of these WFs; a set of Bloch functions $|0nk\rangle = e^{in(k)} |\hat{n}k\rangle$ results in Wannier functions $|w_nR\rangle$ that are not identical to the $|w_nR\rangle$. In practice, the gauge is often set by some criterion that keeps the WFs well localized in real space, such as the minimum quadratic spread criterion introduced by Marzari and Vanderbilt [20]. However, we should expect that any physical quantity, such as the electronic polarization arising from band n , should be invariant with respect to the phase twist $P_n(k)$. A typical WF constructed from the oxygen p-like valence bands of BaTiO₃ in its cubic centrosymmetric phase is shown in Fig. 5(a).

Once we have the Wannier functions, we can locate the “Wannier centers” $r_nR = \langle w_nR | r | w_nR \rangle$. Returning momentarily to one band in 1D, the

phân cực điện tử (PT 30) theo các hàm Wannier (các WF). Các WF là các hàm cục bộ được đặt tên là w_n , trong đó n chỉ vùng n và ô đơn vị R , các hàm này được xây dựng bằng cách thực hiện biến đổi unita của các trạng thái Bloch $|0nk\rangle$. Do đó, các WF và các hàm Bloch có thể được xem là hai biểu diễn trực giao khác nhau của cùng một không gian Hilbert bị chiếm. Quá trình rút ra hàm này được thực hiện thông qua biến đổi Fourier có dạng

(41)
 Trong đó các trạng thái Bloch được chuẩn hóa trong một ô đơn vị. Cũng có một “tự do gauge” nào đó trong việc lựa chọn các WF này; một tập hợp hàm Bloch $|0nk\rangle = e^{in(k)} |\hat{n}k\rangle$ Cho ra các hàm Wannier không đồng



Wannier center of the WF in the unit cell at the origin is just

Fig. 5. Oxygen 2p-like Wannier functions in BaTiO₃ as derived from the maximal-localization algorithm of Ref. [20]. An isocontour of Wannier-function amplitude is shown, illustrating the hybridization of O 2p and Ti 3d orbital character in the Wannier function. Oxygen atom is at center, four second-neighbor Ba atoms also appear, and two first-neighbor Ti atoms are hidden under the d-like lobes of the Wannier function. Left: Centrosymmetric paraelectric structure. Right: Distorted ferroelectric structure, in which the Ti—O bond is shortened in the upper half of the figure and lengthened in the lower half, resulting in enhanced p — d hybridization in the upper portion of the figure and suppressed hybridization below. (See also Ref. [34].)

If Eq. (41) is rewritten as $\langle \mathbf{k} | \mathbf{e}_i(\mathbf{k}) | \mathbf{k} \rangle$,

then it follows that

$$\langle \mathbf{N} | = \int d\mathbf{k} (\langle \mathbf{k} | \mathbf{e}_i(\mathbf{k}) | \mathbf{k} \rangle) = \int d\mathbf{k} \langle \mathbf{k} | \mathbf{e}_i(\mathbf{k}) | \mathbf{k} \rangle, \quad (45)$$

where an integration by parts has been used. Then

Comparing with Eq. (32) of the previous section, we find that that is, the Berry phase θ introduced earlier is nothing other than a measure of the location of the Wannier center in the unit cell. The fact that θ was previously shown to be invariant with respect to choice of gauge implies that the same is true of the Wannier center \mathbf{x}_0 .

where θ_{nj} is given by Eq. (39). That is, the location of the n'th Wannier



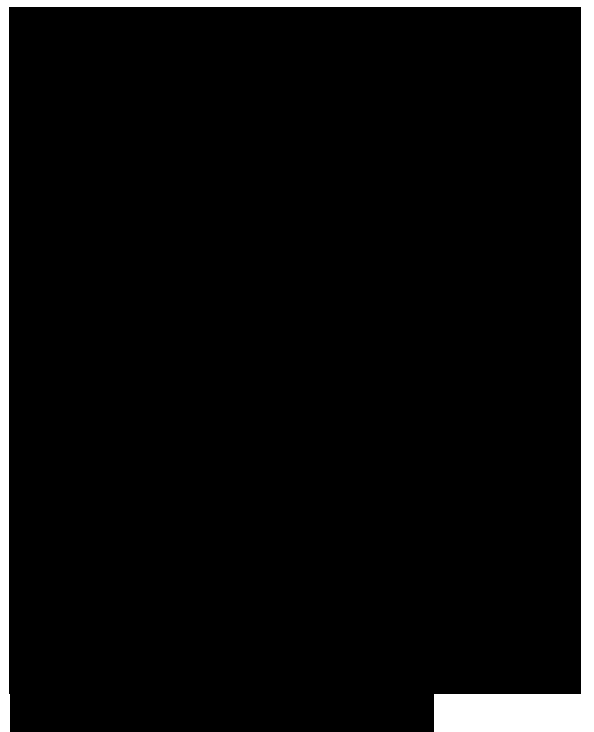
center in the unit cell is just given by the three Berry phases θ_{nj} of band n in the primitive lattice vector directions R_j . In fact, the polarization is just related to the Wannier centers by

(49)

This formula is very similar to the ionic one given in Eq. (31), but now the electron charge is taken to reside at the Wannier centers while the ionic charges reside at the nuclear positions.

The Berry-phase theory can thus be regarded as providing a mapping of the distributed quantum-mechanical electronic charge density onto a lattice of negative point charges of charge $-e$, as illustrated in Fig. 6. Then, the change of polarization resulting from any physical change, such as the displacement of one atomic sublattice or the application of an electric field, can be related in a simple way to the displacements of the Wannier centers $r_n R$ occurring as a result of this change.

This viewpoint is illustrated for the case of BaTiO_3 by returning to Fig. 5, which shows the oxygen 2p-like WF not only before (Panel (a)) but also after (Panel (b)) a displacement of the Ti sublattice by a small distance along the $-Z$ direction. We can think of this WF as being centered on the bottom oxygen atom shown in the left panel of Fig. 1. A calculation of the corresponding displacement of the Wannier center shows that it displaces strongly upward in response. This occurs because the hybridization between O 2p and Ti 3d orbitals is strengthened in the top lobe of the WF, and



weakened in the bottom lobe, leading to the “swelling” and “shrinkage” of the d-like lobes that is evident Fig. 5(b). This analysis provides an insightful microscopic explanation for the “anomalous dynamical effective charges” [$Z^*(O) \sim -5e$, $Z^*(Ti) \sim +7e$] that have been observed in this class of materials [35,36].

6 The quantum of polarization and the surface charge theorem

The alert reader may have noticed that the formulas for the polarization given in Eqs. (30), (38), and (49) have an arbitrariness modulo (e/O) times a lattice vector R . This is perhaps most obvious in connections with Eq. (49), where the decision as to which of the periodic array of WFs is to be taken as belonging to the home unit cell (the one labeled $|n_0\rangle$) is arbitrary in Eq. (48). (Actually, a similar indeterminacy is also present in the ionic contribution, Eq. (31).) It is also fairly obvious if Eq. (38) is evaluated via Eqs. (40) and (37), in which case each Berry phase (n is indeterminate modulo $2n$). In Eq. (30), or in the continuum evaluation (39) of Eq. (38), the difficulty is more subtle. Returning for the moment to the 1D, single-band case, we pointed out in Eq. (36) that, in general, a permissible gauge change (phase twist) of the Bloch functions allows for the phase to evolve by $2n$ as k is transported around the Brillouin zone. Evaluating Eq. (32) using Eq. (34), it follows that $\phi = \phi + 2n$ and $P = P - em$. The polarization is therefore only well-defined modulo an electron charge. In 3D, the

corresponding statement is that one can apply a gauge twist

$$|U_{n\mathbf{k}}\rangle = e^{-i\mathbf{n}\cdot\mathbf{k}} |U_{\mathbf{k}}\rangle \quad (50)$$

obeying

$$P_{n(\mathbf{k} + \mathbf{G}_j)} = P_{n\mathbf{k}} + 2\pi n m_j, \quad (51)$$

where \mathbf{G}_j is the primitive reciprocal lattice vector in direction j . Then $(n_j + 2\pi n m_j)$ in Eq. (39), so that e^3

$$P = P - 5E''_B, \quad (52)$$

$$O_{j=1}$$

where $m_j = n m_j$. Once again, the Berry-phase polarization is seen to be ill-defined modulo eR/O , that is, an electron charge times a lattice vector divided by cell volume. This uncertainty is sometimes known as the “quantum of polarization.”

It is instructive to recall the argument leading to Eq. (29), which can be summarized by saying that where dP/dA is given by Eq. (28). The symbol “:=” has been introduced here to emphasize that this equation needs a special interpretation, namely, that the two sides are equal modulo the quantum eR/O , where R is an arbitrary lattice vector. It is important to understand that while each quantity on the left-hand side is actually ill-defined up to this modulus, the right-hand side has a definite and unambiguous value for a given evolution of the system. That is, the evaluation of the polarization change via Eq. (29) or (30) has a fundamental limitation; some of the information contained in the original definition, Eq. (23), is lost—namely, the information about the “choice of branch” of the polarization modulus eR/O .

Fortunately this limitation is rarely

serious in practice. In most cases, the change in polarization that can be induced by a practical perturbation, such as a small sublattice displacement or electric field, is insufficient to cause P to change by a large fraction of eR/O . Where exceptions exist, as for the case of some strongly polarized ferroelectrics such as $PbTiO_3$, the ambiguity can be resolved by subdividing the adiabatic path into several shorter intervals, for each of which the change in P is unambiguous for practical purposes.

Nevertheless, the ambiguity inherent in Eq. (53) is an essential aspect of the theory. For example, for the case of a closed cyclic adiabatic evolution of the system, in which the parameter values A_1 and A_2 label the same physical state of the system, Eq. (53) becomes

$$\oint c \frac{eR}{d} \frac{dP}{dA} = 0 \text{ modulo } \dots (54)$$

(As always, such equations are defined under the assumption that the system remains insulating everywhere along the path in A space.) The modulus cannot be removed, because there are situations (e.g., sliding charge-density waves) in which the value of the integral is not zero [37]. In such cases, one says that there is “quantized adiabatic charge transport” and the cyclic evolution of A acts as a charge pump that transfers an integral number of electrons from one side of the unit cell to the other in one cycle.

It is amusing to consider the meaning of such a situation in the

context of the Wannier-function picture introduced in the previous section. Because the initial and final states of the system are identical, the arrangement of Wannier

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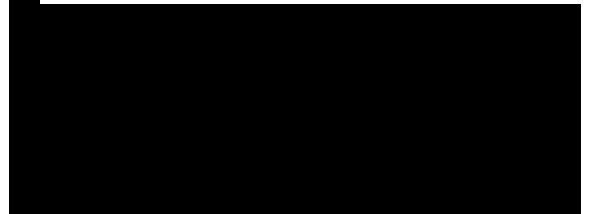
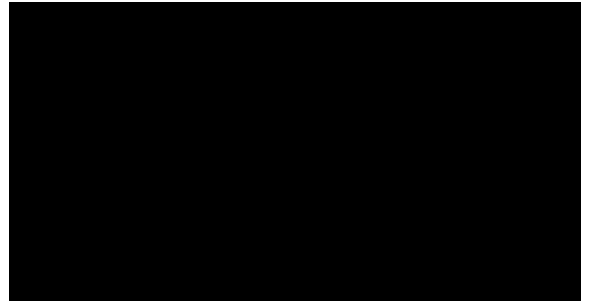
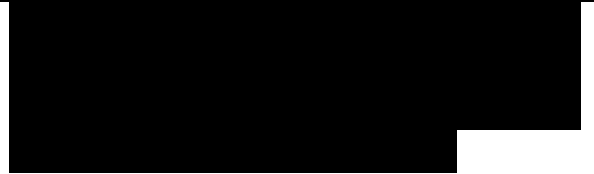
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Fig. 7. Cyclic evolution in which quantum of polarization does not, or does, appear. Possible evolution of positions of Wannier centers (—), relative to lattice of ions (+), as Hamiltonian evolves adiabatically around a closed loop. Wannier functions must return to themselves, but can do so either (a) without, or (b) with, a coherent shift by a lattice vector.

functions must be identical.

However, if one follows individual Wannier centers during the evolution as illustrated in Fig. 7, they need not describe closed loops. If they do all describe closed loops, then the circuit integral in Eq. (54) does vanish. On the other hand, if the evolution results in the pumping of Wannier centers across the unit cell, then the system represents an example of adiabatic charge transport.

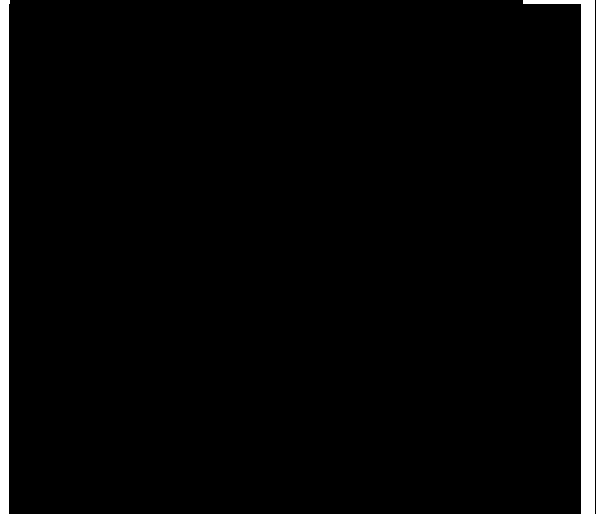
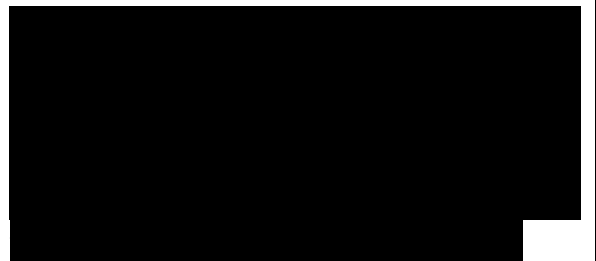
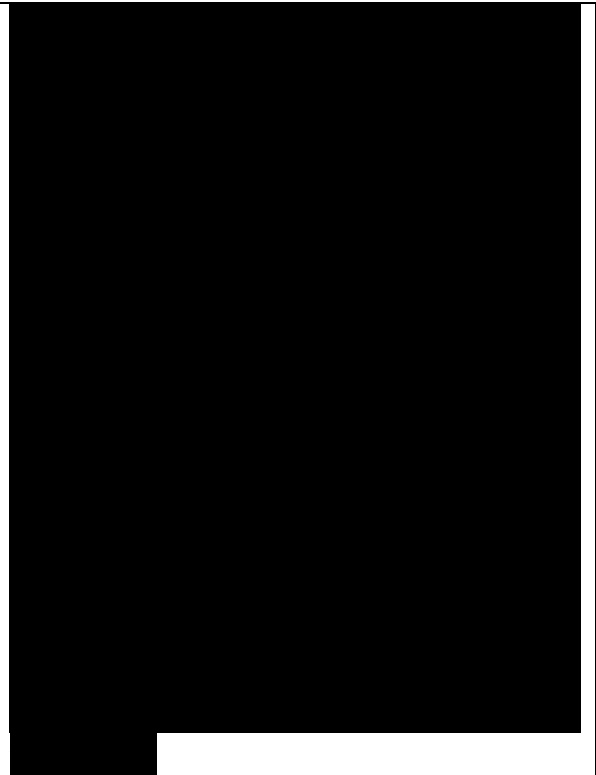
There is one more way in which the indeterminacy of P modulo eR/Q may be understood in a natural way. In elementary electrostatics, one learns that the macroscopic bound surface charge density σ_b residing on the surface of a sample is related to the polarization in the interior by $\sigma_b = \mathbf{n} \cdot \mathbf{P}$, where \mathbf{n} is the surface normal. One defines the bound charge σ_b by saying that no free charge is present, but what, precisely, does this mean? The



surface must be insulating, with the electron chemical potential lying in a gap that is common to both bulk and surface. But this is not a unique prescription. Consider, for example, the case of an insulating crystal having a surface band that lies entirely inside the bulk band gap. Then this surface band may either be completely occupied or completely empty, as indicated schematically in the density-of-states plots shown in Panels (a) and (d), respectively, of Fig. 8. From the point of view of the Wannier-function representation, this corresponds to the question of how many Wannier functions exist at the surface, as illustrated in the remaining Panels (b-c) and (e-f). In either case, the condition of absence of bound charge is satisfied. But the surface charge densities clearly differ by an integer number of electron charges per primitive surface cell area A_{surf} , so we conclude that [38]

However, this is perfectly consistent with the fact that P is ill-defined modulo eR/Q , since $n \cdot R = mc = mQ/A_{\text{surf}}$, where m is an integer and c is the lattice constant of the crystal in the surface-normal direction.

Fig. 8. Ambiguity of bound surface charge. Panels (a) and (d) illustrate the density of states of an insulating crystal having a full valence band (left) and empty conduction band (right), and a surface band lying entirely within the bulk gap (center) that may either be entirely (a) occupied, or (d) empty. Panels (b) and (e) show the corresponding charge densities, while (c) and (f) illustrate the mapping to Wannier



centers in these two cases. As can be seen by comparing (c) and (f), the surface charges differ by precisely one electron charge (or two for spin) per surface unit cell area.

From arguments of this type, it should have been possible to anticipate this essential indeterminacy in the definition of crystal polarization. As a historical aside, it is interesting to note that the presence of this indeterminacy was not widely understood and appreciated until it was forced into the light by the efforts of the computational electronic-structure community to understand precisely how polarization should be computed in practice. For further discussion of the subtleties associated with the “quantum of polarization,” the reader is referred to Refs. [7], [38], and [39].

