Geometrodynamics of electrons in a crystal under position and time-dependent deformation

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The semiclassical dynamics of Bloch electrons in a crystal under slowly varying deformation is developed in the geometric language of a lattice bundle. Berry curvatures and gradients of energy are introduced in terms of lattice covariant derivatives, with the corresponding connections given by the gradient and rate of strain. A number of physical effects are discussed: an effective post-Newtonian gravity at band bottom, polarization induced by spatial gradient of strain, orbital magnetization induced by strain rate, and the electron energy-stress tensor.

I. INTRODUCTION

The semiclassical dynamics of Bloch electrons was developed in the early days of solid state physics to give an intuitive picture of electron motion in the ionic background in a crystal. Combined with the Boltzmann equation, many equilibrium and transport phenomena are well described [1]. The theory can also be quantized [2] to describe quantum energy levels, such as the Wannier-Stark ladder in a constant electric field and Landau levels in a constant magnetic field [1]. Much later, Berry phases [3] were found to play an important role in the semiclassical equations of motion in the form of Berry curvatures [4]. They account for quite a few phenomena such as the quantum Hall effect [5], the intrinsic anomalous Hall effect [6], and charge pumping [7]. The description of electric polarization [8] and orbital magnetization [9] in crystals is also closely related to the notion of the Berry phase.

The wave-packet method developed by Sundaram and Niu provides a systematic way to derive the semiclassical dynamics in perturbed crystals [10] with various types of Berry curvatures appearing in the equations of motion. In their work, besides the effect of electromagnetic field, they studied the crystal deformation. Some interesting results are found such as the dragging effect due to lattice motion and the real space Berry phase associated with a dislocation. Their theory is based on the displacement field of ions, and the wave-packet method can easily account for the effects of first-order derivatives in space and time of the displacement field, i.e., the strain and lattice velocity. However, it is very difficult to extend to the next order of derivatives, such as strain gradient, lattice acceleration, and strain rate in this formalism, which are related to phenomena such as flexoelectricity [11,12] and viscosity [13].

In this paper, we advocate another picture by viewing the whole crystal under deformation as a lattice bundle. For a given time and about each spatial point, a locally periodic lattice can be identified, which well describes the distribution of ions in a region smaller than the length scale of the variation of periodicity. The local lattice also moves rigidly at the average velocity of ions around the position point. By identifying the local lattice at each space and time point, we have a bundle of locally periodic lattices on the spacetime manifold. Each local lattice contains information to the arbitrary order of strain (defined relative to some reference lattice). Strain gradient, strain rate, and lattice acceleration are manifested in the difference between local lattices. In this sense, a periodic crystal can be viewed as a special case where all local lattices are identical.

Based on the lattice bundle picture, we have two geometrical structures, which are extended phase space and the Hilbert bundle [14]. Noticing each local lattice gives rise to a Brillouin zone, all the Brillouin zones together with the spacetime make up the extended phase space $(\boldsymbol{k}; \boldsymbol{x}, t)$, where crystal momentum $\boldsymbol{k}$ denotes points in the Brillouin zone of the local lattice at spacetime point $(\boldsymbol{x}, t)$. However, in a crystal under deformation, the sizes of local Brillouin zones are different in general. This is in contrast to an ideal crystal where all local Brillouin zones are the same and can be viewed as a single one. This special geometry brings up the question of how to express the electron equations of motion in phase space. Particularly, we are faced with the difficulty of defining the change rate of crystal momentum $\boldsymbol{k}$ since at different time slices crystal momentums belong to different Brillouin zones.

Moreover, the definition of Berry connections in terms of the spacetime parameter is also problematic. The naive idea from previous experience is to define, for example, $A_t = i \langle u | \partial_t u \rangle$ using the eigenstates of the $\boldsymbol{k}$-dependent Hamiltonian $\hat{H}(\boldsymbol{k}; \boldsymbol{x}, t)$ given by the local lattice. However, $|\partial_t u\rangle$ involves the difference between two Bloch functions of different periodicities which is not a periodic function in general and gives rise to ill-defined results. In fact, this problem involves the second geometrical structure we mentioned earlier, called the lattice Hilbert bundle. Noticing that all the eigenstates of Hamiltonian $\hat{H}(\boldsymbol{k}; \boldsymbol{x}, t)$ labeled by different band indexes form a complete basis for periodic functions that thus gives rise to a local Hilbert space defined at a particular extended phase space point $(\boldsymbol{k}; \boldsymbol{x}, t)$, the lattice Hilbert bundle appears as the collection of all local Hilbert spaces together with

the extended phase space. Local Hilbert spaces at different spacetime points are distinct in periodicities inherited from the corresponding local lattices. So the definition of the Berry connection actually involves the comparison between states in different Hilbert spaces.

To resolve the aforementioned problem, with the same spirit in differential geometry [15], we introduce the concept of lattice covariant derivatives to take the place of partial derivatives in comparing local quantities such as crystal momentum, Bloch functions, and band energy. This gives mathematically and physically reasonable results as shown later in this paper. With lattice covariant derivatives, we achieve our main result in this paper: the equations of motion of electrons accurate to the first order of strain gradient, strain rate, and lattice acceleration. The results are expressed in terms of the Bloch functions given by the local periodic lattice, which are solvable numerically. A few interesting effects are discussed based on our lattice covariant formalism. First neglecting the Berry phase effects, we show the similarity of the electron dynamics at band bottom to that of a test particle in post-Newtonian gravity. An equivalent metric tensor is identified in terms of the effective mass and lattice deformation. Then we focus on the Berry phase related effects. For a band insulator at zero temperature, we calculate the current induced by deformation. Particularly, we identify the polarization contribution and give an explicit expression for the proper piezoelectric constant [16] in terms of Berry curvatures expressed with lattice covariant derivatives. Then we discuss the Chern-Simons part of the strain gradient induced polarization and strain rate induced orbital magnetization. Finally, for the spatially homogeneous case, we discuss the electron energy-stress tensor and its responses to ionic velocity gradient and acceleration.

This paper is organized as follows: Section II introduces the basic idea of the lattice bundle picture and clears the mathematical notion. In Sec. III, we discuss the special geometry of phase space. The equations of motion without the Berry phase effect are discussed in comparison to the gravitational effect. In Sec. IV, we discuss the lattice covariant Berry curvatures and their related effects. Section IV C concludes the paper with the aforementioned applications.

II. LATTICE BUNDLE PICTURE

A. Local lattice

In this paper, our main results are expressed in the laboratory frame $(\boldsymbol{x}, t)$, which is a Cartesian coordinate representing Minkowski spacetime. $\boldsymbol{x}$ is the position coordinate which has three components denoted by $\{i, j, k\}$ running at 1,2,3. t is the time coordinate. A compound notion like $x^{u,v,\xi}$ is also used in this paper where $u, v, \xi = 0, 1, 2, 3$ to include the time component represented by 0.

The description of an ideal crystal in the laboratory frame is given by its Bravais lattice, which is a set of lattice points periodically aligned in space. Each lattice point may represent several ions and has an integer label $\{\boldsymbol{l}\}$. Its displacement vector from the laboratory frame origin is denoted as $\{\boldsymbol{R}_l = l^\alpha \boldsymbol{c}_\alpha + \boldsymbol{u}\}$. Here we use $\{\alpha, \beta, \gamma\}$ running at 1,2,3 to denote crystalline directions. $\boldsymbol{l}$ is short for $\{l^\alpha\}$ which has three components. $\{\boldsymbol{c}_\alpha\}$ are the three primitive lattice vectors and
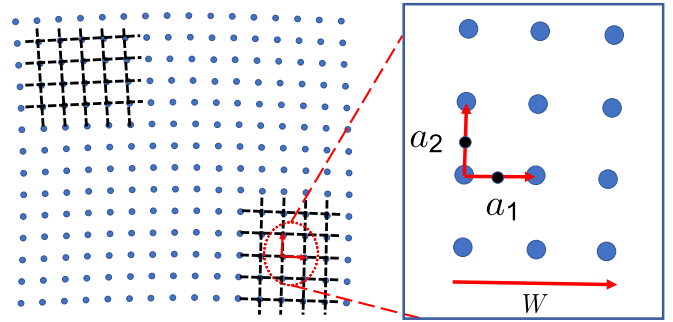

FIG. 1. A schematic picture of how to identify the local lattices in a deforming crystal. Blue circles represent the lattice points of a deforming crystal. Dashed lines represent the crystalline lines of the fictitious periodic local lattice. As can be seen, the local distribution of lattice points is well described by the local lattice only with deviation far away from the local point. The right panel is the zooming-in picture. The lattice vector of a local lattice is given by the relative displacement between lattice points and located in the middle denoted by the black dots on the arrows. And a local lattice moves rigidly at velocity $\boldsymbol{W}$.

$\boldsymbol{u}$ is the position of the zeroth lattice point. The Einstein summation rule is applied throughout this paper.

In the lattice bundle picture, local lattices are expressed in the same way as ideal lattices only with $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t), \boldsymbol{u}(\boldsymbol{x}, t)\}$ becoming position and time-dependent vector fields denoting the property at a particular spacetime point $(\boldsymbol{x}, t)$. Reciprocal lattice vector fields $\{\boldsymbol{b}^\alpha(\boldsymbol{x}, t)\}$ are defined through the relation $\boldsymbol{b}^\alpha \cdot \boldsymbol{c}_\beta = \delta^\alpha_\beta$, where the "crystallographer's definition" is used and δ^α_β is the Kronecker delta function. We use the bold symbol to denote tensors. The normal symbol with the same letter denotes their components. For example, lattice vectors are written as $\boldsymbol{c}_\alpha = (c^1_\alpha, c^2_\alpha, c^3_\alpha)$ and reciprocal lattice vectors as $\boldsymbol{b}^\alpha = (b^\alpha_1, b^\alpha_2, b^\alpha_3)$. Vectors and covectors are indicated by their upper and lower indices of their components, respectively. Thus the orthogonal relation written in components reads $b^\alpha_i c^i_\beta = \delta^\alpha_\beta$. If we only consider the three-dimensional space, $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t)\}$ provides a basis for real space vector fields, e.g., electron velocity, and $\{\boldsymbol{b}^\alpha(\boldsymbol{x}, t)\}$ provides a basis for covector fields, e.g., electron momentum. The completeness relation for this basis reads $b^\alpha_j c^i_\alpha = \delta^i_j$.

On the other hand, we know a crystal under deformation is described by the position of its lattice points $\{\boldsymbol{R}_l(t)\}$. Thus we need to establish the relation between $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t), \boldsymbol{u}(\boldsymbol{x}, t)\}$ and $\{\boldsymbol{R}_l(t)\}$. This relation is schematically shown in Fig. 1 and is given by the following formula:

$$\boldsymbol{c}_\alpha\left(\frac{\boldsymbol{R}_l + \boldsymbol{R}_{l+1_\alpha}}{2}, t\right) = \boldsymbol{R}_{l+1_\alpha} - \boldsymbol{R}_l, \qquad (1)$$

where 1_α means one increment in the αth crystalline direction. To achieve the continuous lattice vector fields $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t)\}$, an interpolation procedure should be applied. A detailed discussion is given in Appendix A. We should note that once the lattice vector fields are given, they can determine the total crystal up to a rigid body displacement since given the position of a particular lattice point, Eq. (1) can be applied repeatedly to recover all the lattice points. The rigid body center position is described by the field $\boldsymbol{u}(\boldsymbol{x}, t)$; however

it is insignificant due to the translational invariance of the Minkowski spacetime. Thus $\boldsymbol{u}(\boldsymbol{x}, t)$ will not be discussed.

However, due to the time dependence of the problem, it is convenient to introduce a velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ to describe the motion of local lattices. It is determined by the property that

$$\boldsymbol{W}(\boldsymbol{R}_l, t) = \dot{\boldsymbol{R}}_l(t), \tag{2}$$

where again the interpolation procedure should be applied to achieve a continuous field. Then the four fields $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t), \boldsymbol{W}(\boldsymbol{x}, t)\}$ with $\alpha = 1, 2, 3$ define at each spacetime point $(\boldsymbol{x}, t)$ a periodic lattice of periodicity $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t)\}$ moving rigidly at velocity $\boldsymbol{W}(\boldsymbol{x}, t)$ as observed in the laboratory frame. Thus we have a lattice bundle over the spacetime.

It is worth pointing out that the above argument is always applicable to cases where the primitive unit cell only contains one ion. For multi-ion cases, we need to check whether there exists a one-to-one correspondence between the ionic positions in a unit cell and the instantaneous positions of Bravais lattice points, i.e., whether all degrees of freedom are contained in lattice points. Examples where such correspondence exists are deformation caused by a particular acoustic phonon branch, the adiabatic case where ions are always relaxed to their minimal energy position at each time slice, or crystals satisfying the clamped-ion approximation where at each time the distribution of ions within a unit cell follows the instantaneous strain of the unit cell (although there can be an internal strain contribution [17]). Exceptions are cases where deformation is caused by optical phonons or there is an internal strain.

Each local lattice automatically gives rise to a local "static" Hamiltonian as

$$\hat{H}(\boldsymbol{k}; \boldsymbol{x}, t) = \frac{1}{2m_e} \left(\frac{1}{i} \frac{\partial}{\partial \boldsymbol{r}} + \boldsymbol{k} \right)^2 + V\left(\{l^\alpha \boldsymbol{c}_\alpha(\boldsymbol{x}, t) - \boldsymbol{r}\}\right). \tag{3}$$

$\boldsymbol{r}$ is the real space representation. $\boldsymbol{k}$ is the crystal momentum. Both $\boldsymbol{r}$ and $\boldsymbol{k}$ should be viewed as local quantities as well. The domain of $\boldsymbol{r}$ is chosen to be the first Wigner-Seitz cell of the local lattice. And the domain of $\boldsymbol{k}$ is chosen to be the first Brillouin zone. The detailed derivation to achieve this Hamiltonian is given in Appendices A through D and the relation between $\boldsymbol{r}$ and $(\boldsymbol{x}, t)$ is given by Eq. (D9).

The above Hamiltonian has translational symmetry and is solvable in principle. Its eigenstates are the periodic part of the Bloch functions denoted by $u_n(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$, where n is the band index. We will call $u_n(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$ Bloch functions in this paper just for simplicity. The corresponding eigenvalue is band energy denoted by $\varepsilon_n(\boldsymbol{k}; \boldsymbol{x}, t)$. In the following discussion, we assume those eigensolutions are given by first-principles calculations and all our results will be given based on them.

Here are a few comments about this local Hamiltonian. In the crystal potential term, information about the center position of a local lattice is discarded as the zeroth ion is always located at $\boldsymbol{r} = 0$. As pointed out earlier, this will not cause trouble since the lattice vector fields contain structural information of the whole crystal up to a rigid body displacement. Also, the local lattice velocity $\boldsymbol{W}(\boldsymbol{x}, t)$ is absent. As can be seen later, the effects of velocity field are to shift the

crystal momentum by $-m_e \boldsymbol{W}(\boldsymbol{x}, t)$ and the electron energy by a centrifugal potential $-\frac{1}{2} m_e W^2$ while not changing electron Bloch functions. The shifted crystal momentum and energy have the physical meaning of electron momentum and energy in the reference frame comoving with ions. Rather than being discussed in the Hamiltonian level, we will introduce the effect of velocity directly in the semiclassical equations of motion in Sec. III B. Again, this procedure can be rigorously proved in Appendix D.

To make sure the above local Hamiltonian gives a good approximation to the real lattice Hamiltonian, we must assume the crystal potential at a given position is mainly determined by ions within some finite spatial length scale ξ, and ξ is much smaller than the variation length scale of lattice vectors λ, i.e., $\xi \ll \lambda$. Also, because we have applied the adiabatic approximation where the instantaneous Bloch function and band energy are used, the variation timescale of lattice vectors denoted by τ should satisfy $\frac{\hbar}{\tau} \ll \Delta$, where Δ is the minimal direct band gap of the adiabatic Hamiltonian. However, for polar materials, there does exist a nonlocal contribution to the crystal potential due to polarization. Although this part of the contribution is not the focus of this paper, we expect that the polarization contribution to the crystal potential can be accounted for by combining the static Poisson equation self-consistently with our formula of polarization given in Sec. IV C. Then our theory takes care of the local potential part within this complete approach.

B. Lattice connection as strain rate and gradient

The major motivation of this work is to study the effects of inhomogeneity, i.e., lattice acceleration, strain gradient, and strain rate, on electron semiclassical dynamics, which are described by the spacetime derivative of the fields $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t), \boldsymbol{W}(\boldsymbol{x}, t)\}$. In formulating the theory, we find it is more convenient to define a quantity that is directly related to inhomogeneity called lattice connection.

Consider the lattice vectors change $\delta \boldsymbol{c}_\alpha = \partial_\mu \boldsymbol{c}_\alpha(\boldsymbol{x}, t) dx^\mu$ given by a small increment in position and time dx^μ; we can define the lattice connection to encode this variation as

$$\delta \boldsymbol{c}_\alpha(\boldsymbol{x}, t) = \boldsymbol{\Gamma}_\mu(\boldsymbol{x}, t) \cdot \boldsymbol{c}_\alpha(\boldsymbol{x}, t) dx^\mu, \tag{4}$$

where $\boldsymbol{\Gamma}_\mu(\boldsymbol{x}, t)$ is the lattice connection and can be viewed as a second-rank tensor with its element denoted by $\{\Gamma^i_{j\mu}\}$. In components, the above equation reads $\delta a^i_\alpha = \Gamma^i_{j\mu} a^j_\alpha dx^\mu$. If we define the infinitesimal strain as $\delta s = dx^\mu \boldsymbol{\Gamma}_\mu$, it simply reads $\delta \boldsymbol{c}_\alpha = \delta s \cdot \boldsymbol{c}_\alpha$, which is the strain induced lattice vector change. Thus the physical meaning of lattice connection $\boldsymbol{\Gamma}_\mu$ is just the gradient $\mu = 1, 2, 3$ and rate $\mu = 0$ of the unsymmetrized strain tensor. The antisymmetric part between the upper and first lower index is the relative rotation between local lattices and the symmetric part is the relative symmetrized strain. Particularly, the unit-cell volume change is described by $\Gamma^i_{i\mu}$. Since we choose the local lattice as the reference, strain is no longer present in our theory; instead the strain gradient denoted by the lattice connection gives the leading order correction. Multiplying the reciprocal lattice vector $\boldsymbol{b}^\alpha$ on both sides of Eq. (4) and summing over α, we can have an
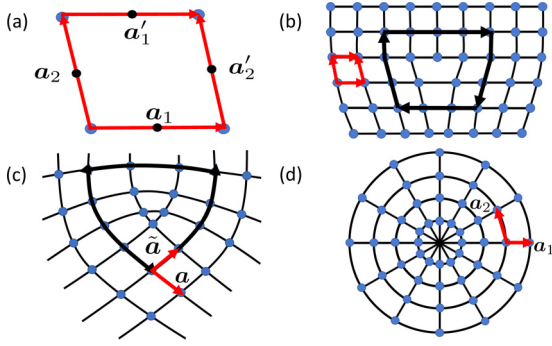
FIG. 2. (a) Elastic condition of lattice vectors. The dots on the four corners represent lattice points, which determine the local lattice vectors denoted by the four edges of the quadrilateral. The dot in the middle of each edge denotes where these lattice vectors reside. According to Eq. (1), it is straightforward to derive the condition for the four lattice vectors to form a closed quadrilateral. (b) Schematics of dislocation in a square lattice. Along the closed trajectory denoted by the bold line, if we count the change of lattice label, we always find a unit mismatch in the crystalline direction. (c) Schematics of a disclination in a square lattice. Along the closed trajectory denoted by the bold line, we find that the lattice vector continuously changes from c to $\tilde{c}$ as shown in the picture. (d) A special case of disclination in a rectangular lattice, which is characterized by the 2π rotation of lattice vectors along the defect center. In the region far enough from the center, locally we have a rectangular lattice, whose two lattice vectors $c_1 = c_1\theta$, $c_2 = c_2 r$ are along the angle direction and radius direction, respectively, in a polar coordinate. The disclination located at the origin is characterized by the rotation of lattice vectors by 2π along the complete circle.

explicit expression of the lattice connection as

$$\Gamma^i_{j\mu} = b^\alpha_j \partial_\mu c^i_\alpha. \quad (5)$$

The lattice connection represents how local lattices are connected together to form the total lattice structure. If in a local region the deformation is elastic, i.e., can be continuously deformed to a periodic crystal, the gradient of the fields $\{c_\alpha(x, t), W(x, t)\}$ is not independent, which is directly manifested in the property of lattice connection. As seen from Fig. 2, the four adjacent local lattice vectors forming a closed quadrilateral lead to the conclusion that

$$(c_\alpha \cdot \partial)c_\beta - (c_\beta \cdot \partial)c_\alpha = 0, \quad (6)$$

where the second-order derivatives of $\{c_\alpha(x, t)\}$ are ignored. On the other hand, if we consider the relative velocity between two adjacent lattice points, it can be expressed either as the total time derivative of the lattice vector fields from Eq. (1) or as the gradient of the velocity field from Eq. (2). Equating both expressions leads to the relation that

$$\partial_t|_x c_\alpha + (W \cdot \partial)c_\alpha = (c_\alpha \cdot \partial)W, \quad (7)$$

where again second-order derivatives of $W(x, t)$ are neglected. Both Eqs. (6) and (7) can be reformulated in terms of the lattice connection as

$$\Gamma^k_{ij} - \Gamma^k_{ji} = 0, \quad (8)$$

$$\Gamma^k_{i0} + \Gamma^k_{ji} W^j = \partial_i W^k. \quad (9)$$

The first relation is the torsion-free condition for a connection form in a coordinate basis, which tells us that the two lower indexes of lattice connection are symmetric. Equation (9) shows that the strain rate experienced by ions on the left-hand side equals the gradient of the velocity field on the right-hand side, where the first term on the left-hand side is the strain rate observed at a fixed position. From the above expression, we see that the angular velocity field given by $\omega = \partial \times W$ is also related to the lattice connection as $\omega^k = \varepsilon^{ijk}(\Gamma^j_{i0} + \Gamma^j_{li} W^l)$ with ε^{ijk} the Levi-Civita symbol. Thus angular velocity is just the antisymmetric part of the strain rate experienced by ions. However, we should notice that the lattice acceleration field a is not directly related to the lattice connection, which is given by $a = (W \cdot \partial)W + \partial_t W$.

Besides its geometrical meaning, the lattice connection also gives rise to an important gradient correction to local Hamiltonian (3). This gradient correction term is for the electron wave packet, which is localized in real space with center position x and expressed as the superposition of the local Bloch states of local Hamiltonian (3) [10]. For such a wave-packet state, the gradient correction reads

$$\Delta H(r; x, t) = \frac{1}{2}\Gamma^m_{ni}\hat{O}^{ni}_m + \frac{1}{2}\Gamma^m_{ni}[(r - r_c)^i \hat{D}^n_m + \text{c.c.}], \quad (10)$$

where r_c is the expectation value of operator r under the wave-packet state. The derivation is given in Appendix B and Appendix C. The first term comes from the difference between local lattice and real lattice away from the particular point where the local lattice resides. The second term comes from the difference between local lattices. Because wave-packet states have finite sizes usually as large as several unit cells, electrons can feel the influence from adjacent local lattices as well. Both terms are proportional to the spatial part of the lattice connection.

$\hat{O}^{ni}_m = \sum_l \frac{\partial V(\{\tilde{R}_l - r\})}{\partial \tilde{R}^m_l}(\tilde{R}_l - r)^n(\tilde{R}_l - r)^i$ is a periodic operator with respect to r, where $\{\tilde{R}^i_l(x, t) = l^\alpha c^i_\alpha(x, t)\}$ are the local lattice points. The second term breaks the translational symmetry due to the factor $\{r - r_c\}$. However, it still has a well-defined expectation value under the wave-packet state due to localization in real space. $\hat{D}^n_m = \mathcal{V}^n_m - \frac{1}{m_e}(\frac{1}{i}\frac{\partial}{\partial r^m} + k_m)(\frac{1}{i}\frac{\partial}{\partial r^n} + k_n)$ is the deformation potential operator [18] with $\mathcal{V}^n_m = \sum_l \frac{\partial V(\{r - \tilde{R}_l(x, t)\})}{\partial \tilde{R}^m_l}(r - \tilde{R}_l)^n$. $\mathcal{V}^n_m$ has the same form as assumed in the rigid ion model [19] and automatically vanishes in the deformable ion model. Actually, following the argument in Sec. IV B, we believe this form of $\mathcal{V}^m_n$ is rather general as long as there is a one-to-one correspondence between all lattice points and the crystal potential. The deformation potential operator is a second-rank symmetric tensor operator with respect to lattice symmetries. Its expression in momentum space is discussed in Appendix G, which might be more useful in first-principles calculations.

Local Hamiltonian (3) together with gradient correction (10) gives the total Hamiltonian of the electron wave packet in the first-order of strain gradient or lattice connection. Although in principle the gradient correction also modifies local Bloch states, the eigenstates of local Hamiltonian (3) are enough to achieve the equations of motion up to first order.

C. Characterizing line defects in the lattice bundle picture

In this subsection, we discuss how to describe line defects within the lattice bundle picture. Although our theory is limited in regions where locally deformation is slowly varying and elastic, the topology of line defects can still be described by the loops enclosing the defect line [20]. Here we consider the cases of dislocation and disinclination.

These two kinds of defects correspond to the redundant freedom to describe a Bravais lattice. For an ideal crystal described by $\{\boldsymbol{c}_\alpha, \boldsymbol{u}\}$, we can change the lattice labels by some integer $\boldsymbol{Z} = \{Z^\alpha\}$ with $\boldsymbol{u}$ fixed, which gives the same lattice. This is associated with dislocation. If we travel along the loop enclosing the dislocation line, after going back to the initial point, we find the lattice labels are changed by some integer. Also, we may choose other crystalline directions $\tilde{\boldsymbol{c}}_\alpha = U_\alpha^\beta \boldsymbol{c}_\beta$, such that $\{\tilde{\boldsymbol{c}}_\alpha, \boldsymbol{u}\}$ gives the same lattice. This degree of freedom is related to disclination. In the lattice bundle picture, if we keep track of the local lattice vectors' change along the loop enclosing the disclination, after returning to the starting point, we end up with another set of equivalent local lattice vectors. Dislocation and disclination are topological in the sense that $\boldsymbol{Z}$ is an integer vector and U is an integer matrix.

The above argument is schematically shown in Figs. 2(b) and 2(c). Here, we show how they can be described mathematically. First, for dislocation, Eq. (6) tells us that the primitive lattice vector equals the position change of lattice points per integer label increment. This can be written in a discrete form as

$$\delta x^i = c_\alpha^i \left(\boldsymbol{x} + \frac{\delta \boldsymbol{x}}{2}, t \right) \delta l^\alpha. \tag{11}$$

The above expression relates the change in $\boldsymbol{x}$ space and $\boldsymbol{l}$ space. With it, we can calculate the change of $\boldsymbol{x}$ or $\boldsymbol{l}$ along some trajectory. If the trajectory is a loop in $\boldsymbol{l}$ space, the displacement in $\boldsymbol{x}$ space gives the Burgers vector. On the other hand, if the trajectory forms a loop in $\boldsymbol{x}$ space, the total change of $\boldsymbol{l}$ gives the mismatch of lattice label $\boldsymbol{Z}$ mentioned before. Here we adopt the latter perspective. Considering a loop in $\boldsymbol{x}$ space far away from and enclosing the dislocation line, the change of lattice label can be written as an integral as

$$\oint_C b_i^\alpha(\boldsymbol{x}) dx^i = Z^\alpha, \tag{12}$$

where the integer on the right-hand side describes the topological "charge" of the dislocation. According to whether the crystalline direction $\boldsymbol{Z}$ is perpendicular or parallel to the plane of the loop, we can characterize the dislocation as either a screw dislocation, edge dislocation, or mixed type. For example, in Fig. 2(b), we have an edge dislocation in a square lattice with $\boldsymbol{Z} = (1, 0, 0)$ denoting one associated with the dislocation line.

Next we discuss disclination. Equation (4) gives a formal description of how local lattice vectors change in position and time. Given lattice connection and the initial value of lattice vectors $\{\boldsymbol{c}_\alpha\}$, this equation determines the final value $\{\tilde{\boldsymbol{c}}_\alpha\}$ along some trajectory. For a loop enclosing the disclination line, in general, the initial and final values of the lattice vectors are different. They are related to each other as $\tilde{\boldsymbol{c}}_\alpha = U \cdot \boldsymbol{c}_\alpha$ and

the matrix U can be formally expressed as

$$U = \mathcal{T} \exp \left(\oint dx^i \boldsymbol{\Gamma}_i \right), \tag{13}$$

where $\mathcal{T}$ is the path ordering operator which is necessary when the matrices $\boldsymbol{\Gamma}_i(x, t)$ at different points along the loop do not commute. Given the lattice connection expressed in the laboratory frame basis $\{\Gamma_{ni}^m\}$, U will have the form of $\{U_n^m\}$. However, to see its topological property, we express it in the lattice vector basis as $U_\alpha^\beta = c_\alpha^n U_n^m b_m^\beta$. Then the final and initial values of lattice vectors are related as $\tilde{\boldsymbol{c}}_\alpha = U_\alpha^\beta \boldsymbol{c}_\beta$. Because $\{\tilde{\boldsymbol{c}}_\alpha\}$ and $\{\boldsymbol{c}_\alpha\}$ represent the same local lattice, the matrix U and its inverse are both integer matrices with determinant ± 1.

It is important to realize that in the presence of disinclination, lattice vector fields are not globally well defined. This restricts our previous discussion only to a local region. To study the global effect of disinclination, at least two sets of lattice vector fields are needed. However, lattice connection is still a good quantity globally. As seen from its expression (5), the summation over all crystalline directions makes lattice connection single-valued even in the presence of disinclination. It is also worth pointing out that because elastic the condition (8), (9), locally the lattice connection is trivial in the sense it can be made zero by a particular coordinate transformation. However, in the presence of a topological defect, the lattice connection is no longer trivial globally.

Here, we give a demonstration calculation for disinclination shown by Fig. 2(d). In polar coordinates $\boldsymbol{c}_1 = c_1 \boldsymbol{\theta}$, $\boldsymbol{c}_2 = c_2 \boldsymbol{r}$, where c_1, c_2 are constant representing the magnitude of the lattice vector. Then according to Eq. (4), we have $\Gamma_{x\theta}^x = \Gamma_{y\theta}^y = 0$ and $\Gamma_{x\theta}^y = -\Gamma_{y\theta}^x = \frac{1}{R}$, where R is the radius of the circle we are considering enclosing the disinclination. The lattice connection can be treated as a matrix

$$\Gamma_\theta = \begin{pmatrix} 0 & -\frac{1}{R} \\ \frac{1}{R} & 0 \end{pmatrix}, \tag{14}$$

which is just the generator of the SO(2) group multiplied by $\frac{1}{R}$. Because the lattice connection is constant along the path, the ordering operator can be omitted and we have

$$U = \exp \begin{pmatrix} 0 & -2\pi \\ 2\pi & 0 \end{pmatrix} = \begin{pmatrix} \cos(2\pi) & -\sin(2\pi) \\ \sin(2\pi) & \cos(2\pi) \end{pmatrix}, \tag{15}$$

which is the expected 2π rotation of the lattice vectors.

III. LATTICE COVARIANT PHASE SPACE

A. Phase space geometry

At a given time t, the electron wave-packet state with center position $\boldsymbol{x}$ and center wave vector $\boldsymbol{k}$ locates at the point $(\boldsymbol{k}; \boldsymbol{x})$ in phase space. Phase space is the base manifold for the semiclassical electron motion. However, for the case of deforming crystals, it takes an unusual geometry comparing to periodic lattices as shown in Fig. 3, which is the one-dimensional case. In the lattice bundle picture, for given time t, at each position $\boldsymbol{x}$ the local lattice gives rise to a local Brillouin zone according to its own periodicity. All the Brillouin zones together with the position space $\boldsymbol{x}$ constitute the phase space. However, the shapes of local Brillouin zones are different. Noticing the topology of the Brillouin zone, we
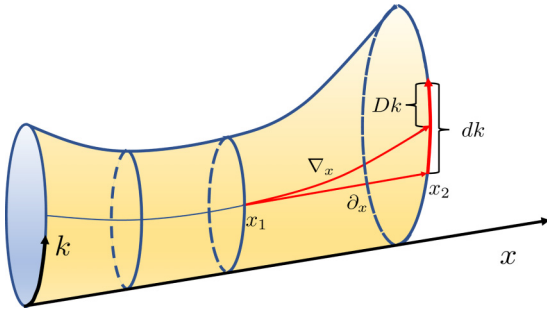
FIG. 3. The phase space of electrons in the one-dimensional case. The straight line at the bottom denotes the position space $\boldsymbol{x}$. Local Brillouin zones are denoted by circles at each position. The intersection between each circle and the straight line is the $\boldsymbol{k} = 0$ point. The phase space is a "tube" with a varying radius. To compare two points in phase space, we show two alternatives. One is along the path denoted by ∂_x where the value of $\boldsymbol{k}$ is fixed, which then goes along the circle by the total change of wave vector $d\boldsymbol{k}$. Another path is to go along the correspondence line formed by parallel transport denoted by ∇_x, then go along the circle by the mechanical change of wave vector $D\boldsymbol{k}$.

have a bundle of smoothly varying toruses as the phase space. As shown in the one-dimensional case, the phase space is an irregular tube.

Mathematically, each point in a local Brillouin zone is labeled by $\boldsymbol{k}$ and we choose the domain of $\boldsymbol{k}$ as $[-\frac{\pi \boldsymbol{b}(\boldsymbol{x},t)}{2}, \frac{\pi \boldsymbol{b}(\boldsymbol{x},t)}{2}]$, with $-\frac{\pi \boldsymbol{b}}{2}$ and $\frac{\pi \boldsymbol{b}}{2}$ denoting the same point and forming a torus. The position and time dependence of $\boldsymbol{b}(\boldsymbol{x},t)$ shows how the local Brillouin zones vary along spacetime. Due to this geometry, unlike periodic crystals, the meaning of wave vector $\boldsymbol{k}$ is incomplete without pointing out which local Brillouin zone it belongs to. This property brings up the question about how to compare wave vectors in different local Brillouin zones. To answer this question, a correspondence between local Brillouin zones is needed. Thus we introduce the concept of correspondence curves in phase space. Given a wave vector $\boldsymbol{k}$ at some initial position point $\boldsymbol{x}$, we move the wave vector in real space while at the same time deforming the wave vector with local Brillouin zones. This is essentially the same concept of parallel transport in differential geometry. The trajectory of parallel transport in phase space is the line of correspondence as shown in Fig. 3. Particularly, the infinitesimal change of wave vector by a small shift in position is given by $\delta k_m = -\Gamma^n_{mi} k_n dx^i$.

Wave vectors on the same correspondence line are treated equivalently. Thus it is useful to introduce a derivative operation ∇_{x^μ} to encode this equivalence, which we call the lattice covariant derivative. The lattice covariant derivative is crucial for the semiclassical dynamics. For example, the band energy $\varepsilon(\boldsymbol{k}, \boldsymbol{x}, t)$ given by Hamiltonian (3) is a time-dependent phase space function and its derivative in position gives the "force" term responsible for the acceleration of electrons. An important property of ε is that it is periodic in $\boldsymbol{k}$ which makes it compatible with the torus topology of the Brillouin zone. Thus it is natural to require that their lattice covariant derivatives are also periodic:

$$\nabla_{x^\mu} f|_{(\boldsymbol{k}+2\pi\boldsymbol{b},\boldsymbol{x},t)} \equiv \nabla_{x^\mu} f|_{(\boldsymbol{k};\boldsymbol{x},t)}, \qquad (16)$$

where f is an arbitrary periodic function, ∇_{x^μ} is the lattice covariant derivative, and $\mu = 0$ accounts for the time derivative. It is easy to see that the partial derivative with $\boldsymbol{k}$ fixed does not satisfy the above relation. To find the right derivative operation, we consider the total differential change of $f(\boldsymbol{k}; \boldsymbol{x}, t)$:

$$df(\boldsymbol{k}; \boldsymbol{x}, t) = \left[dx^\mu \nabla_{x^\mu} + Dk_i \partial_{k_i} \right] f, \qquad (17)$$

with

$$\nabla_{x^\mu} f = \left(\partial_{x^\mu} - k_l \Gamma^l_{j\mu} \partial_{k_j} \right) f, \qquad (18)$$

$$Dk_i = dk_i + k_j \Gamma^j_{i\mu} dx^\mu, \qquad (19)$$

where instead of using partial derivatives to express the total differential, we rearrange the terms to write it in a lattice covariant form. $dx^\mu \nabla_{x^\mu} f$ is the differential change along the correspondence line and $Dk_i \partial_{k_i}$ is the change along $\boldsymbol{k}$, which is schematically shown in Fig. 3.

Equation (18) gives the desired lattice covariant derivative operation. It is easy to check that the lattice covariant derivative of f is still periodic. As a bonus, we get another quantity $D\boldsymbol{k}$. Noticing that $-\Gamma_\mu k dx^\mu$ is the geometrical change of wave vector due to deformation, $D\boldsymbol{k}$ is the total change subtracting the geometrical change. So we call $D\boldsymbol{k}$ the mechanical change of wave vectors. It is worth pointing out that the mechanical change of wave vector defined this way is also periodic in $\boldsymbol{k}$.

When $f(\boldsymbol{k}, \boldsymbol{x}, t) = \varepsilon(\boldsymbol{k}, \boldsymbol{x}, t)$, its lattice covariant derivative is related to the deformation potential as

$$\nabla_{x^\mu} \varepsilon(\boldsymbol{k}; \boldsymbol{x}, t) = D^n_m(\boldsymbol{k}; \boldsymbol{x}, t) \Gamma^m_{n\mu}, \qquad (20)$$

where $D^n_m \equiv (c^n_\alpha \partial_{c^m_\alpha} - k_m \partial_{k_n})\varepsilon$ is the deformation potential defined in the entire Brillouin zone [21]. Here a trick has been used that when the position and time dependence is through the lattice vectors, partial derivatives can be written as $\partial_{x^\mu} = \Gamma^m_{n\mu} c^n_\alpha \partial_{c^m_\alpha}|_k$. Usually, the deformation potential is defined relative to a particular reference crystal. Here we have a deformation potential tensor field from all local lattices.

B. Electron equations of motion

Next, we show how the equations of motion of electrons can be written in a covariant form with the help of lattice covariant derivatives. In this subsection, we neglect the Berry phase effect first. Without the Berry phase, the electron position $\boldsymbol{x}$ and wave vector $\boldsymbol{k}$ are a pair of canonical variables. Under single-band approximation, for a static deformed crystal, it is straightforward to write down the equations of motion:

$$\dot{\boldsymbol{x}} = \partial_{\boldsymbol{k}} \varepsilon, \qquad (21)$$

$$\dot{\boldsymbol{k}} = -\partial_{\boldsymbol{x}} \varepsilon, \qquad (22)$$

where ε and $\boldsymbol{k}$ are the eigenenergy and eigenstate of the local Hamiltonian (3). Although this form is mathematically correct, the equations of motion are not compatible with the phase space geometry mentioned before since $\partial_{\boldsymbol{x}} \varepsilon$ is not a periodic function in $\boldsymbol{k}$ and breaks the torus topology of Brillouin zones. We can then rewrite the above equations with lattice covariant derivatives as

$$\dot{\boldsymbol{x}} = \partial_{\boldsymbol{k}} \varepsilon, \qquad (23)$$

$$D_t \boldsymbol{k} = -\nabla_{\boldsymbol{x}} \varepsilon, \qquad (24)$$

where not only every term in the above equations can be interpreted as a quantity in phase space but also Eq. (24) acquires the new geometrical meaning that the mechanical change of wave vector is induced by the deformation potential force noticing Eq. (20).

For the time-dependent case, the above equations of motion need to be further modified. We pointed out earlier that the Hamiltonian is written in the co-moving frame of ions; thus ε and $\boldsymbol{k}$ denote the energy and crystal momentum relative to ions, respectively. Keeping this in mind, the equations of motion need to be revised in two aspects. First, the energy dispersion represents the relative velocity of electrons to ions; thus the left-hand side of (23) should be replaced by $\dot{\boldsymbol{x}} - \boldsymbol{W}$ instead. Second, due to the noninertial motion of ions, inertial force should also contribute to the change of the relative crystal momentum $\boldsymbol{k}$ in Eq. (24).

By adding those corrections, we achieve the equations of motion in the most general case as

$$D_t \boldsymbol{x} = \partial_{\boldsymbol{k}} \varepsilon, \qquad (25)$$

$$D_t \boldsymbol{k} = -\nabla_{\boldsymbol{x}} \varepsilon + m_e D_t \boldsymbol{x} \times 2\boldsymbol{\omega} - m_e \boldsymbol{a}, \qquad (26)$$

where $D_t \boldsymbol{x} \equiv \dot{\boldsymbol{x}} - \boldsymbol{W}$ is the relative velocity to ions. $m_e D_t \boldsymbol{x} \times 2\boldsymbol{\omega}$, $-m_e \boldsymbol{a}$ are the inertial forces due to lattice rotation and acceleration, respectively, where $\boldsymbol{\omega} = \frac{1}{2} \boldsymbol{\partial} \times \boldsymbol{W}$ is the angular velocity field and $\boldsymbol{a} = (\boldsymbol{W} \cdot \boldsymbol{\partial})\boldsymbol{W} + \partial_t \boldsymbol{W}$ is the acceleration field. The mechanical change rate of the wave vector is defined as $D_t \boldsymbol{k} \equiv \frac{D\boldsymbol{k}}{dt}$ and in components, it reads

$$D_t k_i \equiv \left(\dot{k}_i + \Gamma^n_{it} k_n + \dot{x}^j \Gamma^n_{ij} k_n \right). \qquad (27)$$

The geometrical meaning of the above equations of motion becomes explicit with the help of lattice covariant derivatives. In fact, if we compare the equations of motion to those of a test particle moving in the real gravitational field [22], we can see they share a lot of similarities. Equation (25) is just the expression of the covariant velocity with $\boldsymbol{W}$ resembling the effect of the spatiotemporal component of the metric tensor. However, the free particle energy dispersion on the right-hand side replaced by the band energy dispersion. $D_t \boldsymbol{k}$ has the form of the covariant derivative of the crystal momentum along the electron trajectory in spacetime, which is the same as the test particle case. However, in real gravity the right-hand side of Eq. (26) vanishes for spinless particles. One of the reasons for this distinction is that our lattice connection is only for the spatial part of the tangent space of the spacetime manifold while the Levi-Civita connection in general relativity is for the total tangent space including the time component. We expect a more complete analogy to gravity can be made by considering the deformation of a Bloch-Floquet crystal [23]. Another reason is that the deformation effect is not completely geometrical in the sense that different crystals have different forms of deformation potential. It is also worth pointing out that the equations of motion have the covariant property under Newtonian coordinate transformation. Particularly, each term in Eq. (25) transforms like a vector and each term in Eq. (26) transforms as a covector. This property allows us to get the equations of motion in other coordinates related by Newtonian coordinate transformation with time universal in all coordinate choices.

Chronologically, we derived the above equations of motion from the following zeroth-order Lagrangian:

$$L_e^0 = -\left[\varepsilon(\boldsymbol{k}; \boldsymbol{x}, t) + \boldsymbol{W} \cdot \boldsymbol{k} + \tfrac{1}{2} m_e \boldsymbol{W}^2 \right] + (\boldsymbol{k} + m_e \boldsymbol{W}) \cdot \dot{\boldsymbol{x}}, \qquad (28)$$

where the first-order terms such as Berry connections and gradient energy are discarded. This Lagrangian can be understood in terms of its free electron limit, where $\varepsilon = \frac{k^2}{2m_e}$ and by defining the laboratory frame canonical momentum $\boldsymbol{p} \equiv \boldsymbol{k} + m_e \boldsymbol{W}$, we have the expected free electron Lagrangian $L_e^0 = p\dot{x} - \frac{p^2}{2m_e}$. Direct variation of the Lagrangian (28) gives the following equations of motion expressed in terms of partial derivatives:

$$\dot{\boldsymbol{x}} = \partial_{\boldsymbol{k}} \varepsilon + \boldsymbol{W}, \qquad (29)$$

$$\dot{\boldsymbol{k}} = -\partial_{\boldsymbol{x}} \varepsilon - \partial_{\boldsymbol{x}} \boldsymbol{W} \cdot \boldsymbol{k} + m_e (\dot{\boldsymbol{x}} - \boldsymbol{W}) \times 2\boldsymbol{\omega} - m_e \boldsymbol{a}. \qquad (30)$$

However, as mentioned earlier the geometrical meaning of this form is less obvious and cannot be interpreted as the equations of motion in phase space. By using the lattice covariant derivative and the local elastic relation $\Gamma^k_{i0} + \Gamma^k_{ji} W^j = \partial_i W^k$, they can be rewritten in the covariant form (25) and (26).

C. Post-Newtonian gravity at band bottom

Motivated by the similarity to the gravitational effect, we study the low-energy dynamics around band extrema and find that the electron dynamics is described by an effective post-Newtonian gravity. Since we only consider the deformation of crystals with spatial periodicity and adopt the Newtonian point of view about time passing uniformly regardless of the deformation, we are unlikely to get a full analogy to the four-dimensional gravity. However, it is reasonable to compare to post-Newtonian gravity, which is the low energy and speed limit of the complete gravitational theory. At band minimum, expanding local energy to the second order of $\boldsymbol{k}$ and expressing the electron wave vector $\boldsymbol{k}$ in terms of $\dot{x}$, we have the Lagrangian (28) as

$$\tilde{L}_e = \tfrac{1}{2} m_{ij}^*(\boldsymbol{x}, t) \dot{x}^i \dot{x}^j - (m_{ij}^* - m_e \delta_{ij}) W^j(\boldsymbol{x}, t) \dot{x}^i$$
$$+ \tfrac{1}{2} (m_{ij}^* - m_e \delta_{ij}) W^i W^j - \Phi(\boldsymbol{x}, t), \qquad (31)$$

where m_{ij}^* is the effective mass, and $\Phi(\boldsymbol{x}, t)$ is the energy at band extrema. It reduces to the Lagrangian of the Newtonian free particle when electron and lattice are decoupled. We compare it with the Lagrangian of an electron in post-Newtonian gravity. By assuming both the velocities of the massive object generating gravity and the test particle are small compared to the velocity of light and keeping to the second-order of velocity, the test particle's Lagrangian reads

$$\tilde{L}_g \approx \tfrac{1}{2} m_e g_{ij} \dot{x}^i \dot{x}^j + m_e g_{0i} \dot{x}^i + m_e \phi, \qquad (32)$$

where $g_{00} = -c^2 + 2\phi$ and ϕ is Newton's gravitational potential. The rest energy of the electron is discarded. Direct comparison of both Lagrangians leads to the equivalent metric

tensor in lattice as

$$\frac{m_{ij}^*}{m_e} \sim g_{ij}, \quad -\left(\frac{m_{ij}^*}{m_e} - \delta_{ij}\right)W^j \sim g_{0i},$$

$$\frac{1}{2}\left(\frac{m_{ij}^*}{m_e} - \delta_{ij}\right)W^i W^j - \frac{\Phi}{m_e} \sim \phi. \quad (33)$$

We emphasize that this effective metric is expressed in the laboratory frame. The motion of electrons follows the geodesic equation given by the above equivalent metric. The first relation between the effective mass tensor and the spatial part of the metric tensor is well known in general solid state physics [24]. The energy at band bottom as a static potential that serves as Newton's gravitational potential is also expected. The new discovery here is the contribution from ionic motion. Particularly the g_{0i} component comes directly from the ionic velocity. It acts as the vector potential of the gravitational electromagnetic field thus can be coupled to the energy magnetization [25] in the system (energy magnetization is analogous to charge magnetization, which is the circular motion of energy current and couples to gravitomagnetic field similarly to Zeeman coupling). It also gives a dynamical contribution to the gravitational potential. The factor $\frac{m_{ij}^*}{m_e} - \delta_{ij}$ which is proportional to the difference between effective mass and bare mass is a manifestation of the dragging effect. For free electrons whose effective mass is just the bare mass this effect vanishes. For effective mass larger and smaller than the bare mass, g_{0i} just have opposite effects. It is also interesting to study the effective gravitational effect for Dirac semimetals or Weyl semimetals.

IV. LATTICE COVARIANT FORMULATION OF BERRY PHASE EFFECTS

In this section, we focus on the Berry phase effects. From the previous discussion, we know that evolution of an electron is described by its trajectory in phase space with a special geometry. Under the adiabatic approximation, the electron Bloch functions will change adiabatically along the trajectory. If the trajectory forms a loop, the initial and final states of the Bloch functions only differ by a phase term called the Berry phase. The corresponding Berry connection and Berry curvature will modify the previous equations of motion (25), (26).

A. Lattice covariant Berry connections and Berry curvatures

The mathematical expressions of the Berry connections involve derivatives of the local Bloch states $u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$ with respect to the extended phase space parameters $(\boldsymbol{k}; \boldsymbol{x}, t)$. However, this is nontrivial in the deforming crystal system. On top of the special geometry of extended phase space mentioned before, there is another difficulty due to Bloch states at different positions and times having different periodicities in $\boldsymbol{r}$. A complete understanding of this problem calls for the concept of the Hilbert bundle [14]. Noticing that all the eigenstates of the local Hamiltonian (3) form a complete basis for the Hilbert space of complex periodic functions with the same periodicity as the local lattice, we can assign such a local Hilbert space to each position $\boldsymbol{x}$, time t, and wave vector $\boldsymbol{k}$. Then we have a Hilbert bundle with its fiber

the local Hilbert space denoted by $\mathcal{F}(\boldsymbol{k}; \boldsymbol{x}, t)$ and the base manifold the extended phase space. $\mathcal{F}(\boldsymbol{k}; \boldsymbol{x}, t)$ is characterized by the local periodicity given by $\{\boldsymbol{c}_\alpha(\boldsymbol{x}, t)\}$. The local Hamiltonian $\hat{H}(\boldsymbol{k}; \boldsymbol{x}, t)$ and local Bloch states $u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$ are operator and states in $\mathcal{F}(\boldsymbol{k}; \boldsymbol{x}, t)$. Thus the problem arises from comparing states in different Hilbert spaces.

Next, we discuss how to resolve this problem. Since Bloch functions of all bands form a complete basis, for convenience we use them to discuss the properties of states in the Hilbert bundle. Under a particular choice of smooth gauge, the Bloch functions satisfy the following boundary conditions:

$$u(\boldsymbol{r} + \boldsymbol{c}_\alpha(\boldsymbol{x}, t), \boldsymbol{k}; \boldsymbol{x}, t) = u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t), \quad (34)$$

$$u(\boldsymbol{r}, \boldsymbol{k} + 2\pi \boldsymbol{b}^\alpha(\boldsymbol{x}, t); \boldsymbol{x}, t) = e^{i\phi^\alpha(\boldsymbol{k}; \boldsymbol{x}, t)} e^{i2\pi \boldsymbol{r} \cdot \boldsymbol{b}^\alpha} u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t). \quad (35)$$

The first condition identifies the periodicity of the local Hilbert space $\mathcal{F}(\boldsymbol{k}; \boldsymbol{x}, t)$, to which the Bloch function belongs. The second condition shows that Bloch functions are quasiperiodic functions in $\boldsymbol{k}$ where "quasi" is due to the Berry phase term $e^{i\phi^\alpha(\boldsymbol{k}; \boldsymbol{x}, t)}$. The factor $e^{i2\pi \boldsymbol{r} \cdot \boldsymbol{b}^\alpha}$ is completely artificial because we denote the Brillouin zone torus with a single domain $\boldsymbol{k} \in [-\pi \boldsymbol{b}(\boldsymbol{x}, t), \pi \boldsymbol{b}(\boldsymbol{x}, t)]$. The Berry phase term cannot be eliminated by single-valued and continuous gauge transformation. For example, in the two-dimensional case, the Berry phase accumulated along the Brillouin zone boundary equals the Chern number.

We view (34), (35) as the boundary conditions characterizing a Hilbert bundle state. Then it is natural to require that the correct derivative operation of Bloch states is still a quantity in this Hilbert bundle and satisfies the above boundary conditions. Along the $\boldsymbol{k}$ direction, it can be verified easily that the gauge invariant derivative $\partial_{\boldsymbol{k}} + i A_{\boldsymbol{k}}$ satisfies this requirement, where $A_{\boldsymbol{k}}$ is defined with $\partial_{\boldsymbol{k}}$ as $A_{\boldsymbol{k}} = \langle u|i\partial_{\boldsymbol{k}}u \rangle$. However, the gauge invariant partial derivative of position $\boldsymbol{x}$ and time t does not satisfy our requirement. Thus we introduce the lattice covariant derivative in the Hilbert bundle denoted by ∇_{x^μ}, whose property is given in Table I. The corresponding gauge invariant derivative $\nabla_{x^\mu} + i A_{x^\mu}$ satisfies the boundary conditions.

Our discussion in the last section is the case where the lattice covariant derivative acts on phase space functions and is given in the first row. The last row in Table I shows how the lattice covariant derivative acts on Bloch functions. Comparing the first row and the last row, we see that when the lattice covariant derivative acts on Bloch functions, in addition to the first two terms which treat Bloch functions in the same way as phase space functions, the third term resolves the issue of the periodicity difference of Bloch functions at different position and time in the same manner.

With the lattice covariant derivative, the definition of the Berry connection is straightforward:

$$A_{x^\mu}(\boldsymbol{k}; \boldsymbol{x}, t) \equiv i\langle u(\boldsymbol{k}; \boldsymbol{x}, t)|\nabla_{x^\mu} u(\boldsymbol{k}; \boldsymbol{x}, t)\rangle, \quad (36)$$

$$A_k(\boldsymbol{k}; \boldsymbol{x}, t) \equiv i\langle u(\boldsymbol{k}; \boldsymbol{x}, t)|\partial_k u(\boldsymbol{k}; \boldsymbol{x}, t)\rangle, \quad (37)$$

where the Bloch functions are normalized with the inner product:

$$\langle u_1|u_2\rangle = \frac{(2\pi)^3}{v(\boldsymbol{x}, t)} \int_v d^3r \, u_1^*(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t) u_2(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t), \quad (38)$$

TABLE I. Lattice covariant derivatives of different phase space subjects. The definition comes naturally once we identify $(\boldsymbol{r}, \boldsymbol{k})$ as local quantities and introduce lattice connections to compare them. For example, $\partial_{\boldsymbol{k}}$ and $d^3 k$ are also local quantities inherited from $\boldsymbol{k}$, whose lattice covariant derivatives are responsible for the second term and third term in the vector density case, respectively.

Phase space quantities	Examples	Lattice covariant derivatives
Scalar functions	$\varepsilon(\boldsymbol{k}; \boldsymbol{x}, t)$	$\nabla_{x^\mu} \varepsilon \equiv \partial_{x^\mu} \varepsilon - \Gamma^n_{m\mu} k_n \frac{\partial \varepsilon}{\partial k_m}$
Vectors	$A_{\boldsymbol{k}}(\boldsymbol{k}; \boldsymbol{x}, t)$	$\nabla_{x^\mu} A_{k_i} \equiv \partial_{x^\mu} A_{k_i} - \Gamma^n_{m\mu} k_n \partial_{k_m} A_{k_i} - \Gamma^i_{j\mu} A_{k_j}$
Vector density	$\boldsymbol{P} = \int \frac{d^3 k}{(2\pi)^3} A_{\boldsymbol{k}}$	$\nabla_{x^\mu} P^i \equiv \partial_{x^\mu} P^i - \Gamma^i_{j\mu} P^j + \Gamma^j_{j\mu} P^i$
Bloch functions	$u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$	$\nabla_{x^\mu} u \equiv \partial_{x^\mu} u - \Gamma^n_{m\mu} k_n \frac{\partial u}{\partial k_m} + \Gamma^m_{n\mu} r^n \frac{\partial u}{\partial r^m}$

where $u_1(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$ and $u_2(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$ are two local Bloch functions of different bands. Here because $\nabla_{x^\mu} u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$ is periodic in $\boldsymbol{r}$, the integral in a unit cell becomes reasonable. The factor $\frac{(2\pi)^3}{v(\boldsymbol{x},t)}$ in Eq. (38) can be viewed as the volume measure and is position and time dependent, which is another indication that laboratory frame is "curved" for electrons. This factor is also necessary for the lattice covariant derivative to satisfy the Leibniz rule: $\nabla_{x^\mu} \langle u' | u \rangle = \langle \nabla_{x^\mu} u' | u \rangle + \langle u' | \nabla_{x^\mu} u \rangle$, where the total inner product on the left-hand side is treated as a phase space function.

The corresponding Berry curvature is defined with the lattice covariant derivative as

$$\Omega_{k_i k_j} \equiv i \left[\langle \partial_{k_i} u | \partial_{k_j} u \rangle - \langle \partial_{k_j} u | \partial_{k_i} u \rangle \right], \quad (39)$$

$$\Omega_{k_i x^\mu} \equiv i \left[\langle \partial_{k_i} u | \nabla_{x^\mu} u \rangle - \langle \nabla_{x^\mu} u | \partial_{k_i} u \rangle \right]; \quad (40)$$

Ω_{xx} and Ω_{xt} are second-order quantities, which will not be discussed here. However, from the above definition the relation between Berry curvatures Ω_{kx} and Berry connections is not so trivial. It turns out that the relation $\Omega_{k_i x^\mu} = \partial_{k_i} A_{x^\mu} - \nabla_{x^\mu} A_{k_i}$ is valid only if the lattice covariant derivative of Berry connection $A_{\boldsymbol{k}}$ is defined as

$$\nabla_{x^\mu} A_{k_i} \equiv \partial_{x^\mu} A_{k_i} - \Gamma^n_{m\mu} k_n \partial_{k_m} A_{k_i} - \Gamma^i_{j\mu} A_{k_j}, \quad (41)$$

where the first two terms treat the Berry connection as a normal phase space scalar function. However, we have an additional term. If looking back at the form of Eq. (27) which is the covariant derivative of a covector form $\boldsymbol{k}$, we can see that the last term in Eq. (41) is a manifestation of the vector property of Berry connection $A_{\boldsymbol{k}}$. We summarize this property in the second row of Table I. It can be easily checked that indeed $A_{\boldsymbol{k}}$ transforms in the same way as the coefficient of a three-dimensional vector under Newtonian coordinate transformation. Mathematically, this additional term is due to the commutation relation $[\nabla_{x^\mu}, \frac{\partial}{\partial k_i}] u = \Gamma^i_{m\mu} \frac{\partial}{\partial k_{cm}} u$, where u is the local Bloch function. It is necessary for the gauge invariance of Berry curvatures. And Berry curvatures $\Omega_{k_i k_j}$, $\Omega_{k_i x^j}$ can be viewed as second-rank tensors.

B. Energy correction and complete equations of motion

We have discussed the lattice covariant derivative of Bloch functions and the corresponding Berry connections. A complete discussion should also include the property of lattice covariant derivatives acting on quantum operators such as the local Hamiltonian. This can be achieved by imposing the

Leibniz rule such that

$$\nabla_{x^\mu} [\hat{S} u](\boldsymbol{k}; \boldsymbol{x}, t) \equiv (\nabla_{x^\mu} \hat{S}) u(\boldsymbol{k}; \boldsymbol{x}, t) + \hat{S}(\boldsymbol{k}; \boldsymbol{x}, t) \nabla_{x^\mu} u, \quad (42)$$

where $\hat{S}(\boldsymbol{k}; \boldsymbol{x}, t)$ is some operator in Hilbert bundle which keeps the periodicity of Bloch functions. With the above requirement, we can directly define the deformation potential operator $\hat{D}^n_m$ in arbitrary crystal system as

$$\nabla_{x^\mu} \hat{H}(\boldsymbol{k}; \boldsymbol{x}, t) \equiv \Gamma^m_{n\mu}(\boldsymbol{x}, t) \hat{D}^n_m. \quad (43)$$

We find that for a generic lattice Hamiltonian as shown in Eq. (3), $\hat{D}^n_m = \mathcal{V}^n_m - \frac{1}{m_e} (\frac{1}{i} \frac{\partial}{\partial r^m} + k_m)(\frac{1}{i} \frac{\partial}{\partial r^n} + k_n)$, which is exactly the one appearing in Eq. (10). Historically, the deformation potential operator is first derived using Lagrangian coordinates [18]. Here we show that it is simply the lattice covariant derivative of the local Hamiltonian. This conclusion only relies on the existence of one-to-one correspondence between ionic distribution and the local Bravais lattice.

With the lattice covariant derivative, most well-known results have the same analytical form only with partial derivatives replaced by lattice covariant derivatives. For example the Hellmann-Feynman theorem in the deformation crystal case can be written as

$$\nabla_{x^\mu} \varepsilon(\boldsymbol{k}; \boldsymbol{x}, t) = \langle u(\boldsymbol{k}; \boldsymbol{x}, t) | \hat{D}^m_n | u(\boldsymbol{k}; \boldsymbol{x}, t) \rangle \Gamma^n_{m\mu}, \quad (44)$$

where the left-hand side is to treat the local band energy as a phase space function and the right-hand side comes from the lattice covariant derivative of the expectation values of local Hamiltonian in Bloch states. Comparing to Eq. (20), it is obvious that deformation potential D^m_n is just the expectation value of the deformation potential operator.

Next, we discuss the first-order correction to energy. It contains a static part and dynamical part. The static contribution comes from the expectation value of the gradient correction Eq. (10) in the wave-packet states, which has two terms: the potential correction $\Gamma^i_{jk}(\boldsymbol{x}, t) \langle u | \hat{O}^{jk}_i | u \rangle$ and the gradient correction $\Gamma^m_{ni} \text{Im}[\langle u | D_{mn} - \hat{D}_{mn} | \partial_{k_i} u \rangle]$. The dynamical part comes from the coupling between lattice rotation and self-rotation of the wave packet: $2\boldsymbol{\omega} \cdot \boldsymbol{J}$, which is a Zeeman type coupling with $\boldsymbol{J} = m_e \frac{i}{2\hbar} \langle \partial_{\boldsymbol{k}} u | \times (\varepsilon - \hat{H}) | \partial_{\boldsymbol{k}} u \rangle$ the angular momentum of the wave packet. This can be understood from the similarity between the form of the Coriolis force in Eq. (26) to the Lorentz force. The detailed derivation of these correction terms is given in Appendix D. In summary, the total energy up to first order reads

$$\varepsilon_{\text{tot}} = \varepsilon + \boldsymbol{\Gamma}_i \text{Im} \langle u | \boldsymbol{D} - \hat{\boldsymbol{D}} | \partial_{k_i} u \rangle + \Gamma \langle \hat{O} \rangle + 2\boldsymbol{\omega} \cdot \boldsymbol{J}. \quad (45)$$

TABLE II. Covariant strain derivatives of different phase space subjects.

Phase space quantities	Examples	Lattice covariant derivatives
Phase space functions	$\varepsilon(\boldsymbol{k}; \boldsymbol{x}, t)$	$\nabla_n^m \varepsilon \equiv c_\alpha^m \frac{\partial \varepsilon}{\partial c_\alpha^n} - \Gamma_{m\mu}^n k_n \frac{\partial \varepsilon}{\partial k_m}$
Phase space vectors	$A_k(\boldsymbol{k}; \boldsymbol{x}, t)$	$\nabla_n^m A_{k_i} \equiv c_\alpha^m \frac{\partial A_{k_i}}{\partial c_\alpha^n} - k_n \partial_{k_m} A_{k_i} - \delta_n^i A_{k_m}$
Vector density	$\boldsymbol{P} = \int \frac{d^3k}{(2\pi)^3} A_k$	$\nabla_n^m P^i \equiv c_\alpha^m \frac{\partial P^i}{\partial c_\alpha^n} - \delta_n^i P^m + \delta_n^m P^i$
Bloch functions	$u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)$	$\nabla_n^m u \equiv c_\alpha^m \frac{\partial u}{\partial c_\alpha^n} - k_n \frac{\partial u}{\partial k_m} + r^n \frac{\partial u}{\partial r^m}$

Up till now, we have all the ingredients to write down the equations of motion up to first order. They are achieved by adding Berry curvatures to Eqs. (25), (26) and using the total energy instead of local band energy. The results are

$$D_t \boldsymbol{x} = \partial_k \varepsilon_{\text{tot}} - D_t \boldsymbol{k} \times \Omega_k - \Omega_{kT}, \tag{46}$$

$$D_t \boldsymbol{k} = -\nabla_x \varepsilon_{\text{tot}} + m_e D_t \boldsymbol{x} \times 2\boldsymbol{\omega} - m_e \boldsymbol{a}, \tag{47}$$

which have a similar analytical form as the result in [10]. However, partial derivatives are replaced by lattice covariant derivatives and the geometrical meaning of each term is more transparent. Equation (46) is the relative velocity of an electron to ions and each term can be viewed as a spatial vector while Eq. (47) is the mechanical change of crystal momentum and each term can be viewed as a spatial covector. This geometrical property guarantees the covariant form of the equations of motion and allows us to directly write down the equations of motion in other coordinates related by Newtonian coordinate transformation. Ω_k is the pseudovector constructed from Ω_{kk}. $\Omega_{kT} = \Omega_{kx} \cdot \dot{\boldsymbol{x}} + \Omega_{kt}$ will give rise to the adiabatic current induced by strain rate and strain gradient. Although Ω_{xx} and Ω_{xt} are not included in the equations of motion as second-order quantities, they play the same role as a magnetic field and electric field, respectively, as discussed in [10]. And the above equations of motion can be derived from the complete first-order Lagrangian:

$$L_e = -\left(\varepsilon_{\text{tot}} + \boldsymbol{W} \cdot \boldsymbol{k} - \tfrac{1}{2} m_e \boldsymbol{W}^2\right) + (\boldsymbol{k} + m_e \boldsymbol{W}) \cdot \dot{\boldsymbol{x}}$$
$$+ (A_t + \dot{\boldsymbol{x}} \cdot A_x) + D_t \boldsymbol{k} \cdot A_k. \tag{48}$$

C. Applications

In the following discussion, we study the response of electrons to deformation, i.e., the four fields describing the lattice bundle $\{c_\alpha(\boldsymbol{x}, t), \boldsymbol{W}(\boldsymbol{x}, t)\}$. This is related to quite a few phenomena such as piezoelectricity, flexoelectricity, strain rate induced orbital magnetization, and electron stress tensors as well as their responses to deformation. Frequently, we need to extract a factor which is related to deformation, e.g., strain, strain gradient, and velocity gradient, to get the corresponding response coefficient. This is achieved by defining the covariant strain derivative ∇_n^m, which has the physical meaning as the differentiation to the unsymmetrized strain tensor and is related to the lattice covariant derivative as $\nabla_{x^\mu} = \Gamma_{n\mu}^m \nabla_n^m$. However, we should notice that this is true only when the position and time dependence of the system comes from the lattice vectors $\{c_\alpha(\boldsymbol{x}, t)\}$ such that $\partial_{x^\mu} = \Gamma_{n\mu}^m c_\alpha^n \partial_{c_\alpha^m}$. Similarly, we summarize the derivative's action on various phase space quantities in Table II.

1. Charge density

The first point to notice is that in general a deformed band insulator is not locally charged neutral due to lattice rotation and strain gradient. Particularly, the electron charge density is given by the integration of the modified density of states [9] in phase space: $D = \frac{1}{(2\pi)^3}[1 + \text{tr}(\Omega_{kx}) - m_e 2\boldsymbol{\omega} \cdot \boldsymbol{\Omega}]$. The form of D comes from the fact that due to the Berry phase effect, electron coordinate $\boldsymbol{x}$ and crystal momentum $\boldsymbol{k}$ are not canonical to each other. While the density of states is $\frac{1}{(2\pi\hbar)}$ for a pair of canonical variables, the Berry phase gives rise to a correction to the density of states as denoted by the Berry curvature terms $\text{tr}(\Omega_{kx}) - m_e 2\boldsymbol{\omega} \cdot \boldsymbol{\Omega}$. Then the electron charge density in real space is given by $-e \sum \int \frac{d^3k}{(2\pi)^3} D f$, where $f(\boldsymbol{k}, \boldsymbol{x}, t)$ is the distribution function which can be achieved for example by solving the Bolzmann equation and the summation $\sum$ is over all bands.

For insulators at zero temperature, f is a step function and it is just the integration of D in $\boldsymbol{k}$ space and summation over all occupied bands. Then the electron density in real space reads $-\frac{en_e}{v} + em_e 2\boldsymbol{\omega} \cdot \sum \int \frac{d^3k}{(2\pi)^3} \Omega_k - e \sum \int \frac{d^3k}{(2\pi)^3} \text{tr}(\Omega_{kx})$ [9]. n_e is the number of itinerate electrons per unit cell. The exact meaning of n_e depends on the first-principles method used. In the "all electron" calculation, n_e includes all the electrons outside the nuclei while in the pseudopotential method, the core electrons are excluded. Under the clamped-ion approximation, the first term is canceled by the ionic charge density. The second term is analogous to the effect of Fermi sea volume change due to the magnetic field in a Chern insulator, where $\boldsymbol{\Omega} = \int \frac{d^3k}{(2\pi)^3} \Omega_k$ is quantized. The third term comes from inhomogeneous piezoelectricity. The physical meaning becomes more transparent if we chose the periodic gauge for A_x in $\boldsymbol{k}$. Then the third term reads $-\partial_i P^i$, where $\boldsymbol{P} = -\frac{e}{(2\pi)^3} \sum \int d^3k A_k$ is the Vanderbilt polarization [8].

2. Deformation induced adiabatic charge current

For simplicity, in the discussion of deformation induced adiabatic charge current, we only consider band insulators at zero temperature such that the distribution function is simply a step function. First, we study the total current of both ions and electrons under the clamped-ion approximation. This approximation states that at each time the distribution of ions within a unit cell follows the instantaneous strain of the unit cell (although there can be an internal strain contribution [17]).

Next, we show that for band insulators at zero temperature, the total current is adiabatic and can be categorized as either electric polarization current or electric magnetization current besides the anomalous current. Particularly, the magnetization due to the motion of the polarization dipole modifies the

charge pumping picture and leads to the concept of proper piezoelectricity [16,26].

Using the equations of motion, it is straightforward to write down the total current density up to first order (Appendix E):

$$\boldsymbol{j}_{\text{tot}} = - e m_e \boldsymbol{a} \times \boldsymbol{\Omega} + \partial \times \boldsymbol{M} + \partial_t \boldsymbol{P} + \partial \times (\boldsymbol{P} \times \boldsymbol{W}), \quad (49)$$

where e is the absolute value of electron charge and the integral is in local $\boldsymbol{k}$ space. And the periodic gauge for the real space Berry connections, $A_{x^\mu}(\boldsymbol{k}) = A_{x^\mu}(\boldsymbol{k} + \boldsymbol{b})$, is used. The first term is the well-known anomalous current density [27], with $\boldsymbol{\Omega} = \frac{1}{(2\pi)^3} \int d^3 k \Omega_{\boldsymbol{k}}$. The anomalous current density here is driven by the inertial force due to ionic acceleration. The second term is the magnetization current density, where $\boldsymbol{M} = -\frac{1}{(2\pi)^3} \frac{e}{2\hbar} \sum_n \int i \langle \partial_{\boldsymbol{k}} u_n | \times (\varepsilon_n + \hat{H} - 2\mu) | \partial_{\boldsymbol{k}} u_n \rangle$ is the orbital magnetization at zero temperature [28]. The third term is the polarization current density. Attention should be paid to the last term. It is the curl of $\boldsymbol{P} \times \boldsymbol{W}$, which indicates that $\boldsymbol{P} \times \boldsymbol{W}$ should be interpreted as the magnetization density. This term comes from the motion of a polarized material, which is actually a well-known phenomenon in classical electromagnetism. As magnetization and polarization form a (3+1)-dimensional antisymmetric tensor, they transform into each other under material motion. The picture is as follows: consider an initially stationary dipole moment $\boldsymbol{P}$ composed by a pair of spatially separated positive and negative charges; if it begins to move at velocity $\boldsymbol{W}$, the two charges give rise to currents of opposite directions and thus an effective current circuit is formed which gives rise to the orbital magnetization density $\boldsymbol{P} \times \boldsymbol{W}$. This effect shows the consistency between the classical electromagnetism and the modern quantum theory of polarization and magnetization in solids.

We then consider the case where the lattice vectors are constant in space and only change slowly with time, and we further assume that at each fixed time t, the lattice has time-reversal symmetry. Then the first term and the second term in Eq. (49) vanish and using the elastic condition (8), (9) the remaining terms can be written in an intriguing form as

$$j_{\text{tot}}^i = \partial_t P^i - \Gamma_{m0}^i P^m + \Gamma_{m0}^m P^i. \quad (50)$$

The first term is the absolute change of polarization density under deformation. The second term is the directional change due to the deformation of crystalline directions. The last term is the magnitude change due to the deformation of unit-cell volume. Equation (50) shows that the last two geometrical changes of polarization density should be subtracted to give the experimentally observed current density. This confirms the argument by Nelson and Vanderbilt [16,29] that only the proper change of polarization can be observed experimentally. Substituting $\boldsymbol{P} = -\frac{e}{(2\pi)^3} \int d^3 k A_{\boldsymbol{k}}$ and $\partial_t = \Gamma_{n0}^m c_\alpha^n \partial_{c_\alpha^m}$, within our lattice covariant formula, Eq. (50) can be conveniently written as

$$j^i = - e \Gamma_{m0}^n \int \frac{d^3 k}{(2\pi)^3} [\boldsymbol{\nabla}_n^m A_{k_i} - \partial_{k_i} A_n^m], \quad (51)$$

where the periodic gauge condition for $A_t = \Gamma_{m0}^n A_n^m$ is used again to retain this gauge invariant form and $A_n^m = i \langle u | \boldsymbol{\nabla}_n^m u \rangle$. Noticing $\boldsymbol{\Gamma}_0$ denotes the strain rate and by defining the proper piezoelectric constant as $e_n^{mi} = \frac{\partial j^i}{\partial \Gamma_{m0}^n}$, we have an explicit

expression for e_n^{mi} as

$$e_n^{mi} = - e \int \frac{d^3 k}{(2\pi)^3} [i \langle \partial_{k_i} u | \boldsymbol{\nabla}_n^m u \rangle - i \langle \boldsymbol{\nabla}_n^m u | \partial_{k_i} u \rangle], \quad (52)$$

which is nothing but the integral of Berry curvature involving $\boldsymbol{k}$ and strain. And the lattice covariant strain derivative gives an explicit meaning for the strain derivative. Its expression in terms of the deformation potential operator is discussed in Appendix G.

Another consequence of Eq. (50) is that the charge pumping picture should be revised in the deforming crystal case. The usual picture states that when the system varies slowly and periodically in time, the charge pumped through a fixed plane in the laboratory frame during one cycle is quantized [7]. However, due to the last two terms in Eq. (50), this picture is changed due to that the right-hand side is not a total time derivative. To see this, by multiplying a factor $v b^\alpha$ on both sides, Eq. (50) reads

$$j_{\text{tot}}^i v b_i^\alpha = - \partial_t (v b_i^\alpha P^i), \quad (53)$$

where $v(t)$ is the unit-cell volume and $\boldsymbol{b}^\alpha(t)$ is the reciprocal lattice vectors. Now the right-hand side becomes a total time derivative and the left-hand side is the current passing through a lattice plane unit cell, where $\boldsymbol{b}^\alpha$ is the normal direction. After integration in time, the left-hand side gives the total charge pumped through a lattice plane unit cell and the right-hand side is the difference of $v b_l^\alpha P^l$ between initial and final state. Suppose the initial and final states are the same; from the uncertainty of P^l, the charge pumped is quantized to some integer. However, noticing that the lattice plane unit cell is constantly changing during the time cycle, the pumped charge through a fixed surface plane in the laboratory frame is not necessarily quantized.

3. Strain gradient induced polarization and strain rate induced magnetization

The first-order current density comes from the variation of the zeroth-order polarization/magnetization. To study the polarization/magnetization induced by strain gradient/rate, current density accurate to second order is needed. As pointed out in the work [30], polarization/magnetization due to inhomogeneity can be divided into two parts: (1) the zeroth-order polarization/magnetization formula expressed with inhomogeneity modified Bloch functions; (2) the Chern-Simons contribution expressed with the zeroth-order local Bloch function. The former will be deferred to future study. Here we concentrate on the Chern-Simons contribution to polarization/magnetization from electrons.

Two results are discussed here: the polarization induced by the strain gradient denoted by lattice connection and orbital magnetization induced by strain rate denoted by the gradient of the velocity field. The former phenomenon is well known as flexoelectricity [12] while the latter phenomenon we call dynamical magnetization. We find that the Chern-Simons contributions to both effects share the same response tensor coefficient given by

$$\mu_n^{mij} = \int [A_{k_i} \boldsymbol{\nabla}_n^m A_{k_j} + A_{k_j} \partial_{k_i} A_n^m + A_n^m \partial_{k_j} A_{k_i}], \quad (54)$$

where $\int \frac{d^3k}{(2\pi)^3}$ is just the **k**-space integral of a Chern-Simons form involving one strain parameter and two **k** parameters. A_n^m is the Berry connection in terms of strain.

The tensor coefficient μ_n^{mij} is antisymmetric with respect to the indices ij and symmetric to mn. The former property is inherited from the Chern-Simons form and the latter is due to the vanishing of the lattice covariant derivative of Bloch functions under local rotation. In terms of this coefficient, the Chern-Simons polarization and magnetization induced by strain gradient and strain rate, respectively, can be written as

$$P_{cs}^i = e\Gamma_{mj}^n \mu_n^{mij}, \qquad (55)$$

$$M_{cs}^{ij} = -e\partial_m W^n \mu_n^{mij} + \left(P_{cs}^i W^j - P_{cs}^j W^i\right). \qquad (56)$$

Equation (55) is the Chern-Simons contribution to flexoelectricity, where the strain gradient is denoted by lattice connection $\{\Gamma_{mj}^n\}$. The well-known picture to understand flexoelectricity is introduced by Taganstsev, where flexoelectricity is described by the ionic effective Born charge multiplied by the displacement induced by strain gradient [17]. The major challenge is the calculation of the effective charge. The longitudinal polarization can be calculated from the local charge density response to ionic position [26,31]. However, the transverse part involves the current response to strain gradient [31]. As can be seen from Appendix E, indeed we achieve the above formula by considering the response of current to strain gradient and strain rate. The key point is to calculate the Abelian Chern-Simons form (54), which is a tractable problem.

Equation (56) is the dynamical magnetization as clearly indicated by the appearance of the velocity field. The first term is induced by the gradient of the velocity field, which is the strain rate experienced by ions. It couples to the same tensor coefficient of Chern-Simons flexoelectricity. This indicates that materials with large bulk flexoelectricity effect may also demonstrate observable dynamical magnetization. The second term is the transformation from polarization to magnetization due to ionic motion as discussed before.

We conclude by summarizing the different parts of polarization/magnetization in Table III, which includes the zeroth-order contributions intrinsic to local lattices and the Chern-Simons contribution due to inhomogeneity.

4. Stress tensor and its responses

The electron stress tensor response to a geometrical background is a very interesting problem. Particularly, the response to the velocity gradient is known as the viscosity term and is a manifestation of the rigidity of the electron system. Electron viscosity has been studied in different cases such as the integer Hall system [32,33], the fractional quantum Hall state [34–36], topological insulators [37], superfluids [38], and in

the time-dependent density functional theory [39]. Here we give a general formula of the electron energy-stress tensor in a spatially homogeneous band insulator at zero temperature including its response to lattice deformation:

$$\mathcal{T}_j^i = \mathcal{D}_j^i + 2\boldsymbol{\omega}\cdot\nabla_j^i\mathcal{J} + \Gamma_{m0}^n\eta_{nj}^{mi} + \boldsymbol{a}\cdot\nabla_j^i\boldsymbol{P}_{m_e}$$
$$+ \frac{m_e}{v}W^iW^j - \left[W^j j_{m_e}^i + i \leftrightarrow j\right], \qquad (57)$$

where the left-hand side is the stress-energy tensor. The derivation is given in Appendix F. First we would like to point out that the indices i and j are symmetric on both sides of the equation. This is because the energy-stress tensor can be viewed as the unsymmetrized strain derivative of electron energy. And this covariant strain derivative vanishes when strain is antisymmetric, i.e., a crystal under rigid body rotation.

The above expression is for a particular filled band while the total energy-stress tensor is the sum of all occupied bands. $\mathcal{D}_j^i = \int \frac{d^3k}{(2\pi)^3}D_j^i$ is the contribution from the deformation potential. It gives the leading order contribution to the stress tensor. The second term is the response of the stress tensor to the rotation of lattices in time, which is the antisymmetric part of the ionic velocity gradient. $\mathcal{J}$ is the orbital angular momentum for a filled band:

$$\nabla_i^j\mathcal{J}^{mn} = a_\alpha^j\frac{\partial\mathcal{J}^{mn}}{\partial a_\alpha^i} - \delta_i^m\mathcal{J}^{jn} - \delta_i^n\mathcal{J}^{mj} + \delta_i^j\mathcal{J}^{mn}, \qquad (58)$$

where $\mathcal{J}^{mn} = m_e\int\frac{d^3k}{(2\pi)^3}\text{Im}\langle\partial_{k_m}u\,|\,(\varepsilon+\hat{H})\,|\,\partial_{k_n}u\rangle$. The first three terms in Eq. (C6) are the strain derivative of a second-rank tensor in retrospect to the first-rank vector case exemplified by the Berry connection term in Table II. The last term comes from the strain derivative of the volume element in **k** space, which reads $\nabla_n^m(d^3k) = -\delta_n^m d^3k$. If we are to put the strain derivative outside the integral $\int d^3k$, this term always appears. Equivalently, we can view a phase space quantity after integration in **k** space as a real space density quantity. The last term is a manifestation of this density property.

The third term in Eq. (57) is the response to strain rate, which is often referred to as the viscosity term. The viscosity tensor has the following explicit form:

$$\eta_{nj}^{mi} = \int d^3k\left[i\langle\nabla_n^m u\,|\,\nabla_j^i u\rangle - i\langle\nabla_j^i u\,|\,\nabla_n^m u\rangle\right], \qquad (59)$$

which is simply the integral of the Berry curvature in terms of the strain parameter in **k** space. Again the meaning of the strain derivative is only clear within our theory as given in Table II. This term is automatically antisymmetric between the two groups of indices mn and ij, and thus is dissipationless. And both mn and ij are symmetric within their own groups. This symmetric property is inherited from the fact that $|\nabla_n^m u\rangle = 0$ when m,n are antisymmetric, i.e.,

TABLE III. Electric polarization and orbital magnetization.

	Polarization	Orbital magnetization
Intrinsic contribution	$\boldsymbol{P}_{in} = e\int A_{\boldsymbol{k}}$	$\boldsymbol{M}_{in} = \boldsymbol{M} + \boldsymbol{P}\times\boldsymbol{W}$
Chern-Simons contribution	$P_{cs}^i = e\Gamma_{mj}^n\mu_n^{mij}$	$M_{cs}^{ij} = -e\partial_m W^n\mu_n^{mij} + \left(P_{cs}^i W^j - P_{cs}^j W^i\right)$

rigid body rotation. Its expression in terms of the deformation potential operator is given in Appendix G.

The fourth term in Eq. (57) is the response to acceleration. $P_{m_e} = m_e \int d^3k A_k$ is the mass polarization of the electron and

$$\nabla_i^j P_{m_e}^n = a_\alpha^j \frac{\partial P_{m_e}^n}{\partial a_\alpha^i} - \delta_i^n P_{m_e}^j + \delta_i^j P_{m_e}^n. \qquad (60)$$

Comparing to Eq. (58), it is easily to see this is the strain derivative of a vector density. Noticing the periodic gauge condition for A_n^m, actually $\nabla_i^j P_{m_e}^n = \frac{m_e}{e} e^{in}_j$ is just the proper piezoelectric constant multiplied by a factor $\frac{m_e}{e}$.

The last two terms in Eq. (57) have the signature of a perfect fluid with energy density and energy current density $(\frac{m_e}{v}, -j_{m_e})$ in coordinates relative to ions. After transforming back to laboratory frame with relative velocity $-W$, we have those terms as part of the energy-stress tensor. And j_{m_e} is the mass current density with expression $j_{m_e}^i = \frac{m_e}{e} \Gamma_{n0}^m e_m^{ni} + \frac{m_e W^i}{v} - m_e^2 (a \times \Omega)^i + (\partial \times \mathcal{J})^i$ in the spatially homogeneous case.

Here we only discussed the spatially homogeneous case for band insulators. The physical meaning of the above stress-energy tensor is to provide a force effect on the dynamics of ions as shown in the derivation of Appendix F. And we did not include the strain gradient contribution to the energy-stress tensor, which will be referred to in future study.

Also, we want to point out the direction to extend the current formalism to study the deformation effect in metals. The equations of motion (46), (47) hold regardless of whether the system is metallic or insulating. The difference between metallic and insulating systems lies in the distribution function which can be calculated, for example, from the Boltzmann equation. Near equilibrium, the distribution function can be divided into a local equilibrium part which is responsible for the intrinsic property and a nonequilibrium part. The nonequilibrium correction can be calculated in the simplest case with relaxation time approximation or more accurately by considering the scattering process introduced by impurities, phonons, or electron-electron interaction. In the hydrodynamic limit, we expect the lattice deformation provides a platform to study the curved space hydrodynamics. It is also interesting to study the electron energy-stress tensor from the hydrodynamic point of view.

V. CONCLUSION

In summary, we have developed a theory describing the semiclassical dynamics of electrons in deforming crystals up to the first order of strain gradient, strain rate, and lattice acceleration. Our theory is based on the lattice bundle picture, where local lattices are introduced to account for the local property of deforming crystals. To compare quantities associated with local lattices with different periodicities, a derivative operation called the lattice covariant derivative is introduced. It takes the place of the partial derivative in expressing the equations of motion including the Berry phase effect. In general, the lattice covariant derivative allows our results to be expressed in a familiar and covariant form under Newtonian coordinate transformation. The geometrical effect of lattice deformation is made explicit in terms of our lattice covariant

formalism. Many deformation effects resemble the effects in a curved spacetime even if expressed in the Euclidean laboratory frame coordinates.

Our formula considers the deformation of an original periodic Hamiltonian and makes no other particular assumption about the property of the Hamiltonian. Thus we expect the results can be easily applied to other periodic systems such as the photonic crystal or cold atom systems. Moreover, our approach provides a way to generate nontrivial geometry for particles coupled to a deformed background. In other systems of different order parameters (in our case the lattice vectors), we expect other types of geometry can be achieved. As the focus of this paper is to set up the framework of our lattice covariant formula, many discussions in the application part are not complete. The most obvious direction to pursue is to include the strain gradient contribution to Bloch functions and the electron energy-stress tensor.

APPENDIX A: LATTICE FRAME

In the main text, the results are expressed in the laboratory frame. This has the advantage that the physical picture is more transparent. However, it is more convenient to derive the results in another curvilinear frame called the lattice frame. This is similar to the relation between Euclidean and Lagrangian description in fluid dynamics. This coordinate transformation method in dealing with the deforming crystal problem is introduced by Whitfield [18].

Here we introduce the lattice frame and discuss its relation with the lattice bundle picture. Lattice frame coordinates are denoted as $\{x'^\alpha, t'\}$, with $\alpha = 1, 2, 3$ representing three crystalline directions. Given the positions of all lattice points in the laboratory frame $\{R_l(t)\}$, we define a smooth lattice field $R(x', t')$ in terms of lattice frame coordinates, which satisfies

$$R_l(t) \equiv R(l, t')|_{t=t'}. \qquad (A1)$$

Then the laboratory frame coordinates are related to lattice frame coordinates as

$$x = R(x', t'), \qquad (A2)$$
$$t = t'. \qquad (A3)$$

From (A1), we see that lattice frame coordinates can be viewed as the continuity of the lattice points label. Any deforming crystal is mapped to a unit cubic lattice in the lattice frame. We require that in a local region deformation is elastic which means the relation (A2) is reversible and x' is also a

function of $\boldsymbol{x}$ and t. In later discussion, we will frequently use this reversibility and change the independent variables of the same fields from $(\boldsymbol{x}', t')$ to $(\boldsymbol{x}, t)$ or vice versa.

To connect to the lattice bundle picture introduced in the main body of this paper, we can define the lattice vector fields and velocity field as

$$\boldsymbol{c}_\alpha(\boldsymbol{x}', t') \equiv \partial_{x'^\alpha} \boldsymbol{R}(\boldsymbol{x}', t'), \tag{A4}$$

$$\boldsymbol{W}(\boldsymbol{x}', t') \equiv \partial_{t'} \boldsymbol{R}(\boldsymbol{x}', t'). \tag{A5}$$

The physical property of the lattice vector fields and velocity field comes naturally from (A1) that

$$\boldsymbol{c}_\alpha\left(\frac{\boldsymbol{l} + (\boldsymbol{l} + 1^\alpha)}{2}, t'\right) = \boldsymbol{R}_{l+1^\alpha}(t') - \boldsymbol{R}_l(t'), \tag{A6}$$

$$\boldsymbol{W}(\boldsymbol{l}, t') = \dot{\boldsymbol{R}}_l(t'). \tag{A7}$$

However, from the definition (A1), Eq. (A6) does not necessarily hold exactly. Here we impose the second requirement for the lattice field such that the left-hand and right-hand sides of Eq. (A6) equal. This is to keep our theory accurate in the first-order gradient of lattice fields at least in the case of constant strain gradient. In the constant strain gradient case, we have the following form of lattice field $\boldsymbol{R}(\boldsymbol{x}', t')$:

$$\boldsymbol{R}(\boldsymbol{x}', t') = N_\alpha^1(t') x'^\alpha + \tfrac{1}{2} N_{\alpha\beta}^2(t') x'^\alpha x'^\beta + N^0(t'), \tag{A8}$$

where $N_{\alpha\beta}^2$ describes a constant strain gradient in space. After substituting Eq. (A8) into Eq. (A6), we can see that Eq. (A6) holds exactly.

From the above definition of lattice vector fields and velocity fields, it is straightforward to show that

$$(\boldsymbol{c}_\alpha \cdot \boldsymbol{\partial}) \boldsymbol{c}_\beta - (\boldsymbol{c}_\beta \cdot \boldsymbol{\partial}) \boldsymbol{c}_\alpha = 0, \tag{A9}$$

$$(\boldsymbol{c}_\alpha \cdot \boldsymbol{\partial}) \boldsymbol{W} - (\boldsymbol{W} \cdot \boldsymbol{\partial}) \boldsymbol{c}_\alpha = \partial_t \boldsymbol{c}_\alpha, \tag{A10}$$

which is the elastic relation addressed by Eq. (67). This shows the consistency between the definition here and the discussion in the main body of this paper. Actually, the elastic condition is the necessary condition for the existence of local lattice fields $\boldsymbol{R}(\boldsymbol{x}', t)$.

Next, we discuss the metrics in the lattice frame. In the lattice frame, lattice points always have unit cubic lattice coordinates and the deformation is described by the metric tensor in this curvilinear coordinate system. This is in contrast to the laboratory frame description where coordinates of lattice points are crucial. The four-dimensional metric tensor in lattice frame is

$$G_{\alpha\beta} = \frac{\partial x^i}{\partial x'^\alpha} \frac{\partial x^i}{\partial x'^\beta} = c_\alpha^i c_\beta^i, \tag{A11}$$

$$G_{0\alpha} = \frac{\partial x^i}{\partial t'} \frac{\partial x^i}{\partial x'^\alpha} = W^i c_\alpha^i, \tag{A12}$$

where we choose $(-1, 1, 1, 1)$ for the Minkowski metric signature. We see that from the above expression the spatial part of the metric is just the contraction between two lattice vectors and the time-space component of the metric is just the velocity field projected to lattice frame coordinate directions. This is consistent with the geometric method of describing the deformation effect [40,41] where the metric tensor is introduced to account for strain effect. Next, we discuss how

the metric fields couple to the first-principles Hamiltonian of electrons written in the lattice frame.

APPENDIX B: GRADIENT EXPANSION TO CRYSTAL POTENTIAL

Viewed in laboratory frame, the total crystal potential which depends on deformed lattice points is responsible for all the deformation effects. However, this potential is not easy to deal with since it has no periodicity. So it is crucial to write the potential in a tractable form. In the case of slowly varying deformation, this is done by expanding the total potential in the first order of strain gradient. Here we show how this process can be conducted with the help of lattice frame defined previously.

In general, the crystal potential is a function of the relative position between electrons and all ions:

$$\bar{V}(\{\boldsymbol{R}_{l\tau} - \boldsymbol{x}\}), \tag{B1}$$

where $\boldsymbol{x}$ is the position of electrons expressed in the laboratory frame. $\boldsymbol{l}$ is the lattice point label and τ is the label of ions inside a unit cell. Here we assume that the position of ions inside a unit cell is completely determined by the lattice points positions while there are exceptions as mentioned earlier in this paper. Thus $\boldsymbol{R}_{l\tau}(\{\boldsymbol{R}_{l'}\})$ can be written as a function of all the lattice points. Due to translational invariance of the whole crystal, when we displace all lattice points by the same amount, all ions in a unit cell will be translated by the same value as well. This property is described by the formula $\boldsymbol{R}_{l\tau}(\{\boldsymbol{R}_{l'}\}) - \boldsymbol{C} = \boldsymbol{R}_{l\tau}(\{\boldsymbol{R}_{l'} - \boldsymbol{C}\})$ with $\boldsymbol{C}$ some constant displacement. Thus we can absorb the overall constant translation of $\boldsymbol{R}_{l\tau}$ into its $\{\boldsymbol{R}_{l'}\}$ dependence. Thus when $\boldsymbol{C} = \boldsymbol{x}$, the total crystal potential can be written as a function of the position difference between electron and lattice points:

$$\bar{V}(\{\boldsymbol{R}_{l\tau} - \boldsymbol{x}\}) = \bar{V}(\{\boldsymbol{R}_{l\tau}(\{\boldsymbol{R}_{l'} - \boldsymbol{x}\})\}) \equiv V(\{\boldsymbol{R}_l - \boldsymbol{x}\}), \tag{B2}$$

where by defining the crystal potential as $V(\{\boldsymbol{R}_l - \boldsymbol{x}\})$ we eliminate the label of ions within a unit cell.

The distribution of $\{\boldsymbol{R}_l\}$ is not periodic in general for a deforming crystal. However, for slowly varying deformation, we can apply a local approximation to transform it into a more tractable form. It is based on the assumption that only ions within some length scale that is much smaller than the length scale of strain variation contribute to the above crystal potential. This is true for metals and nonpolar insulators. For polar materials, the macroscopic electric field caused by polarization needs to be attended to the potential and the argument here applies to the local part. With the lattice field defined in (A1), we have $\boldsymbol{R}_l(t) = \boldsymbol{R}(\boldsymbol{l}, t)$. Expanding $\boldsymbol{l}$ with respect to the electron position in lattice frame $\boldsymbol{x}'$, we have

$$\begin{aligned} \boldsymbol{R}_l(t) - \boldsymbol{x} &= \boldsymbol{R}(\boldsymbol{l}, t) - \boldsymbol{R}(\boldsymbol{x}', t) \\ &\approx (\boldsymbol{l} - \boldsymbol{x}')^\alpha \boldsymbol{c}_\alpha(\boldsymbol{x}, t) \\ &\quad + \tfrac{1}{2}(\boldsymbol{l} - \boldsymbol{x}')^\alpha (\boldsymbol{l} - \boldsymbol{x}')^\beta (\boldsymbol{c}_\beta \cdot \boldsymbol{\partial}) \boldsymbol{c}_\alpha(\boldsymbol{x}, t), \end{aligned} \tag{B3}$$

where the last term is a first-order small quantity proportional to the spatial gradient of lattice vector fields. Substituting back into (B2) and utilizing the property of lattice connection Eq. (5), the Taylor expansion of the potential with respect to

the second term in Eq. (B3) gives the potential as

$$V(\{\boldsymbol{R}_l - \boldsymbol{x}\}) \approx V(\{(l^\alpha - x'^\alpha)\boldsymbol{c}_\alpha(\boldsymbol{x}, t)\}) + \tfrac{1}{2}\Gamma^i_{jk}\hat{O}^{jk}_i, \quad (\text{B4})$$

where $\{\boldsymbol{\Gamma}_k\}$ is the lattice connection introduced in Eq. (4). We call the above procedure the gradient expansion to the crystal potential.

The first term is the potential given by the local lattice at the electron $\boldsymbol{x}$. It is still not periodic due to the position dependence of $\boldsymbol{c}_\alpha(\boldsymbol{x}, t)$. This can be expected in the lattice bundle picture; as the electron moves it experiences different local lattices with potentials of different periodicities. However, the advantage here is that if we transform to the lattice frame and apply the local approximation, the first term becomes periodic and tractable. Actually, due to the invariance of the crystal potential under rigid body rotation of all ions and electrons at the same time, we can rotate three lattice vectors freely without changing the crystal potential, i.e., $V(\{(l^\alpha - x'^\alpha)c^i_\alpha\}) = V(\{(l^\alpha - x'^\alpha)O^i_j c^j_\alpha\})$ with $O^i_j O^i_k = \delta_{jk}$. This property means that the first term actually only depends on the lattice frame metric $\{G_{\alpha\beta} = c^i_\alpha c^i_\beta\}$.

The second term is the gradient correction to the potential, where $\hat{O}^{jk}_i = \sum_l \frac{\partial V(\{\tilde{\boldsymbol{R}}_l - x'^\alpha \boldsymbol{c}_\alpha\})}{\partial \tilde{R}^i_l}(\tilde{R}^k_l - x'^\alpha c^k_\alpha)(\tilde{R}^j_l - x'^\alpha c^j_\alpha)$ with $\tilde{\boldsymbol{R}}_l(\boldsymbol{x}, t) = l^\alpha \boldsymbol{c}_\alpha(\boldsymbol{x}, t)$. It can be understood as the response of the crystal potential operator to the strain gradient denoted by $\{\boldsymbol{\Gamma}_k\}$, and $\hat{O}^{jk}_i$ is the response coefficient.

APPENDIX C: SCHRÖDINGER EQUATION IN LATTICE FRAME

Given the expression of total crystal potential (B4) up to first order of the strain gradient, the Schrödinger equation in the laboratory frame reads

$$i\partial_t \psi = \left[-\frac{1}{2m_e}\Delta + V_{\text{tot}}(\{(l^\alpha - x'^\alpha)\boldsymbol{c}_\alpha\}) \right]\psi, \quad (\text{C1})$$

where $\Delta = \partial^2_x$ is the Laplace operator in the laboratory frame and

$$V_{\text{tot}} = V(\{l^\alpha - x'^\alpha\}\boldsymbol{c}_\alpha) + \tfrac{1}{2}\Gamma^i_{jk}\hat{O}^{jk}_i \quad (\text{C2})$$

comes from Eq. (B4). It is very tempting to express the Schrödinger equation lattice frame $(\boldsymbol{x}', t')$ due to the fact that the potential only depends on $\{l^\alpha - x'^\alpha\}$ and the lattice frame metric.

During the transformation to the lattice frame, if we require that the wave function be invariant under the coordinate transformation, then the Schrödinger equation in the lattice frame simply reads

$$i\partial_{t'}\psi = \left\{ -\frac{1}{2m}\Delta' - iW'^\alpha\partial'_\alpha + V_{\text{tot}}(\{(l^\alpha - x'^\alpha)\boldsymbol{c}_\alpha\}) \right\}\psi, \quad (\text{C3})$$

where $\Delta' = \frac{1}{\sqrt{G'}}\partial'^\alpha(\sqrt{G}\partial'_\alpha)$ is the Laplacian in the lattice frame with $\partial'^\alpha = G^{\alpha\beta}\partial'_\beta$, $\partial'_\beta = \frac{\partial}{\partial x'^\beta}$, and $G' = \det(G_{\alpha\beta})$. $\{G^{\alpha\beta}\}$ is the inverse matrix of $\{G_{\alpha\beta}\}$ and satisfies $G^{\alpha\beta}G_{\beta\gamma} = \delta^\alpha_\gamma$, with repeated indices summed. It has the explicit expression as

$$G^{\alpha\beta} = \frac{\partial x'^\alpha}{\partial x^i}\frac{\partial x'^\beta}{\partial x^i} = b^\alpha_i b^\beta_i, \quad (\text{C4})$$

where $\{\boldsymbol{b}^\alpha\}$ is the reciprocal lattice vector. In order to be more transparent about the meaning of $G_{0\alpha}$, we use the symbol $W'_\alpha = G_{0\alpha}$ to denote this component of the metric tensor. Then we only have spatial indices and the spatial part of metric tensor $\{G'^{\alpha\beta}, G'_{\alpha\beta}\}$ can be used to raise and lower indices. For example, we have

$$W'^\alpha = G^{\alpha\beta}W'_\beta = b^\alpha_i W^i. \quad (\text{C5})$$

However, there is a problem with the Schrödinger equation (C3) that the Hamiltonian on the right-hand side is not Hermitian with respect to the inner product $\int dx'\sqrt{G}$. This inner product is inherited from the definition in the laboratory frame. Since during the transformation the wave function is kept invariant, to ensure that the probability of finding an electron in a given volume is the same expressed in both coordinates, i.e., $\Delta\rho = |\psi|^2 d^3x = |\psi|^2\sqrt{G}d^3x'$, we have to define the inner product in the lattice frame as $\int dx'\sqrt{G}$. To resolve the non-Hermiticity problem, instead of keeping the wave function invariant, we require that the wave function in lattice frame ψ' satisfies the following relation:

$$|\psi|^2 d^3x = |\psi'|^2 d^3x', \quad (\text{C6})$$

as a result of which the physical meaning of the wave function is still kept while the inner product in the lattice frame becomes $\int dx'$. Then we can choose the transformation of the wave function and define the inner product in the lattice frame as

$$\psi' \equiv (G)^{\frac{1}{4}}\psi, \quad (\text{C7})$$

$$\langle\varphi'|\psi'\rangle' \equiv \int \varphi'^* \psi' d^3x'. \quad (\text{C8})$$

As can be seen later, this choice restores the Hermiticity of the Hamiltonian in the lattice frame.

To complete the argument, the transformation relation for operators should also be specified. This can be done by requiring that physical observables have the same value calculated in both frames:

$$\int \varphi^* \hat{S}\psi d^3x = \int \varphi'^* \hat{S}'\psi' d^3x', \quad (\text{C9})$$

where $\hat{S}$ and $\hat{S}'$ are operators in the laboratory frame and lattice frame, respectively. Thus we see that operators transform as

$$\hat{S}' = G^{\frac{1}{4}}\hat{S}G^{-\frac{1}{4}}. \quad (\text{C10})$$

Equipped with this transformation relation, after some long but tedious algebra, we finally have the Schrödinger equation for ψ' in the lattice frame as

$$\begin{aligned}
i\partial_{t'}\psi' = \Big[&-\frac{1}{2m_e}(\partial'_\alpha - im_e W'_\alpha)[G'^{\alpha\beta}(\partial'_\beta - im_e W'_\beta)] \\
&+ V_{\text{tot}}(\{(l^\alpha - x'^\alpha)\boldsymbol{c}_\alpha(\boldsymbol{x}', t')\}) \\
&- \frac{1}{2}m_e W'_\alpha W'^\alpha + V_g \Big]\psi', \quad (\text{C11})
\end{aligned}$$

where $V_g = \frac{1}{8m_e}\partial'_\alpha\partial'^\alpha\ln G + \frac{1}{32m_e}G^{\alpha\beta}(\partial'_\alpha\ln G)(\partial'_\beta\ln G)$ is a pure geometrical quantity. It is second order in strain gradient and thus will be discarded in our first-order theory. It can

be checked that the Hamiltonian in the above Schrödinger equation is Hermitian with respect to the inner product (C8). From Eq. (C3) to Eq. (C11), the derivation is exact and the geometrical potential V_g is the only remembrance of this process. The probability balance equation can be easily deduced from Eq. (C11), which reads

$$\partial_{t'}\rho' + \partial_\alpha' j'^\alpha = 0, \qquad (C12)$$

with $\rho' = |\psi'|^2$ and $j'^\alpha = \frac{1}{2m_e}G'^{\alpha\beta}\{\psi'^* \frac{1}{i}\partial_\beta'\psi' - \psi' \frac{1}{i}\partial_\beta'\psi'^* - 2m_e W_\beta'\rho'\}$. Noticing that $\rho' dx'$ denotes the probability to find the particle in the volume denoted by d^3x', which has the same form as the one in a Cartesian coordinate, it is easy to understand that the probability balance equation (C12) also has the same form expressed with partial derivatives. The first two terms of the current density can be interpreted as the current density of laboratory frame projected to lattice frame basis directions and the third term comes from the relative motion between the lattice frame and laboratory frame.

APPENDIX D: LAGRANGIAN OF WAVE PACKET

The Schrödinger equation in the lattice frame is still hard to solve. The Hamiltonian in Eq. (C11) is neither periodic nor static. However, it is easily seen that both the aperiodicity and time dependence come from the fields $\{W'^\alpha(\mathbf{x}', t'), G^{\alpha\beta}(\mathbf{x}', t')\}$. So if deformation varies slowly in position and time, local approximation and adiabatic approximation can be applied to solve this problem. This can be done systematically with the wave-packet method. We refer to the paper by Sundaram and Niu [10] for a more complete discussion of this method. The basic idea is that if we have a wave-packet state of an electron that is localized both in real space and reciprocal space, with its center position in the lattice frame as $\mathbf{x}_c'$ and $\mathbf{q}_c'$, respectively, the effective Hamiltonian is given by the Taylor expansion of the position operator in metric fields relative to the center position of the wave packet. The zeroth-order and first-order Hamiltonians for the wave-packet state thus read

$$\hat{\tilde{H}}_c' = -\frac{1}{2m}G_c^{\alpha\beta}(\partial_\alpha' - im_e W_{c\alpha}')(\partial_\beta' - im_e W_{c\beta}') \\ + V(\{(l^\alpha - x'^\alpha)\mathbf{c}_{c\alpha}\}) - \frac{1}{2}m_e W_{c\alpha}' W_c'^\alpha, \qquad (D1)$$

$$\Delta\hat{\tilde{H}}_c' = \frac{1}{2}\left[(x'^\alpha - x_c'^\alpha)\frac{\partial \hat{H}_c'}{\partial x_c'^\alpha} + \frac{\partial \hat{H}_c'}{\partial x_c'^\alpha}(x'^\alpha - x_c'^\alpha)\right] \\ + \frac{1}{2}\Gamma_{jk}^i(x_c', t')\hat{O}_i^{jk}\{(l^\alpha - x'^\alpha)\mathbf{c}_{c\alpha}\}, \qquad (D2)$$

where $\{G_c'^{\alpha\beta}, W_{c\alpha}'\}$ are fields evaluated at position $(\mathbf{x}_c', t')$.

The Hamiltonian (D1) seems complicated but is actually easy to solve since it is periodic and the metric tensor and velocity field are just parameters. To solve this eigenproblem, first we define the gauge invariant wave vector k_c' as

$$\mathbf{k}_c' = \mathbf{q}_c' - m_e \mathbf{W}_c'. \qquad (D3)$$

Then the eigenstate and eigenvalue of Hamiltonian (D1) read

$$\tilde{\psi}_c'(\mathbf{x}'; \mathbf{q}_c', \mathbf{x}_c', t') = e^{i\mathbf{q}_c'\mathbf{x}'}u'(\mathbf{x}'; \mathbf{k}_c', \mathbf{x}_c', t'), \qquad (D4)$$

$$\tilde{\varepsilon}_c'(\mathbf{q}_c', \mathbf{x}_c', t') = \varepsilon_c'(\mathbf{k}_c', \mathbf{x}_c', t') - \frac{1}{2}m_e W_c'^\alpha W_{c\alpha}', \qquad (D5)$$

where $u'(\mathbf{x}'; \mathbf{k}_c', \mathbf{x}_c', t')$ and $\varepsilon_c'(\mathbf{k}_c', \mathbf{x}_c', t')$ are eigenstates and eigenenergies of the Hamiltonian without velocity field:

$$\hat{H}_c'(\mathbf{k}_c', \mathbf{x}_c', t') = -\frac{1}{2m}G_c^{\alpha\beta}(\partial_\alpha' + ik_{c\alpha}')(\partial_\beta' + ik_{c\beta}') \\ + V(\{(l^\alpha - x'^\alpha)\mathbf{c}_{c\alpha}\}). \qquad (D6)$$

As a first-order theory in inhomogeneity, we do not need to consider the correction to the wave function from the first-order Hamiltonian (D2). But we do need to consider its correction to energy. To calculate this gradient correction, we first superpose the eigenstates (D4) to construct an electron wave-packet state. Then we calculate the expectation value of the first-order Hamiltonian (D2) in this wave-packet state. Again this process is quite standard in the wave-packet method [10]; we just list the result here:

$$\Delta\tilde{\varepsilon}_c'(\mathbf{q}_c', \mathbf{x}_c', t') = -\operatorname{Im}\langle\partial_{\mathbf{x}_c'}|_{\mathbf{q}_c'}u'| \cdot (\varepsilon_c' - \hat{H}_c')|\partial_{\mathbf{q}_c'}u'\rangle' \\ + \frac{1}{2}\Gamma_{cjk}^i\langle u'|\hat{O}_i^{jk}|u'\rangle', \qquad (D7)$$

where the first and second terms come from the two terms in (D2), respectively. After expressing $(\partial_{\mathbf{q}_c'}, \partial_{\mathbf{x}_c'})$ in terms of $(\partial_{\mathbf{k}_c'}, \partial_{\mathbf{x}_c'})$, the first term gives rise to two terms: $2\boldsymbol{\omega}_c' \cdot \mathbf{J}'$ and $\operatorname{Im}\langle\partial_{\mathbf{x}_c'}|_{\mathbf{k}_c'}u'| \cdot (\varepsilon_c' - \hat{H}_c')|\partial_{\mathbf{k}_c'}u'\rangle'$. $\boldsymbol{\omega}_c'$ defined as $\boldsymbol{\omega}_c' = \frac{1}{2}\partial_{\mathbf{x}_c'}\times \mathbf{W}_c'$ is the angular velocity of lattice and $\mathbf{J}' = \frac{m_e}{2}\operatorname{Im}\langle\partial_{\mathbf{k}_c'}u'| \times (\varepsilon_c' - \hat{H}_c')|\partial_{\mathbf{k}_c'}u'\rangle'$ is the angular momentum of electron.

Then the Lagrangian for the wave packet in the lattice frame reads

$$L_e' = -\left(\varepsilon_{\text{tot}}' - \frac{1}{2}m_e W_c'^\alpha W_{c\alpha}'\right) + (\mathbf{k}_c' + m_e\mathbf{W}_c') \cdot \dot{\mathbf{x}}_c' \\ + \langle\tilde{u}'|i\partial_{\mathbf{x}_c'}\tilde{u}'\rangle' \cdot \dot{\mathbf{x}}_c' + \langle u'|i\partial_{\mathbf{k}_c'}u'\rangle' \cdot \dot{\mathbf{k}}_c' \\ + \langle u'|i\partial_{t'}u'\rangle', \qquad (D8)$$

where $\varepsilon_{\text{tot}}' = \varepsilon_c' - \frac{1}{2}m_e W_c'^\alpha W_{c\alpha}' + 2\boldsymbol{\omega}_c' \cdot \mathbf{J}' + \frac{1}{2}\boldsymbol{\Gamma}_c\langle\mathbf{O}\rangle' + \operatorname{Im}\langle\partial_{\mathbf{x}_c'}u'| \cdot (\varepsilon_c' - \hat{H}_c')|\partial_{\mathbf{k}_c'}u'\rangle'$ is the energy depending on the Bloch functions.

The Lagrangian of the wave packet in the lattice frame (D8) is very useful in deriving results but its physical meaning is usually less clear since we are more accustomed to understanding a physical problem in the laboratory frame. Also, we are left with the question of how to calculate the eigenproblem of Hamiltonian (D6) with *ab initio* calculations. Furthermore, the lattice frame is not globally well defined in the presence of defects so we are unable to consider the topological effect associated with defects in the lattice frame. Based on the above reasons, it is more desirable to express the results in the laboratory frame.

First, we rewrite the Hamiltonian (D6) in orthonormal coordinates defined as

$$r^i = x'^\alpha c_{c\alpha}^i. \qquad (D9)$$

Then the Hamiltonian written in these orthonormal coordinates denoted by $\hat{H}_c$ reads

$$\hat{H}_c(k_c; x_c, t) = \frac{1}{2m_e}\left(\frac{1}{i}\frac{\partial}{\partial r} + k_c\right)^2 + V(\{l^\alpha c_{c\alpha}(x_c, t) - r\}),$$
(D10)

which is exactly the Hamiltonian (3) evaluated at x_c with $k_{ci} \equiv k'_{c\alpha}b^\alpha_{ic}$. Thus we automatically get the transformation rule for the wave vector from the lattice frame to laboratory frame,

$$k_{ci} = k'_{c\alpha}b^\alpha_i(x_c, t),$$
(D11)

which denotes points in the Brillouin zone of the local lattice at (x_c, t).

Then the eigensolution of (D6) is related to the eigensolution of (D10) as

$$u'(x'; k'_c, x'_c, t') = u(x'^\alpha c_{c\alpha}; k'_{c\alpha}b^\alpha_c, x_c(x'_c, t), t),$$
(D12)

$$\varepsilon'_c(k'_c, x'_c, t') = \varepsilon_c(k'_{c\alpha}b^\alpha_c, x_c(x'_c, t), t),$$
(D13)

where $u(r; k_c, x_c, t)$ and $\varepsilon_c(k_c, x_c, t)$ are the eigenstates and eigenenergies of Hamiltonian (D10). Then the Berry connection in the Lagrangian (D8) takes the form

$$\langle u'|i\partial_{x'^\mu_c}u'\rangle' = \frac{\partial x^\nu_c}{\partial x'^\mu_c}\left[\frac{(2\pi)^3}{v_c(x_c, t)}\int d^3r u^* i\nabla_{x^\nu_c}u\right],$$
(D14)

where $v_c(x_c, t)$ is the unit-cell volume at point (x_c, t) and the lattice covariant derivative $\nabla_{x^\nu_c}$ arises naturally. Thus through this line of derivation, we have proved the validity of the lattice covariant derivative.

If we define the Berry connection in the laboratory frame as

$$A_{x^\nu_c} \equiv i\langle u|\nabla_{x^\nu_c}|u\rangle \equiv \frac{(2\pi)^3}{v_c}\int d^3r u^*\nabla_{x^\nu_c}u,$$
(D15)

$$A_{k_{ci}} \equiv i\langle u|\partial_{k_{ci}}|u\rangle \equiv \frac{(2\pi)^3}{v_c}\int d^3r u^*\partial_{k_{ci}}u,$$
(D16)

then the relation between Berry connections in the lattice frame and laboratory frame reads $A_{x'^\mu_c} = \frac{\partial x^\nu_c}{\partial x'^\mu_c}A_{x^\nu_c}$ and $A'_{k'_{c\alpha}} = \frac{\partial x'^\alpha_c}{\partial x^j_c}A_{k_{cj}}$.

The next step is to transform the Lagrangian back to the laboratory frame. Since time is the same for both coordinates, their Lagrangians can also be chosen to be equal for a particular gauge. Then we can write down the Lagrangian in the laboratory frame as

$$L_e = -\left(\varepsilon_{\text{tot}} + W_c \cdot k_c + \frac{1}{2}m_e W^2\right) + (k_c + m_e W_c)\cdot \dot{x}_c$$
$$+ (A_t + \dot{x}_c \cdot A_{x_c}) + D_t k_c \cdot A_{k_c},$$
(D17)

where

$$\varepsilon_{\text{tot}} = \varepsilon_c + \Gamma_c \text{Im}\langle u|D - \hat{D}|\partial_k u\rangle + \Gamma_c\langle\hat{O}\rangle + 2\omega_c \cdot J.$$ (D18)

The first term is the eigenenergy of local Hamiltonian (3) evaluated at x_c. The second and third term come from the gradient correction to local Hamiltonian Eq. (10). The last term is due to lattice rotation and J is the angular momentum of electrons. After omitting the indices c we have the Lagrangian appearing in the main text (48).

APPENDIX E: ORBITAL MAGNETIZATION AND POLARIZATION

Here, we deduce the result in Eq. (49). For an insulator, the total current density up to first order is given by two contributions:

$$j^i_a = \int \dot{x}^i D d^3k,$$
(E1)

$$j^i_b = \partial_j \int \frac{dk}{(2\pi)^3}\text{Im}\left[\left\langle\frac{\partial u_{nk}}{\partial k_i}\Big|H - \varepsilon\Big|\frac{\partial u_{nk}}{\partial k_j}\right\rangle\right],$$
(E2)

where $D = 1 + \text{tr}(\Omega_{kx}) - m_e 2\omega \cdot \Omega_k$ is the density of states. j_b comes from the dipole moments of velocity operator [4]. We can combine Eq. (46) and (47) to solve for $\dot{x}$.

Especially the last two terms in Eq. (49) come from the following terms in j_a:

$$j^i_a = e\int d^3k[-\Omega_{k_ix^j}W^j + \Omega_{k_it} + W^i\text{tr}(\Omega_{kx})].$$
(E3)

To get the same form in Eq. (49), we will frequently use the following identity:

$$\partial_{x^\mu}\int dkf(k, x, t) = -\Gamma^i_{i\mu}\int dkf + \int dk\nabla_{x^\mu}f,$$
(E4)

where f is any phase space function. Choosing the periodic gauge $A_{x^\mu}(k + 2\pi b; x, t) = A_{x^\mu}(k; x, t)$ and noticing that $\nabla_{x^j}A_{k_j} = \partial_{x^j}A_{k_j} - \Gamma^n_{mj}k_n\partial_{k_m}A_{k_j} - \Gamma^j_{ij}A_{k_i}$, we have

$$\int -\Omega_{k_ix^j}W^j = W^j\left(\partial_j P^i - \Gamma^i_{lj}P^l + \Gamma^l_{lj}P^i\right),$$
(E5)

$$\int \Omega_{k_it} = \partial_t P^i - \Gamma^i_{l0}P^l + \Gamma^l_{l0}P^i,$$
(E6)

$$\int W^i\text{tr}(\Omega_{kx}) = -W^i\left(\partial_j P^j - \Gamma^j_{lj}P^l + \Gamma^l_{lj}P^j\right),$$
(E7)

where $P = -\frac{e}{(2\pi)^3}\int A_k$. Substituting back to Eq. (E3) and utilizing the elastic condition $\Gamma^k_{i0} + \Gamma^k_{ji}W^j = \partial_i W^k$, we have the last two terms in Eq. (49):

$$\partial_t P - \partial\times(W\times P).$$
(E8)

Next, we deduce the Chern-Simons contribution to flexoelectricity and dynamical magnetization. We start from the expressions in the lattice frame then transform back to the laboratory frame. Because the lattice connection vanishes in the lattice frame, the results in [30] can be applied directly in the lattice frame. We can directly write down the Chern-Simons contribution to current density as

$$j'^i_{cs} = -e\int dk'\left[\Omega'_{k'_ik'_j}\Omega'_{x'_jt'} + \Omega'_{k'_jx'^j}\Omega'_{k'_it'} + \Omega'_{x'_jk'_i}\Omega'_{k'_jt'}\right]$$

$$= e\partial_{t'}\int dk'\partial_{k'_i}A'_{k'_j}A'_{x'_j} + \partial_{k'_j}A'_{x'_j}A'_{k'_i} + \partial_{x'_j}A'_{k'_i}A'_{k'_j}$$

$$- e\partial_{x'_j}\int dk'\partial_{k'_i}A'_{k'_j}A'_t + \partial_{k_j}A'_t A'_{k_i} + \partial'_t A'_{k_i}A'_{k_j},$$
(E9)

where the periodic gauge condition for real space Berry connections has been used:

$$A'_{t'}(k') - A'_{t'}(k' + 2\pi b') = 0,$$
$$A'_{x'}(k') - A'_{x'}(k' + 2\pi b') = 0,$$

where $\boldsymbol{b}'$ is the reciprocal lattice vector in the lattice frame. From (E9), we can easily identify the polarization and magnetization term as

$$P'^i = e \int dk' A_{k'_i} \partial_{x'j} A_{k'_j} + A_{k'_j} \partial_{k'_i} A_{x'j} + A_{x'j} \partial_{k'_j} A_{k'_i}, \quad \text{(E10)}$$

$$M'^{ij} = -e \int dk' \partial_{k'_i} A_{k'_j} A_{t'} + \partial_{k'_j} A_{t'} A_{k'_i} + \partial_{t'} A_{k'_i} A_{k'_j}. \quad \text{(E11)}$$

Then using the transformation rule of the polarization-magnetization tensor under coordinate transformation, which we have verified in zeroth order, we can get the results given by Eqs. (55) and (56).

APPENDIX F: ENERGY-STRESS TENSOR OF ELECTRON

Here we will demonstrate how the concept of the energy-stress tensor appears naturally by considering the role electrons play in the dynamics of ions. From Appendix A, we can see that the fundamental field describing the ionic degrees of freedom is contained in the lattice field $\boldsymbol{R}(\boldsymbol{x}', t')$ given by Eq. (A1). If we are to consider the dynamics of ions in the least action principle, we need to vary the total action including both the electronic part and ionic part with respect to the lattice field.

Here, we focus on the electron part. The electron Lagrangian written in the lattice frame depends on the lattice frame metric field, which is related to the lattice field as

$$G_{\alpha\beta} = \partial_\alpha R^i \partial_\beta R^i = c_\alpha^i c_\beta^i, \quad \text{(F1)}$$

$$G_{0\alpha} = \partial_\alpha R^i \partial_{t'} R^i = c_\alpha^i W^i. \quad \text{(F2)}$$

The variation in the lattice field can be expressed in terms of the variation in the lattice frame metric, which is just the formal definition of the stress-energy tensor. The action of electrons is given by the Lagrangian of the wave packet as discussed before, which has the following form:

$$A = \int_{V_0} d\boldsymbol{x}' dt' \delta(\boldsymbol{x}' - \boldsymbol{y}'(t')) L'_e(W'(\boldsymbol{y}', t'), \{G'_{\alpha\beta}(\boldsymbol{y}', t')\};$$
$$(\boldsymbol{k}'(t'), \dot{\boldsymbol{y}}'(t'), \dot{\boldsymbol{k}}'(t'))), \quad \text{(F3)}$$

where L'_e is given by Eq. (D8). Here we use variables $(\dot{\boldsymbol{k}}'(t'), \dot{\boldsymbol{y}}'(t'), \boldsymbol{y}'(t'), t')$ to denote the degrees of freedom of the electron as a point particle, all of which are functions of time t'. And we add a factor $\delta(\boldsymbol{x}' - \boldsymbol{y}'(t'))$ to express the action in a field form so that we can apply the variation principle in field theories directly.

Then we vary the above action with respect to the lattice field $\boldsymbol{R}(\boldsymbol{x}', t')$. After some long and tedious calculation, we have

$$F^i = \frac{\delta A_e}{\delta R^i}(\boldsymbol{x}', t') = \frac{\partial L_e}{\partial G_{\alpha\beta}} [\partial_{y'\alpha} \delta(\boldsymbol{x}' - \boldsymbol{y}') \partial_{y'\beta} R^i + \alpha \leftrightarrow \beta]|_{t'}$$

$$+ \frac{\partial L_e}{\partial (\partial_\gamma G_{\alpha\beta})} \partial_{y'\gamma} [\partial_{y'\alpha} \delta(\boldsymbol{x}' - \boldsymbol{y}') \partial_{y'\beta} R^i + \alpha \leftrightarrow \beta]$$

$$- \left\{ \tilde{\partial}_{t'} \left[\frac{\partial L_e}{\partial (\partial_{t'} G_{\alpha\beta})} \right] \partial_{y'\beta} R^i \partial_{y'\alpha} \delta(\boldsymbol{x}' - \boldsymbol{y}') + \alpha \leftrightarrow \beta \right\}$$

$$+ \left[\frac{\partial L_e}{\partial G_{0\alpha}} \partial_{y'\alpha} \delta(\boldsymbol{x}' - \boldsymbol{y}') \partial_{t'} R^i \right.$$

$$- \delta(\boldsymbol{x}' - \boldsymbol{y}') \tilde{\partial}_{t'} \left(\frac{\partial L_e}{\partial G_{0\alpha}} \partial_{y'\alpha} R^i \right) \right]$$

$$+ \frac{\partial L_e}{\partial (\partial_\gamma G_{0\alpha})} \partial_{y'\gamma} [\partial_{y'\alpha} \delta(\boldsymbol{x}' - \boldsymbol{y}') \partial_{t'} R^i]$$

$$- \tilde{\partial}_{t'} \left\{ \frac{\partial L_e}{\partial (\partial_\gamma G_{0\alpha})} \partial_{y'\gamma} [\delta(\boldsymbol{x}' - \boldsymbol{y}') \partial_{y'\alpha} R^i] \right\}, \quad \text{(F4)}$$

where the derivative operator $\tilde{\partial}_{t'}$ only acts the explicit time dependence while not on the time dependence of those variables $(\dot{\boldsymbol{k}}'(t'), \dot{\boldsymbol{y}}'(t'), \boldsymbol{y}'(t'))$. Here we have not used the expressions of $(\dot{\boldsymbol{k}}', \dot{\boldsymbol{y}}')$ which can be given by the equations of motion in the lattice frame. $\frac{\delta S_e}{\delta R^i}$ describes the force density of electrons exerted on ions. We see from the delta function $\delta(\boldsymbol{x}' - \boldsymbol{y}')$ that the effective interaction between electron and ion is local, which is inherited from the local approximation and adiabatic approximation we used.

Equation (F4) is the contribution from a single electron. However, we have multiple electrons filling in the band structure. Then we need to sum over all electrons in a filled band with the integration of density of states and substitute the expression for $(\dot{\boldsymbol{k}}', \dot{\boldsymbol{y}}')$ given by the equations of motion. For simplicity, here we only consider a particular band in an insulator at zero temperature. Then the total force from all electron contributions reads

$$\mathcal{F}^i(\boldsymbol{x}', t') = \int dy' dk' D' \frac{\delta A_e}{\delta R^i}(\boldsymbol{x}', t'), \quad \text{(F5)}$$

where we adopt the convention to use the script form of the symbol to denote all electron contributions, such as $\mathcal{F}$ as the total contribution from the F of each individual electron.

Then substituting Eq. (F4) into the above expression, we have a very simple form that

$$\mathcal{F}^i(x', t') = \sqrt{G} [\partial_j \mathcal{T}^{ij} + \partial_t \mathcal{T}^{0i}], \quad \text{(F6)}$$

where

$$\mathcal{T}^{ij} = \frac{\partial x^i}{\partial x'^\alpha} \frac{\partial x^j}{\partial x'^\beta} \mathcal{T}^{\alpha\beta} + \mathcal{T}^{0i} W^j + W^i \mathcal{T}^{0j}, \quad \text{(F7)}$$

$$\mathcal{T}^{0i} = \frac{\partial x^i}{\partial x'^\beta} T^{0\beta}, \quad \text{(F8)}$$

and $\mathcal{T}^{\alpha\beta}, \mathcal{T}^{0\beta}$ are the four-dimensional energy-stress tensors of electrons in the lattice frame defined as

$$\mathcal{T}^{\alpha\beta}(\boldsymbol{x}', t') = - \int dk' D' \frac{2}{\sqrt{G}} \left\{ \frac{\tilde{\partial} L}{\tilde{\partial} G_{\alpha\beta}} - \partial_\sigma \frac{\tilde{\partial} L_e}{\tilde{\partial}(\partial_\sigma G_{\alpha\beta})} \right.$$

$$\left. - \tilde{\partial}_{t'} \frac{\tilde{\partial} L_e}{\tilde{\partial}(\partial_{t'} G_{\gamma\delta})} \right\}, \quad \text{(F9)}$$

$$\mathcal{T}^{0\alpha}(\boldsymbol{x}', t') = - \int dk' D' \frac{1}{\sqrt{G}} \left\{ \frac{\tilde{\partial} L_e}{\tilde{\partial} G_{0\alpha}} - \partial_\sigma \frac{\tilde{\partial} L_e}{\tilde{\partial}(\partial_\sigma G_{0\alpha})} \right\}, \quad \text{(F10)}$$

where $\frac{\tilde{\partial}}{\tilde{\partial} G_{\alpha\beta}}, \frac{\tilde{\partial}}{\tilde{\partial}(\partial_\sigma G_{\alpha\beta})}, \frac{\tilde{\partial}}{\tilde{\partial}(\partial_{t'} G_{\gamma\delta})}, \frac{\tilde{\partial}}{\tilde{\partial} G_{0\alpha}}, \frac{\tilde{\partial}}{\tilde{\partial}(\partial_\sigma G_{0\alpha})}$ do not act on the metric dependence of $(\dot{\boldsymbol{k}}', \dot{\boldsymbol{y}}')$ whose expression is given by the equations of motion and $D' = [1 + \text{tr}(\Omega'_{k'x'}) - 2m_e \boldsymbol{\omega}' \cdot \boldsymbol{\Omega}']$

while ∂_σ acts on all the position dependence including that in the expression of $(\dot{\boldsymbol{k}}', \dot{\boldsymbol{y}}')$.

Here we come up with the expressions (F9), (F10) to ensure the physical meaning of energy-stress tensor, i.e., the form of Eq. (F6). Equivalently, we can define the energy-stress tensor directly in the lattice frame following the variation to the metric as

$$T^{\alpha\beta} \equiv -2\frac{1}{\sqrt{G}}\frac{\delta A}{\delta G_{\alpha\beta}}, \qquad (\text{F11})$$

$$T^{0\alpha} \equiv -\frac{1}{\sqrt{G}}\frac{\delta A}{\delta G_{0\alpha}}, \qquad (\text{F12})$$

where the definitions of $T^{\alpha\beta}$ and $T^{0\alpha}$ differ by a factor of two besides their variations to different components of the metric, which is a feature of nonrelativistic theory [42]. Then following the same procedure in calculating $\mathcal{F}^i$ from F^i, we can achieve the expressions (F9), (F10).

To calculate the specific form of energy-stress tensor, we need to substitute the expression of electron Lagrangian Eq. (D8) into Eqs. (F9), (F10). The calculation is very tedious but straightforward; thus we only list the result here:

$$\begin{aligned}
T^{\alpha\beta} = \frac{2}{\sqrt{G}}\int dk' D' &\left\{ \frac{\tilde{\bar{\partial}}\varepsilon'}{\tilde{\bar{\delta}}G_{\alpha\beta}} + \frac{1}{2}m_e G^{0\alpha}G^{0\beta}D' \right.\\
&+ m_e\partial_\sigma G_{0\gamma}\,\text{Im}\,\tilde{\bar{\delta}}_{G_{\alpha\beta}}\langle\partial_{k'_\gamma}u'|(\varepsilon'-\hat{H}')|\partial_{k'_\sigma}u'\rangle'\\
&\left. - \dot{\boldsymbol{k}}'\cdot\frac{\tilde{\bar{\partial}}A'_{k'}}{\tilde{\bar{\partial}}G_{\alpha\beta}} - \partial_{t'}G_{\sigma\gamma}\Omega_{G_{\alpha\beta}G_{\sigma\gamma}} \right\}\\
= 2\int\frac{dk'}{\sqrt{G}}&\left\{ \tilde{\bar{\partial}}_{G_{\alpha\beta}}\varepsilon' + \frac{1}{2}m_e G^{0\alpha}G^{0\beta} \right.\\
&+ m_e\partial_\sigma G_{0\gamma}\,\text{Im}\,\tilde{\bar{\delta}}_{G_{\alpha\beta}}\langle\partial_{k'_\sigma}u'|(\varepsilon'+\hat{H}')|\partial_{k'_\gamma}u'\rangle'\\
&\left. + m_e a^l_\gamma\partial_{t'}W^l\tilde{\bar{\delta}}_{G_{\alpha\beta}}A'_{k'_\gamma} - \partial_{t'}G_{\sigma\gamma}\Omega_{G_{\alpha\beta}G_{\sigma\gamma}} \right\},
\end{aligned}$$

where from the second line to the third line, we substitute the expression of $\dot{\boldsymbol{k}}'$ and use the periodic gauge condition for $\langle u'|i\partial_{G_{\alpha\beta}}u'\rangle'$. $\Omega_{G_{\alpha\beta}G_{\sigma\gamma}} = i[\partial_{G_{\alpha\beta}}\langle u'|\partial_{G_{\sigma\gamma}}u'\rangle' - \partial_{G_{\sigma\gamma}}\langle u'|\partial_{G_{\alpha\beta}}u'\rangle']$ is the Berry curvature with respect to lattice metric. On the other hand,

$$\begin{aligned}
T^{0\alpha} &= -\int dk' D'\frac{1}{\sqrt{G}}\frac{\tilde{\bar{\partial}}L_e}{\tilde{\bar{\partial}}G_{0\alpha}}\\
&= -\int\frac{dk'}{\sqrt{G}}D'(m_e W'^\alpha + m_e\dot{x}'^\alpha).
\end{aligned}$$

Then following Eqs. (F7), (F8) and using the identity $2\frac{\partial}{\partial G_{\alpha\beta}} = b^\beta_i\frac{\partial}{\partial a^i_\alpha}$, we have the energy-stress tensor in the laboratory frame as

$$\begin{aligned}
\mathcal{T}^i_j = \mathcal{D}^i_j - 2\boldsymbol{\omega}\cdot\nabla^i_j\mathcal{J} &+ \nabla^i_j P_{m_e}\cdot a - \Gamma^m_{l0}\int dk\Omega^{jl}_{im}\\
&+ \frac{m_e}{v}W^i W^j - [W^j j^i_{m_e} + i\leftrightarrow j].
\end{aligned} \qquad (\text{F13})$$

We illustrate the physical meaning of each term in the main body of this paper.

APPENDIX G: EXPRESSIONS IN MOMENTUM REPRESENTATION

Although we introduce the concept of the lattice covariant in the position representation in order to contrast with the normal partial derivatives, often it is more convenient to calculate in momentum space. So it is worthwhile to discuss the expression in momentum space. Since the local Hamiltonians and Bloch states all have the same periodicity as local lattices, their expression in momentum space only involves discrete momentum basis $|l\rangle = \exp[2\pi i l_\alpha \boldsymbol{b}^\alpha(\boldsymbol{x}, t)\cdot\boldsymbol{r}]$, where l is some integer and $\boldsymbol{b}(\boldsymbol{x}, t)$ the reciprocal lattice vector at $(\boldsymbol{x}, t)$. If we calculate the lattice covariant derivative of Bloch states expressed on the momentum basis, we have

$$\nabla_{x^\mu}u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t) = \sum_l \left[\partial_{x^\mu}u_l + \Gamma^n_{m\mu}k_n\partial_{k_m}u_l\right]\exp(il_\alpha\boldsymbol{b}^\alpha\cdot\boldsymbol{r}), \qquad (\text{G1})$$

where $u_l(\boldsymbol{k}; \boldsymbol{x}, t) = \int d\boldsymbol{r}\,u(\boldsymbol{r}, \boldsymbol{k}; \boldsymbol{x}, t)\exp[-2\pi i l_\alpha\boldsymbol{b}^\alpha(\boldsymbol{x}, t)\cdot\boldsymbol{r}]$ is the Fourier component of Bloch functions. An important property is that the basis $|l\rangle$ vanishes under the lattice covariant derivative while not under the partial derivative. Thus in the momentum representation the lattice covariant derivative takes a simpler form as

$$\nabla_{x^\mu} = \partial_{x^\mu} + \Gamma^n_{m\mu}k_n\partial_{k_m}, \qquad (\text{G2})$$

which acts on the Fourier components. Then the real space Berry connection can be conveniently expressed as

$$A_{x^\mu} = i\Gamma^n_{m\mu}\sum_l u^*_l\left(a^m_\alpha\partial_{a^n_\alpha} + k_n\partial_{k_m}\right)u_l, \qquad (\text{G3})$$

where the relation $\partial_{x^\mu} = \Gamma^n_{m\mu}a^m_\alpha\partial_{a^n_\alpha}$ is used. The normalization condition for the Bloch function is $\sum_l u^*_l u_l = 1$ from Eq. (38).

For the local Hamiltonian, its matrix element expressed in momentum representation is

$$H_{l,l'} = \frac{(\boldsymbol{G}_l + \boldsymbol{k})^2}{2m}\delta_{l,l'} + V(\boldsymbol{G}_{l-l'}(\boldsymbol{x}, t)), \qquad (\text{G4})$$

where $\boldsymbol{G}_l = 2\pi l_\alpha\boldsymbol{b}^\alpha$, $\boldsymbol{G}_{l-l'} = 2\pi(l-l')_\alpha\boldsymbol{b}^\alpha$, and $V(\boldsymbol{G}) = \frac{1}{v}\int d\boldsymbol{r}\,V(\{\tilde{R}_l - \boldsymbol{r}\})\exp(i\boldsymbol{G}\cdot\boldsymbol{r})$ is the Fourier component of the local crystal potential. Directly applying (G2), we have the lattice covariant derivative of the local Hamiltonian as

$$\nabla_{x^\mu}\hat{H}_{l,l'} = \hat{D}^m_{n;l,l'}\Gamma^n_{m\mu}, \qquad (\text{G5})$$

where $\{\hat{D}^m_{n;l,l'}\}$ is the deformation potential operator in the momentum representation, which reads

$$\hat{D}^m_{n;l,l'} = -\left[\frac{(G_l+k)_m(G_l+k)_n}{2m}\delta_{l,l'} + \nabla^m_n V(\boldsymbol{G}_{l-l'})\right]. \qquad (\text{G6})$$

$\nabla^m_n V(\boldsymbol{G}) = \lim_{\delta G_l\to 0}\frac{V(\boldsymbol{G}+\delta\boldsymbol{G})-V(\boldsymbol{G})}{\delta G^m_\alpha}G^\alpha_n$ is the derivative of the crystal potential to strain expressed in reciprocal space. $V(\boldsymbol{G}+\delta\boldsymbol{G})$ and $V(\boldsymbol{G})$ correspond to two crystals with different periodicities. This has also been touched on in the paper [21]. However, this discussion here is valid in the general case not limited to the rigid ion model.

The energy effect of deformation operator has been discussed thoroughly [43], which is the diagonal part in the Bloch basis. Its off-diagonal part also plays an important role in electron dynamics through Berry curvatures. This can be seen

through the expression of Berry curvatures as a sum over all band contributions. For example, $\Omega_{nk_i}^m$ can be written as

$$\Omega_{nk_i}^m = i \sum_{l \neq 0} \frac{\langle u_0 | \hat{D}_n^m | u_l \rangle \langle u_l | \hat{v}_i | u_0 \rangle - \langle u_0 | \hat{v}_i | u_l \rangle \langle u_l | \hat{D}_n^m | u_0 \rangle}{(\varepsilon_0 - \varepsilon_l)^2},$$

(G7)

where 0 is the band we are interested in and l labels all other bands. The role of the deformation potential operator

is explicit in this expression. Integration in the Brillouin zone $-e \int d^3 k i \sum_{l \neq 0} \frac{\langle 0 | \hat{O}_{mn} | l \rangle \langle l | \hat{v}_i | 0 \rangle - \langle 0 | \hat{v}_i | l \rangle \langle l | \hat{O}_{mn} | 0 \rangle}{(\varepsilon_0 - \varepsilon_l)^2}$ just gives the proper piezoelectric constant.

The viscosity term comes from the Berry curvature Ω_{nq}^{mp} involving strain and can be written as

$$\Omega_{nq}^{mp} = i \sum_{l \neq 0} \frac{\langle u_0 | \hat{D}_n^m | u_l \rangle \langle u_l | \hat{D}_q^p | u_0 \rangle - \langle u_0 | \hat{D}_q^p | u_l \rangle \langle u_l | \hat{D}_n^m | u_0 \rangle}{(\varepsilon_0 - \varepsilon_l)^2}.$$

(G8)

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