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Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and Berry-phase effects

Ganesh Sundaram and Qian Niu
Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081
(Received 8 June 1998)

We present a unified theory for wave-packet dynamics of electrons in crystals subject to perturbations varying slowly in space and time. We derive the wave-packet energy up to the first-order gradient correction and obtain all kinds of Berry phase terms for the semiclassical dynamics and the quantization rule. For electromagnetic perturbations, we recover the orbital magnetization energy and the anomalous velocity purely within a single-band picture without invoking interband couplings. For deformations in crystals, besides a deformation potential, we obtain a Berry-phase term in the Lagrangian due to lattice tracking, which gives rise to new terms in the expressions for the wave-packet velocity and the semiclassical force. For multiple-valued displacement fields surrounding dislocations, this term manifests as a Berry phase, which we show to be proportional to the Burgers vector around each dislocation. [S0163-1829(99)07023-X]

I. INTRODUCTION

Our understanding of electronic properties of crystalline solids is primarily based on the Bloch theory for periodic systems.[1] It has been of great interest to extend this theory to situations where crystals are perturbed in various ways. So far, the most useful description has been the semiclassical theory for electron dynamics within a band supplemented by the semiclassical quantization rule or the Boltzmann transport equations. For example, the equations of motion of Bloch electrons in electromagnetic fields are given by[2]

$$\dot{\mathbf{x}}=\frac{1}{\hbar}\frac{\partial \mathcal{E}_{0,n}(\mathbf{k})}{\partial \mathbf{k}},$$

$$\hbar\dot{\mathbf{k}}=-e\mathbf{E}-e\dot{\mathbf{x}}\times\mathbf{B}, \tag{1.1}$$

where $\mathcal{E}_{0,n}(\mathbf{k})$ is the energy of the nth band of an unperturbed crystal. These equations have played a fundamental role in the physics of metals and semiconductors.

The derivation of Eq. (1.1) dates back to Bloch, Peierls, Jones and Zener in the early 1930s.[3] By assuming that the transition probabilities to other bands are negligible, they showed that Eqs. (1.1) describe the motion of a narrow wave packet obtained by superposing the Bloch states of a band. Various extensions of the theory have been made to deal with perturbations of more general nature and to obtain corrections to Eqs. (1.1) in high fields.

Peierls[4] pioneered the effort of constructing an effective one-band Hamiltonian to describe the quantum dynamics of a Bloch electron. By using the tight-binding model, he was able to show that the effective Hamiltonian in the presence of a magnetic field may be obtained by replacing the crystal momentum $\hbar\mathbf{k}$ by the gauge invariant momentum operator $[-i\hbar\nabla+e\mathbf{A}(\hat{\mathbf{x}})]$ in the unperturbed band energy

$$\hat{H}_{\rm eff}=\mathcal{E}_{0,n}\left[-i\nabla+\frac{e}{\hbar}\mathbf{A}(\hat{\mathbf{x}})\right], \tag{1.2}$$

which later came to be known as the Peierls substitution. Two decades later, Slater[5] and Luttinger[6] gave a more rigorous derivation of the effective Hamiltonian for electromagnetic perturbations, by expanding the wave function in the basis of Wannier functions

$$\Psi(\mathbf{x},t)=\sum_l f_l(t)W(\mathbf{x}-\mathbf{R}_l), \tag{1.3}$$

where $\{\mathbf{R}_l\}$ are the lattice positions. They showed that the envelope function $f(\mathbf{x},t)$, defined by $f(\mathbf{R}_l,t)=f_l(t)$ and a smooth interpolation between the atomic positions, satisfies the effective Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}f=\left\{\mathcal{E}_{0,n}\left[-i\nabla+\frac{e}{\hbar}\mathbf{A}(\mathbf{x})\right]-e\phi(\mathbf{x})\right\}f, \tag{1.4}$$

where $\phi(\mathbf{x})$ is a slowly varying scalar potential. The equations of motion (1.1) then follow from Eq. (1.4) and the correspondence principle.

Further development of the theory was made by taking into account the effects of interband coupling. Adams[7] extended the works of Slater and Luttinger to many-band operator formalism. Karplus, Luttinger, and Kohn derived a correction to the velocity, known as the anomalous velocity, and predicted a spontaneous Hall effect in ferromagnetic materials.[8] Later, Adams and Blount[9,10] showed that this term arises from the noncommutability between the Cartesian components of the intraband position operator. Recently, Chang and Niu[11,12] related the anomalous velocity correction to the Berry phase associated with the electron motion in an energy band.[13–15] Corrections to the effective Hamiltonian as an asymptotic series in the field strength were obtained by eliminating the interband matrix elements

with unitary transformations by Kohn, Blount, and Roth in the early 1960s.[16] Later, Brown[17] extended the Wannier function method to crystals under high magnetic fields using magnetic-translation symmetry. A decade later, a variant of the Wannier function method that treats position and momentum in a symmetric way, known as kq-representation, was developed by Zak.[18] Recently, Rammal and Bellissard used an algebraic approach[19] and Wilkinson an operator approach[20] to derive the first-order field correction for the special case of the Harper's equation.[21,22]

Another approach to this problem involves the use of the WKB expansion to derive a Hamilton-Jacobi equation, and then making the correspondence from the classical variables to the quantum operators. This method was applied by many researchers to understand the nature of the spectrum and the wave function of electrons described by the Harper's equation, particularly in the semiclassical limit.[22] A more general treatment of the problem is based on a two-scale expansion in which the electron coordinate and the slowly varying vector potential are regarded as independent variables.[23]

In this paper, we come back to the original consideration of a wave packet in a band and use a time-dependent variational principle[24,25] to derive the wave-packet energy up to first order in the gradient of the perturbations and Berry-phase corrections to the semiclassical dynamics and the quantization rule. We are able to obtain the magnetization energy and the anomalous velocity entirely from the single-band point of view. Also, our method can be directly extended to the case of slowly perturbed magnetic bands, where methods based on the usual Wannier function approach break down because of the nonexistence of localized Wannier functions for such bands in general.[26]

This program was started with Chang and Niu[11,12] for the special case of a two-dimensional periodic system in a strong magnetic field. Here we establish a unified framework for slowly perturbed crystals whose Hamiltonian can be expressed in the form

$$H[\hat{\mathbf{x}},\hat{\mathbf{p}};\beta_1(\hat{\mathbf{x}},t),\ldots,\beta_r(\hat{\mathbf{x}},t)], \tag{1.5}$$

where $\{\beta_i(\mathbf{x},t)\}$ are the modulation functions characterizing the perturbations. They may represent either deformation strain fields, gauge potentials of electromagnetic fields, or slowly varying impurity potentials. They also appear in model potentials for modulated and incommensurate crystals,[27] and for graded semiconductors.[28]

We shall illustrate our formalism with two special cases of perturbations: electromagnetic fields and deformations in crystals. In the first case, in addition to the corrections of orbital magnetization energy and anomalous velocity mentioned above, we discuss the Peierls substitution, Berry-phase-modified Landau levels, and Zak-phase-modified Wannier-Stark levels. For deformational perturbations, we show that the deformation correction to the wave-packet energy can be obtained from the differential shift in the band energy under uniform strain. Then we obtain for the Lagrangian a Berry phase term due to lattice tracking, which gives rise to new terms in the expressions for the wave packet velocity and the semiclassical force; for multiple-valued displacement fields in the presence of dislocations, this term manifests as a Berry phase, which we show to be proportional to the Burgers vector around each dislocation, and thus, in a sense keeps track of the lattice position. We also discuss the consequences of the Berry phase term on electron transport, and the Aharonov-Bohm-type effects in dislocated crystals.

The paper is organized as follows. We present our formalism in Sec. II, treat electromagnetic and deformational perturbations in Secs. III and IV, respectively, and conclude with a summary in Sec. V.

II. FORMALISM

We shall begin by constructing a basis local to the wave packet and describe the wave packet in detail. Then we derive the Lagrangian, the semiclassical equations of motion, and Berry-phase correction to the semiclassical quantization, and discuss some aspects of formal quantization through the Hamiltonian formalism.

A. The local basis and the wave packet

Consider a wave packet centered at $\mathbf{x}_c$ at a given time, with its spread small compared to the length scale of the perturbations. Then the approximate Hamiltonian that the wave packet ''feels'' may be obtained by linearizing the perturbations about the wave-packet center as

$$\hat{H}\approx\hat{H}_c+\left\{\begin{array}{c}\text{sum of terms}\propto\\ (\hat{\mathbf{x}}-\mathbf{x}_c)\cdot\text{grad}_{\mathbf{x}_c}\beta_i(\mathbf{x}_c,t)\end{array}\right\}, \tag{2.1}$$

where $\hat{H}_c\equiv H(\hat{\mathbf{x}},\hat{\mathbf{p}};\{\beta_i(\mathbf{x}_c,t)\})$ will be called the local Hamiltonian. The terms within the braces are small in the neighborhood of the wave packet and may be treated perturbatively. The local Hamiltonian $\hat{H}_c$ has the required periodicity of the unperturbed crystal, and has an energy spectrum of bands (Bloch bands) with Bloch wave eigenstates satisfying

$$\hat{H}_c(\mathbf{x}_c,t)|\psi_{\mathbf{q}}(\mathbf{x}_c,t)\rangle=\mathcal{E}_c(\mathbf{x}_c,\mathbf{q},t)|\psi_{\mathbf{q}}(\mathbf{x}_c,t)\rangle, \tag{2.2}$$

where $\mathbf{q}$ is the Bloch wave vector and $\mathcal{E}_c(\mathbf{x}_c,\mathbf{q},t)$ is the band energy. Since we will be concerned with only a single band, we have omitted the band index for simplicity of notation. We note that both the wave-packet center $\mathbf{x}_c$ and time t enters in the Bloch states and the band energy parametrically. We shall see that the dependency on the center position of the wave packet will manifest as new types of Berry-phase terms in the equations of motion.

These eigenstates form a convenient basis to expand the wave packet. Specifically, we write

$$|\Psi\rangle=\int d^3q\,a(\mathbf{q},t)|\psi_{\mathbf{q}}(\mathbf{x}_c,t)\rangle, \tag{2.3}$$

where $a(\mathbf{q},t)$ is the amplitude with the normalization

$$\int d^3q|a(\mathbf{q},t)|^2=\langle\Psi|\Psi\rangle=1. \tag{2.4}$$

Here, we have taken the convention that $\langle\Psi_{\mathbf{q}'}|\Psi_{\mathbf{q}}\rangle=\delta(\mathbf{q}'-\mathbf{q})$. It is assumed that the distribution $|a(\mathbf{q},t)|^2$ is narrow compared to the size of the Brillouin zone and has the mean wave vector

$$\mathbf{q}_c = \int d^3q\,\mathbf{q}|a(\mathbf{q},t)|^2. \tag{2.5}$$

To be consistent, the wave packet must yield the preassigned center position

$$\mathbf{x}_c = \langle\Psi|\hat{\mathbf{x}}|\Psi\rangle. \tag{2.6}$$

This condition can be expressed in terms of other wave-packet parameters as follows. Writing the amplitude in the form $a(\mathbf{q},t)=|a(\mathbf{q},t)|\exp[-i\gamma(\mathbf{q},t)]$, and using the matrix elements of position operator $\hat{\mathbf{x}}$ between the Bloch states [Eq. (A1) of Appendix A], we find that

$$\langle\Psi|\hat{\mathbf{x}}|\Psi\rangle = \int d^3q|a|^2\left[\frac{\partial\gamma}{\partial\mathbf{q}} + \left\langle u\left| i\frac{\partial u}{\partial\mathbf{q}}\right\rangle\right], \tag{2.7}$$

where $|u\rangle \equiv |u(\mathbf{x}_c,\mathbf{q},t)\rangle = e^{-i\mathbf{q}\cdot\hat{\mathbf{x}}}|\psi_{\mathbf{q}}(\mathbf{x}_c,t)\rangle$ is the periodic part of the Bloch wave, and inner products involving the periodic part $|u\rangle$ mean an integration over the unit-cell volume v_c with a factor of $(2\pi)^3/v_c$, which implies the normalization $\langle u|u\rangle = 1$. According to our assumption of a narrow wave packet in the $\mathbf{q}$ space, Eq. (2.6) becomes

$$\mathbf{x}_c = \frac{\partial\gamma_c}{\partial\mathbf{q}_c} + \left\langle u\left| i\frac{\partial u}{\partial\mathbf{q}_c}\right\rangle\right., \tag{2.8}$$

where $|u\rangle$ now stands for $|u(\mathbf{x}_c,\mathbf{q}_c,t)\rangle$, and γ_c for $\gamma(\mathbf{q}_c,t)$.

In writing down the expansion (2.3), we have assumed that the wave packet that is initially in a band always lies in the same band. This is justified if the band is separated from other bands by finite gaps, and if the time and the length scales of the perturbations are long compared to those associated with these gaps.[29]

B. The Lagrangian and dynamics

The dynamics of the mean position $\mathbf{x}_c$ and the crystal momentum $\hbar\mathbf{q}_c$ can in principle be derived from the Schrödinger equation for the wave packet. It is more conveniently obtained using a time-dependent variational principle[24,25] with the Lagrangian given by

$$L = \left\langle \Psi\left| i\frac{d}{dt} - \hat{H}\right|\Psi\right\rangle, \tag{2.9}$$

where and hereafter we use the convention $\hbar = 1$. We use d/dt to mean the derivative with respect to the time dependence of the wave function explicitly or implicitly through $\mathbf{x}_c$ and $\mathbf{q}_c$. The partial derivative $\partial/\partial t$, is reserved for those with $\mathbf{x}_c$ and $\mathbf{q}_c$ held fixed.

Under the previously discussed conditions on the widths of the wave packet, we can evaluate the Lagrangian as a function of $\mathbf{x}_c$ and $\mathbf{q}_c$, their time derivatives, and the time t

$$L \approx L(\mathbf{x}_c,\dot{\mathbf{x}}_c,\mathbf{q}_c,\dot{\mathbf{q}}_c,t). \tag{2.10}$$

The terms involving higher moments of the wave packet, which specify its width and shape, are of higher order in the gradient of the perturbations and hence are neglected.[30]

Accordingly, we obtain for the first term in Eq. (2.9),

$$\left\langle \Psi\left| i\frac{d\Psi}{dt}\right\rangle\right. = \frac{\partial\gamma_c}{\partial t} + \left\langle u\left| i\frac{\partial u}{\partial t}\right\rangle\right. + \dot{\mathbf{x}}_c\cdot\left\langle u\left| i\frac{\partial u}{\partial\mathbf{x}_c}\right\rangle\right.. \tag{2.11}$$

The first term comes from the explicit time dependence of γ_c. The contribution from $|a(\mathbf{q},t)|$ is zero because of the normalization condition (2.4) on the amplitude. The second and third terms come about because of the dependence of the basis functions on time explicitly and implicitly through $\mathbf{x}_c$, respectively. Using the relation

$$\frac{\partial\gamma_c}{\partial t} = \frac{d\gamma_c}{dt} - \dot{\mathbf{q}}_c\cdot\frac{\partial\gamma_c}{\partial\mathbf{q}_c} \tag{2.12}$$

and Eq. (2.8), Eq. (2.11) can be recast into the form

$$\left\langle \Psi\left| i\frac{d\Psi}{dt}\right\rangle\right. = \frac{d\gamma_c}{dt} - \dot{\mathbf{q}}_c\cdot\mathbf{x}_c + \dot{\mathbf{q}}_c\cdot\left\langle u\left| i\frac{\partial u}{\partial\mathbf{q}_c}\right\rangle\right. + \dot{\mathbf{x}}_c\cdot\left\langle u\left| i\frac{\partial u}{\partial\mathbf{x}_c}\right\rangle\right. + \left\langle u\left| i\frac{\partial u}{\partial t}\right\rangle\right., \tag{2.13}$$

where γ_c appears only in a total time derivative.

The expectation value of the Hamiltonian, which gives the wave-packet energy $\mathcal{E}$, may be evaluated up to first order in the perturbation gradients using the linearized Hamiltonian (2.1)

$$\mathcal{E} = \langle\Psi|\hat{H}|\Psi\rangle \approx \langle\Psi|\hat{H}_c|\Psi\rangle + \langle\Psi|\Delta\hat{H}|\Psi\rangle, \tag{2.14}$$

where the gradient correction $\Delta\hat{H}$ may be written as[31]

$$\Delta\hat{H} = \frac{1}{2}\left[(\hat{\mathbf{x}}-\mathbf{x}_c)\cdot\frac{\partial\hat{H}_c}{\partial\mathbf{x}_c} + \frac{\partial\hat{H}_c}{\partial\mathbf{x}_c}\cdot(\hat{\mathbf{x}}-\mathbf{x}_c)\right]. \tag{2.15}$$

The expectation value of the local Hamiltonian is just the band energy at the mean wave vector,

$$\langle\Psi|\hat{H}_c|\Psi\rangle = \mathcal{E}_c(\mathbf{x}_c,\mathbf{q}_c,t), \tag{2.16}$$

while the gradient correction requires some calculations [Appendix A], but the result has the simple form

$$\Delta\mathcal{E} = -\mathrm{Im}\left[\left\langle\frac{\partial u}{\partial\mathbf{x}_c}\right|\bullet(\mathcal{E}_c-\hat{H}_c)\left|\frac{\partial u}{\partial\mathbf{q}}\right\rangle\right]\Bigg|_{\mathbf{q}=\mathbf{q}_c}, \tag{2.17}$$

where "$\bullet$" denotes a scalar product between the vectors formed by gradients with respect to $\mathbf{x}_c$ and $\mathbf{q}$.

The Lagrangian thus takes the form

$$L = -\mathcal{E} + \mathbf{q}_c\cdot\dot{\mathbf{x}}_c + \dot{\mathbf{q}}_c\cdot\left\langle u\left| i\frac{\partial u}{\partial\mathbf{q}_c}\right\rangle\right. + \dot{\mathbf{x}}_c\cdot\left\langle u\left| i\frac{\partial u}{\partial\mathbf{x}_c}\right\rangle\right. + \left\langle u\left| i\frac{\partial u}{\partial t}\right\rangle\right., \tag{2.18}$$

where we have neglected a term of total time derivative $d(\gamma-\mathbf{x}_c\cdot\mathbf{q}_c)/dt$ in the Lagrangian, as it does not affect the equations of motion and the quantization rule. The last three terms may be grouped into a single term $\langle u|idu/dt\rangle$, which turns out to be the net rate of change of Berry phase for wave-packet motion within the band. We note that under the transformations $|u\rangle\rightarrow\exp[i\varphi(\mathbf{x}_c,\mathbf{q},t)]|u\rangle$ or $\mathbf{q}\rightarrow\mathbf{q}+\mathbf{K}$, $\mathbf{K}$ being a reciprocal lattice vector, the Lagrangian remains invariant up to a total time derivative of some function of $\mathbf{x}_c$,

$\mathbf{q}_c$, and t. The former corresponds to gauge invariance while the latter to periodicity in the reciprocal space.

From the Lagrangian (2.18) we obtain the following equations of semiclassical motion:

$$\dot{\mathbf{x}}_c = \frac{\partial \mathcal{E}}{\partial \mathbf{q}_c} - (\overleftrightarrow{\Omega}_{\mathbf{qx}} \cdot \dot{\mathbf{x}}_c + \overleftrightarrow{\Omega}_{\mathbf{qq}} \cdot \dot{\mathbf{q}}_c) + \mathbf{\Omega}_{t\mathbf{q}},$$

$$\dot{\mathbf{q}}_c = -\frac{\partial \mathcal{E}}{\partial \mathbf{x}_c} + (\overleftrightarrow{\Omega}_{\mathbf{xx}} \cdot \dot{\mathbf{x}}_c + \overleftrightarrow{\Omega}_{\mathbf{xq}} \cdot \dot{\mathbf{q}}_c) - \mathbf{\Omega}_{t\mathbf{x}}. \qquad (2.19)$$

The components of the tensor $\overleftrightarrow{\Omega}_{\mathbf{qq}}$ are defined by

$$(\overleftrightarrow{\Omega}_{\mathbf{qq}})_{\alpha\beta} \equiv \Omega_{q_\alpha q_\beta} \equiv i\left[\left\langle \frac{\partial u}{\partial q_{c\alpha}} \middle| \frac{\partial u}{\partial q_{c\beta}} \right\rangle - \left\langle \frac{\partial u}{\partial q_{c\beta}} \middle| \frac{\partial u}{\partial q_{c\alpha}} \right\rangle\right], \qquad (2.20)$$

and those of the vector $\mathbf{\Omega}_{t\mathbf{x}}$ by

$$(\mathbf{\Omega}_{t\mathbf{x}})_\alpha \equiv \Omega_{t x_\alpha} \equiv i\left[\left\langle \frac{\partial u}{\partial t} \middle| \frac{\partial u}{\partial x_{c\alpha}} \right\rangle - \left\langle \frac{\partial u}{\partial x_{c\alpha}} \middle| \frac{\partial u}{\partial t} \right\rangle\right], \qquad (2.21)$$

where α and β are Cartesian indices. The other tensors $\overleftrightarrow{\Omega}_{\mathbf{xx}}, \overleftrightarrow{\Omega}_{\mathbf{xq}}$, and $\overleftrightarrow{\Omega}_{\mathbf{qx}}$ and the vector $\mathbf{\Omega}_{t\mathbf{q}}$ are defined similarly. These quantities are known as Berry curvatures.[13,14] We note that these equations involve Berry curvatures between every pair of parameters and that they have symplectic symmetry in the absence of time dependence.

C. Formal and semiclassical quantization

We mentioned in the Introduction that the equations of motion were usually derived from the effective Hamiltonian upon using the correspondence principle. Here, we consider the reverse process to obtain the effective quantum Hamiltonian from the semiclassical dynamics. This requires a knowledge of canonical structure of the wave-packet dynamics. Following the standard procedure of analytical mechanics, we introduce the canonical momenta conjugate to the generalized coordinates

$$\mathbf{P}_1 = \frac{\partial L}{\partial \dot{\mathbf{x}}_c} = \mathbf{q}_c + \left\langle u \middle| i \frac{\partial u}{\partial \mathbf{x}_c} \right\rangle, \qquad (2.22)$$

$$\mathbf{P}_2 = \frac{\partial L}{\partial \dot{\mathbf{q}}_c} = \left\langle u \middle| i \frac{\partial u}{\partial \mathbf{q}_c} \right\rangle, \qquad (2.23)$$

and the semiclassical Hamiltonian $\mathcal{H}$ by the Legendre transformation

$$\mathcal{H} = \dot{\mathbf{x}}_c \cdot \mathbf{P}_1 + \dot{\mathbf{q}}_c \cdot \mathbf{P}_2 - L = \mathcal{E}(\mathbf{x}_c, \mathbf{q}_c, t) - \left\langle u \middle| i \frac{\partial u}{\partial t} \right\rangle. \qquad (2.24)$$

The semiclassical Hamiltonian is independent of $\mathbf{P}_1$ and $\mathbf{P}_2$, because the Lagrangian is linear in the generalized velocities.

Starting with $\mathcal{H}$, regarded formally as a function of $\mathbf{x}_c$, $\mathbf{q}_c$, $\mathbf{P}_1$, and $\mathbf{P}_2$, one cannot obtain the equations of motion (2.19) from the Hamilton equations. This is because the Eqs. (2.22) and (2.23) defining $\mathbf{P}_1$ and $\mathbf{P}_2$ do not depend on the generalized velocities, and hence they should be treated as constraints between the canonical variables.

In the simple case where the Berry-phase terms are zero, these constraints become $\mathbf{P}_1 = \mathbf{q}_c$, and $\mathbf{P}_2 = 0$, and $\mathcal{H} = \mathcal{E}$. These suggest that we treat $(\mathbf{x}_c, \mathbf{q}_c)$ as a canonical pair and forget about the other degrees of freedom. By doing so, we can indeed obtain the equations of motion (2.19) from the Hamilton equations. Having identified the canonical pair, one can proceed with a formal procedure of quantization (''requantization''), $\mathbf{q}_c \to -i\partial/\partial \mathbf{x}_c$, to obtain an effective quantum Hamiltonian. A slightly more general case will be encountered in the case of electromagnetic perturbations in the next section of this article.

When Berry-phase terms are present, constraints (2.22) and (2.23) still imply some hidden canonical relations between $\mathbf{x}_c$ and $\mathbf{q}_c$, but these are entangled in a complicated manner that cannot be expressed explicitly in general. This clearly shows the difficulty of the Hamiltonian formalism in the presence of Berry-phase terms. If one insists on using the Hamiltonian approach, one can employ the method of Lagrange multipliers, which allows the spurious degrees of freedom to be formally treated as independent,[32] and obtain the equations of motion (2.19). The ''requantization'' procedure for this case is quite complicated and needs further investigation.

The semiclassical quantization, on the other hand, is quite straight forward. In order that stationary states and energy levels can be talked about, we shall restrict ourselves to static perturbations. For a wave-packet motion that is regular and is described by closed orbits in the phase space $(\mathbf{x}_c, \mathbf{q}_c)$, semiclassical energy levels are obtained using the quantization procedure[33] due to Einstein, Brillouin, and Keller,

$$\oint_{\mathcal{C}} \mathbf{P}_1 \cdot d\mathbf{x}_c + \oint_{\mathcal{C}} \mathbf{P}_2 \cdot d\mathbf{q}_c = 2\pi\left[m + \frac{\nu}{4}\right], \qquad (2.25)$$

where $\mathcal{C}$ denotes an orbit of constant energy $\mathcal{E}$, m an integer that labels the eigenvalue, and ν the number of caustics traversed. With Eqs. (2.22) and (2.23) for $\mathbf{P}_1$ and $\mathbf{P}_2$, the above condition reduces to

$$\oint_{\mathcal{C}} \mathbf{q}_c \cdot d\mathbf{x}_c = 2\pi\left[m + \frac{\nu}{4} - \frac{\Gamma(\mathcal{C})}{2\pi}\right], \qquad (2.26)$$

where

$$\Gamma(\mathcal{C}) = \oint_{\mathcal{C}} d\mathbf{x}_c \cdot \left\langle u \middle| i \frac{\partial u}{\partial \mathbf{x}_c} \right\rangle + \oint_{\mathcal{C}} d\mathbf{q}_c \cdot \left\langle u \middle| i \frac{\partial u}{\partial \mathbf{q}_c} \right\rangle \qquad (2.27)$$

is the Berry phase acquired by the wave packet upon going round the closed orbit once. The Berry phase correction to the quantization condition made its first appearance in Wilkinson's work[34] on Harper's equation, in Kuratsuji and Iida's work[35] on adiabatic nuclear motion, and also recently in the work of Chang and Niu[12] on wave-packet dynamics in magnetic Bloch bands.

III. ELECTROMAGNETIC FIELDS

So far, our treatment of perturbations has been in general terms, and our results are in an abstract form. Their physical meaning will become clear through the consideration of two special cases in this and the next section. For a class of

perturbations for which the Hamiltonian is of the special form

$$H_0[\hat{\mathbf{x}}+\boldsymbol{\beta}_1(\hat{\mathbf{x}},t),\hat{\mathbf{p}}+\boldsymbol{\beta}_2(\hat{\mathbf{x}},t)]+\beta_3(\hat{\mathbf{x}},t), \tag{3.1}$$

all the results can be expressed in terms of the unperturbed Bloch wave basis. In this section, we shall consider electromagnetic perturbations for which $\boldsymbol{\beta}_1(\hat{\mathbf{x}},t)=0$.

A. The gauge invariant crystal momentum

Let $\hat{H}_0(\mathbf{q})$ denote the Hamiltonian for the bare crystal, with the eigenstate $|u(\mathbf{q})\rangle$ (the periodic part of the Bloch wave) and the band energy $\mathcal{E}_0(\mathbf{q})$ for a particular band. The Hamiltonian gets modified by the gauge potentials $[\mathbf{A}(\mathbf{x},t),\phi(\mathbf{x},t)]$ of an electromagnetic field to

$$\hat{H}=H_0[\mathbf{q}+e\mathbf{A}(\hat{\mathbf{x}},t)]-e\phi(\hat{\mathbf{x}},t). \tag{3.2}$$

This has the form (1.5) and (3.1), with the gauge potentials playing the role of the modulation functions, and hence the local Hamiltonian must have the form

$$\hat{H}_c=\hat{H}_0[\mathbf{q}+e\mathbf{A}(\mathbf{x}_c,t)]-e\phi(\mathbf{x}_c,t). \tag{3.3}$$

As $e\mathbf{A}(\mathbf{x}_c,t)$ is only an additive constant to the crystal momentum $\mathbf{q}$, the basis states have the form $|u(\mathbf{x}_c,\mathbf{q},t)\rangle=|u(\mathbf{k})\rangle$, where $\mathbf{k}=\mathbf{q}+e\mathbf{A}(\mathbf{x}_c,t)$ is the gauge invariant or mechanical crystal momentum. In terms of the gauge invariant crystal momentum $\mathbf{k}$, a number of simplifications can be obtained. First, the eigenenergy can be written in the form

$$\mathcal{E}_c(\mathbf{x}_c,\mathbf{k},t)=\mathcal{E}_0(\mathbf{k})-e\phi(\mathbf{x}_c,t). \tag{3.4}$$

Second, the gradient correction (2.17) becomes the orbital magnetization energy of the wave packet,

$$-\mathbf{M}\cdot\mathbf{B}, \tag{3.5}$$

where $\mathbf{B}\equiv\mathrm{curl}_{\mathbf{x}_c}\mathbf{A}(\mathbf{x}_c,t)$ is the magnetic field, and

$$\mathbf{M}=e\,\mathrm{Im}\left[\left\langle\frac{\partial u}{\partial\mathbf{k}}\right|\times(\mathcal{E}_0-\hat{H}_0(\mathbf{k}))\left|\frac{\partial u}{\partial\mathbf{k}}\right\rangle\right]\Bigg|_{\mathbf{k}=\mathbf{k}_c} \tag{3.6}$$

is the orbital magnetic moment of Bloch electrons. Third, the last three terms of the Lagrangian (2.18) simply become the single term $\dot{\mathbf{k}}_c\cdot\langle u|i\partial u/\partial\mathbf{k}_c\rangle$. Finally, the Lagrangian takes the form

$$L=-\mathcal{E}_M+e\phi(\mathbf{x}_c,t)+\dot{\mathbf{x}}_c\cdot\mathbf{k}_c-e\dot{\mathbf{x}}_c\cdot\mathbf{A}(\mathbf{x}_c,t)+\dot{\mathbf{k}}_c\cdot\left\langle u\left|i\frac{\partial u}{\partial\mathbf{k}_c}\right.\right\rangle, \tag{3.7}$$

where $\mathcal{E}_M\equiv\mathcal{E}_0(\mathbf{k}_c)-\mathbf{M}\cdot\mathbf{B}$.

B. The reciprocal magnetic field and orbital magnetization energy

The equations of motion can either be derived variationally from the above Lagrangian or directly from Eq. (2.19) derived for the general case in the previous section. They have the form

$$\dot{\mathbf{x}}_c=\frac{\partial\mathcal{E}_M}{\partial\mathbf{k}_c}-\dot{\mathbf{k}}_c\times\boldsymbol{\Omega},$$

$$\dot{\mathbf{k}}_c=-e\mathbf{E}-e\dot{\mathbf{x}}_c\times\mathbf{B}, \tag{3.8}$$

where $\mathbf{E}\equiv-\mathrm{grad}_{\mathbf{x}_c}\phi(\mathbf{x}_c,t)-\partial\mathbf{A}(\mathbf{x}_c,t)/\partial t$ is the electric field, and

$$(\boldsymbol{\Omega})_\alpha\equiv\tfrac{1}{2}\epsilon_{\alpha\beta\gamma}(\overleftrightarrow{\Omega}_{\mathbf{kk}})_{\beta\gamma}, \tag{3.9}$$

are the components of the vector form of the antisymmetric tensor $\overleftrightarrow{\Omega}_{\mathbf{kk}}$ given by Eq. (2.20). In Eq. (3.9) and henceforth, repeated Cartesian indices are taken to be summed. Because $\boldsymbol{\Omega}$ occupies a similar position as the magnetic field in the equations of motion, it will be called the reciprocal magnetic field.

The above equations differ from Eqs. (1.1) in two respects. Firstly, the energy $\mathcal{E}$ contains a correction term from the magnetic moment (3.6) of Bloch electron. This term has been derived earlier as a first order correction in the theory of Bloch electrons subject to magnetic fields.[36] A similar term has also been found in the theory of electrons in incommensurate lattices,[19,20] and in the theory of wave-packet dynamics in magnetic Bloch bands.[12] Secondly, the correction term to the velocity, $-\dot{\mathbf{k}}_c\times\boldsymbol{\Omega}$, is the anomalous velocity that was predicted to give rise to a spontaneous Hall conductivity in ferromagnetic materials.[8,9] In the context of the quantum Hall effect, the integral of the Berry curvature $\Omega_{k_\alpha k_\beta}$ over the Brillouin zone was shown to be proportional to the Hall conductivity for a full band and to be quantized (Chern's topological invariant).[37] Recently, Chang and Niu[12] proved this result semiclassically. It seems more appropriate to call this term Hall velocity than anomalous velocity.

The semiclassical Eq. (3.8) should be invariant under time reversal, spatial inversion, or certain rotations if these are symmetries of the unperturbed crystal. Such symmetries impose severe restrictions on the behavior of the reciprocal magnetic field $\boldsymbol{\Omega}$ and the magnetic moment $\mathbf{M}$ as functions of $\mathbf{k}$. Under time reversal, $\dot{\mathbf{x}}_c$, $\mathbf{k}_c$, and $\mathbf{B}$ change sign while $\mathbf{x}_c$, $\dot{\mathbf{k}}_c$, and $\mathbf{E}$ are invariant. If the bare crystal is invariant under time reversal, we must have $\boldsymbol{\Omega}(-\mathbf{k})=-\boldsymbol{\Omega}(\mathbf{k})$, and $\mathbf{M}(-\mathbf{k})=-\mathbf{M}(\mathbf{k})$, which implies in particular that they must vanish at $\mathbf{k}=0$. Under spatial inversion, $\mathbf{E}$, $\mathbf{x}_c$, $\mathbf{k}_c$, and the time derivatives of the last two change sign while $\mathbf{B}$ remains unchanged. If the bare crystal has inversion symmetry, we must have $\boldsymbol{\Omega}(-\mathbf{k})=\boldsymbol{\Omega}(\mathbf{k})$, and $\mathbf{M}(-\mathbf{k})=\mathbf{M}(\mathbf{k})$. Finally, if the system is invariant under certain proper rotations, the reciprocal magnetic field and the magnetic moment should transform like vectors under these rotations.

For monatomic nonmagnetic crystals, both time reversal and spatial inversion symmetries are present, rendering $\boldsymbol{\Omega}$ and $\mathbf{M}$ null everywhere in the Brillouin zone. However, it is not entirely justified to ignore these quantities for magnetic crystals or nonmagnetic crystals without inversion symmetry (such as GaAs). Investigations have been undertaken to see whether the presence of the reciprocal magnetic field and the orbital magnetization lead to observable effects.

The Lagrangian (3.7) and the equations of motion (3.8) were derived earlier by Chang and Niu[12] for perturbed magnetic Bloch electrons in two dimensions in the gauge where

$\phi(\mathbf{x},t)=0$. They used a wave packet that gauges away the vector potential locally so that their magnetic Bloch wave vector is the same as the corresponding gauge invariant crystal momentum $\mathbf{q}+e\mathbf{A}(\mathbf{x}_c,t)=\mathbf{k}$ here. Their derivation was less general in that it is only for two dimensions and more general in that it provides a description of electrons in rational magnetic fields $\mathbf{B}_0$, for which the flux through a unit cell equals a rational fraction $[\sim\mathcal{O}(1)]$ of the flux quantum (h/e). However, our formalism can easily be generalized to this situation, for a more general three-dimensional case, by assuming a background of constant rational magnetic field $\mathbf{B}_0$. All we need to do is to interpret $\mathbf{q}$ as the wave vector of magnetic Bloch states defined within a reduced Brillouin zone (the magnetic Brillouin zone),[12] and to replace $\mathbf{B}$ in (3.8) by $\mathbf{B}-\mathbf{B}_0$.

C. Peierls substitution and Landau levels

It follows from the Lagrangian (3.7) that the canonical momenta are given by

$$\mathbf{P}_1=\mathbf{k}_c-e\mathbf{A}(\mathbf{x}_c,t), \tag{3.10}$$

$$\mathbf{P}_2=\left\langle u\left| i\frac{\partial u}{\partial \mathbf{k}_c}\right\rangle\right., \tag{3.11}$$

and the Hamiltonian by $\mathcal{H}=\mathcal{E}_M(\mathbf{k}_c)-e\phi(\mathbf{x}_c,t)$. In the absence of the Berry-phase term (3.11), we may obtain the Hamiltonian as a function of the canonical pair $(\mathbf{x}_c,\mathbf{P}_1)$ as

$$\mathcal{H}=\mathcal{E}_M[\mathbf{P}_1+e\mathbf{A}(\mathbf{x}_c,t)]-e\phi(\mathbf{x}_c,t). \tag{3.12}$$

The quantization of this Hamiltonian by setting $\mathbf{P}_1=-i\partial/\partial\mathbf{x}_c$ amounts to the Peierls substitution. However, it is not clear how to deal with the case with a Berry-phase term using the Hamiltonian approach.

When only a uniform magnetic field is present, the two equations of motion (3.8) can be combined into a single one for the $\mathbf{k}$-space motion. It is evident that a $\mathbf{k}$-space orbit must lie in a plane normal to $\mathbf{B}$ and must be on a constant energy surface of $\mathcal{E}(\mathbf{k})$. If such an orbit is closed, known as a cyclotron orbit, the EBK formula yields

$$\frac{1}{2}\hat{\mathbf{B}}\cdot\oint_{\mathcal{C}}\mathbf{k}_c\times d\mathbf{k}_c=\frac{e|\mathbf{B}|}{\hbar}\left[m+\frac{1}{2}-\frac{\Gamma(\mathcal{C})}{2\pi}\right], \tag{3.13}$$

where

$$\Gamma(\mathcal{C})=\oint_{\mathcal{C}}d\mathbf{k}\cdot\left\langle u\left| i\frac{\partial u}{\partial\mathbf{k}_c}\right\rangle\right. \tag{3.14}$$

is the Berry phase accumulated by the wave packet upon completing a circuit along the loop $\mathcal{C}$, and we have restored the Planck constant. The left-hand side of Eq. (3.13) is just the $\mathbf{k}$-space area enclosed by the orbit $\mathcal{C}$. As this phase influences energy levels, it affects the density of states. It is shown in Ref. 12 that Γ plays an important role in determining the spectral splitting pattern of magnetic bands.

D. Zak phase and Wannier-Stark ladder

In this subsection, we restrict our discussion to one dimension for simplicity. The semiclassical motion under a uniform electric field is described by the Hamiltonian $\mathcal{H}=\mathcal{E}_0(k_c)+eEx_c$. It follows from the boundedness and the periodicity of the band energy that the motion in real space is also bounded and periodic. Such a closed motion in the real space is known as Bloch oscillations. In the reduced zone scheme, the motion is closed also in the phase space (x_c,k_c), which is a cylinder. Quantizing this motion according to Eq. (2.25) gives the condition

$$-\int_{-\pi/a}^{\pi/a}dk_c x_c(k_c)=2\pi\left(m+\frac{\nu}{4}-\frac{\Gamma}{2\pi}\right), \tag{3.15}$$

where a stands for the lattice constant, and

$$\Gamma=\int_{-\pi/a}^{\pi/a}dk\left\langle u\left| i\frac{\partial u}{\partial k}\right\rangle\right. \tag{3.16}$$

is known as the Zak phase,[38] and $x_c(k_c)$ is the constant energy curve for the mth energy level defined by $W_m=\mathcal{E}_0(k_c)+eEx_c$, m being an integer. Averaging this expression over the orbit, we obtain from Eq. (3.15)

$$W_m=\overline{\mathcal{E}_0}+eEa\left(-m-\frac{\nu}{4}+\frac{\Gamma}{2\pi}\right), \tag{3.17}$$

where $\overline{\mathcal{E}_0}$ is the average of the band energy over the Brillouin zone, and m is any integer between $-\infty$ to ∞, since the mean value of x_c can be anywhere on the cylinder. This spectrum, known as the Wannier-Stark ladder, was first derived by Wannier[39] without the Berry-phase term. The correction was due to Zak, who later interpreted it as a Berry phase.[40]

IV. DEFORMATIONS IN CRYSTALS

We shall now come to deformational perturbations. It turns out that the model Hamiltonian for a deformed crystal also has the special form (3.1) with $\boldsymbol{\beta}_2(\hat{\mathbf{x}},t)=0$, which is $H_0[\hat{\mathbf{x}}+\boldsymbol{\beta}_1(\hat{\mathbf{x}},t),\hat{\mathbf{p}}]+\beta_3(\hat{\mathbf{x}},t)$, and hence all the corrections are expressible in terms of the undeformed basis for this case too.

A. The translated crystal basis

A deformed crystal with atomic displacements $\{\mathbf{u}_l\}$ may be described by the Hamiltonian[41,42]

$$H=\frac{\hat{\mathbf{p}}^2}{2m}+V_0[\hat{\mathbf{x}}-\mathbf{u}(\hat{\mathbf{x}})]+s_{\alpha\beta}(\hat{\mathbf{x}})\mathcal{V}_{\alpha\beta}[\hat{\mathbf{x}}-\mathbf{u}(\hat{\mathbf{x}})], \tag{4.1}$$

where $\mathbf{u}(\mathbf{x})$ is a smooth displacement field[43] satisfying $\mathbf{u}(\mathbf{R}_l+\mathbf{u}_l)=\mathbf{u}_l$, and $s_{\alpha\beta}=\partial u_\alpha/\partial x_\beta$ is the unsymmetrized strain. The justification of the above Hamiltonian and an explicit expression for the last term are given in Appendix B. While the last term of the Hamiltonian, being proportional to the strain, can be treated perturbatively, the other terms are of the form Eq. (1.5), with the displacement field playing the role of the modulation function. The local Hamiltonian is then given by

$$\hat{H}_c=\frac{\hat{\mathbf{p}}^2}{2m}+V_0[\hat{\mathbf{x}}-\mathbf{u}(\mathbf{x}_c)]. \tag{4.2}$$

This is nothing but the Hamiltonian of an undeformed crystal shifted in position by the displacement field at the center of the wave packet, $\mathbf{u}(\mathbf{x}_c)$. The band energy is therefore the same as that of the undeformed crystal, $\mathcal{E}_0(\mathbf{k})$, and the eigenstates are the translated Bloch waves $\{\psi_{\mathbf{k}}[\mathbf{x}-\mathbf{u}(\mathbf{x}_c)]\}$.

Our wave packet will thus be formed out of these translated Bloch states of the undeformed but translated crystal. This procedure is valid so long as the strain is weak, so that the variation of the displacement within the spatial width of the wave packet is small. When the first-order corrections to the Hamiltonian are taken into account, our method should give the same physical results (to the same order) as obtained using a strained basis. However, our formulation should be simpler and easier to interpret, because it avoids the necessity of transformation between the lab and lattice frames of reference.

Although the small strain regime covers the vast majority of practical situations, it is some times necessary to consider the effect of large strains. In the case where a large uniform and static strain is superposed on top of a small varying strain, our formulation can still be applied; one only needs to interpret the basis as that of the uniformly strained crystal. There can be a third possibility in which the strain variation is large over large distances but is small over the size of the wave packet. In this case, it is more appropriate to use a strained local basis, that is, a basis of a homogeneously strained crystal with the strain value given by the actual strain at the center of the wave packet.

B. The crystal deformation potential

The wave-packet energy is obtained by summing the expectation values of the local Hamiltonian (4.2), the gradient correction (2.15), and the last term of Eq. (4.1). Because of the functional form of the basis states, we have

$$\langle\Psi|\hat{H}_c|\Psi\rangle=\mathcal{E}_0(\mathbf{k}_c), \tag{4.3}$$

while the gradient correction becomes

$$-ms_{\alpha\beta}(\mathbf{x}_c)[\langle\hat{v}_\alpha\hat{v}_\beta\rangle-\langle\hat{v}_\alpha\rangle\langle\hat{v}_\beta\rangle]. \tag{4.4}$$

The angular brackets in the above expression represent the expectation value of the enclosed operators in the Bloch state at $\mathbf{k}=\mathbf{k}_c$, and $\hat{v}_\alpha=\partial\hat{H}(\mathbf{k})/\partial k_\alpha$ is the velocity operator. As is well known, $\langle\hat{v}_\alpha\rangle=\partial\mathcal{E}_0/\partial k_\alpha\equiv v_\alpha$ is the group velocity of Bloch electrons. As for the last term of the Hamiltonian (4.1), we may write, in accordance with our approximation [Eq. (2.10)],

$$\langle\Psi|s_{\alpha\beta}(\hat{\mathbf{x}})\hat{\mathcal{V}}_{\alpha\beta}|\Psi\rangle\approx s_{\alpha\beta}(\mathbf{x}_c)\langle\hat{\mathcal{V}}^c_{\alpha\beta}\rangle, \tag{4.5}$$

where $\mathcal{V}^c_{\alpha\beta}=\mathcal{V}_{\alpha\beta}[(\mathbf{x}-\mathbf{u}(\mathbf{x}_c)]$. We again write the energy of the wave packet in the form

$$\mathcal{E}=\mathcal{E}_0(\mathbf{k}_c)+\Delta\mathcal{E}(\mathbf{x}_c,\mathbf{k}_c), \tag{4.6}$$

where, this time, the correction $\Delta\mathcal{E}$, which is to be called the deformation potential for the wave packet,[44] has two contributions [Eqs. (4.4) and (4.5)]. As the latter is proportional to the local deformation, it may be written in the form

$$\Delta\mathcal{E}=s_{\alpha\beta}(\mathbf{x}_c)D^w_{\alpha\beta}(\mathbf{k}_c), \tag{4.7}$$

with

$$D^w_{\alpha\beta}=m[v_\alpha v_\beta-\langle\hat{v}_\alpha\hat{v}_\beta\rangle]+\langle\hat{\mathcal{V}}^c_{\alpha\beta}\rangle. \tag{4.8}$$

We note that this quantity vanishes in the free-electron limit ($V_0\to 0$), which is quite satisfying from a physical point of view: a wave packet should not feel the effect of a deformation of the lattice in the absence of electron-lattice coupling.

Further, from the differential band structure[45] under a uniform strain $\overleftrightarrow{\epsilon}$,

$$\mathcal{E}'(\mathbf{k}')-\mathcal{E}_0(\mathbf{k})=\epsilon_{\alpha\beta}D^b_{\alpha\beta}(\mathbf{k})=\epsilon_{\alpha\beta}[-m\langle\hat{v}_\alpha\hat{v}_\beta\rangle+\langle\hat{\mathcal{V}}^c_{\alpha\beta}\rangle], \tag{4.9}$$

where $\mathbf{k}'=(\overleftrightarrow{1}+\overleftrightarrow{\mathbf{s}})^{-1}\cdot\mathbf{k}$ $\Delta\mathcal{E}$ can be determined by the relation

$$D^w_{\alpha\beta}=D^b_{\alpha\beta}+mv_\alpha v_\beta, \tag{4.10}$$

according to Eqs. (4.8) and (4.9). The same expression has been obtained for the deformation potential for electron-phonon interaction at long wavelengths, showing the equivalence of the latter with our wave-packet deformation potential (4.7).[46]

C. Equations of motion and lattice tracking

Before we proceed further, let us first make the displacements time dependent, $\{\mathbf{u}_l(t)\}$, as we are discussing the dynamical aspect. Accordingly, we extend the results of the previous subsections with the replacements $\mathbf{u}(\mathbf{x})\to\mathbf{u}(\mathbf{x},t)$ and $s_{\alpha\beta}(\mathbf{x})\to s_{\alpha\beta}(\mathbf{x},t)$, and with the Bloch wave basis given by the states $\{\psi_{\mathbf{k}}[\mathbf{x}-\mathbf{u}(\mathbf{x}_c,t)]\}$.

As for the Lagrangian, the functional form of the basis states imply that the last two terms of its general expression (2.18) become

$$\left\langle u\left|i\frac{\partial u}{\partial\mathbf{x}_c}\right.\right\rangle=f_\alpha\frac{\partial u_\alpha}{\partial\mathbf{x}_c},\quad \left\langle u\left|i\frac{\partial u}{\partial t}\right.\right\rangle=f_\alpha\frac{\partial u_\alpha}{\partial t}, \tag{4.11}$$

where

$$\mathbf{f}(\mathbf{k})=\frac{m}{\hbar}\frac{\partial\mathcal{E}_0}{\partial\mathbf{k}}-\hbar\mathbf{k}, \tag{4.12}$$

in which $\hbar$ has been restored. The reader is warned that the displacement field ($\mathbf{u}$ or u_α) should not be confused with the periodic part of the Bloch state, $|u\rangle$. The quantity $\mathbf{f}(\mathbf{k})$, being the difference between the group momentum of a Bloch electron and the momentum of a free electron, denotes that part of the momentum arising from the lattice interaction alone. It has the desired property of vanishing in the free electron limit, where the lattice deformation should not be felt. By substituting Eq. (4.11) into Eq. (2.18), we obtain

$$L=-\mathcal{E}+\dot{\mathbf{x}}_c\cdot\mathbf{k}_c+\dot{\mathbf{k}}_c\cdot\left\langle u\left|i\frac{\partial u}{\partial\mathbf{k}_c}\right.\right\rangle+\dot{\mathbf{u}}\cdot\mathbf{f}(\mathbf{k}_c), \tag{4.13}$$

where $\dot{\mathbf{u}}$ denotes $d\mathbf{u}/dt$. The last term is new and represents the rate of change of the Berry phase due to lattice tracking. We shall see below that there is a tendency for the lattice to drag the electron with its displacement motion, hence the word ''tracking.'' This term also gives rise to the Burgers

vector when integrated around a dislocation, so in a sense it keeps track of the lattice position.

Similarly, the Berry curvatures in Eq. (2.19) take values

$$\Omega_{k_\alpha x_\beta} = -\Omega_{x_\beta k_\alpha} = \frac{\partial u_\gamma}{\partial x_{c\beta}} \frac{\partial f_\gamma}{\partial k_{c\alpha}},$$

$$\Omega_{tk_\alpha} = -\frac{\partial f_\gamma}{\partial k_{c\alpha}} \frac{\partial u_\gamma}{\partial t}, \quad \Omega_{x_\alpha x_\beta} = \Omega_{tx_\beta} = 0, \tag{4.14}$$

and by expressions (4.6) and (4.7) for $\mathcal{E}$, the equations of motion become

$$\dot{x}_{c\alpha} = \frac{\partial \mathcal{E}_0}{\partial k_{c\alpha}} + s_{\beta\gamma} \frac{\partial D^w_{\beta\gamma}}{\partial k_{c\alpha}} - (\dot{\mathbf{k}}_c \times \mathbf{\Omega})_\alpha - \dot{u}_\beta \frac{\partial f_\beta}{\partial k_{c\alpha}}, \tag{4.15}$$

$$\dot{k}_{c\alpha} = -D^w_{\beta\gamma} \frac{\partial s_{\beta\gamma}}{\partial x_{c\alpha}} - s_{\beta\alpha} \frac{\partial f_\beta}{\partial k_{c\gamma}} \dot{k}_{c\gamma}. \tag{4.16}$$

In the above equations, the semiclassical force has two contributions: the first term arises from the deformation potential, and the second term, which arises from the lattice tracking term, will be called the tracking force. For uniform strains the semiclassical force vanishes, so that $\mathbf{k}_c$ is a good quantum number in such a case.

The velocity has three contributions in addition to the usual term given by the gradient of the band energy. The second term corresponds to the group velocity arising from the deformation potential, and the third term, as was seen earlier in Eq. (3.8) of Sec. III, is the Hall velocity. The last term arises from the lattice tracking term of the Lagrangian, and will be similarly called the tracking velocity. To understand this term better, let us rewrite the term using Eq. (4.12) as

$$\dot{u}_\alpha - m\dot{u}_\beta \frac{\partial^2 \mathcal{E}_0}{\partial k_{c\beta} \partial k_{c\alpha}}. \tag{4.17}$$

In the free-electron limit, where electrons and lattice decouple, the adiabatic velocity vanishes identically, for

$$\frac{\partial^2 \mathcal{E}_0}{\partial k_{c\alpha} \partial k_{c\beta}} \to \frac{\delta_{\alpha\beta}}{m}. \tag{4.18}$$

On the other hand, when the band under consideration is full, the second term of Eq. (4.17) averaged over the band is zero, implying a complete adiabatic following of the lattice motion, which confirms an earlier result on adiabatic particle transport.[47]

D. Dislocations and Berry phase

Our formalism is also applicable to dislocation strain fields, which are well defined except in a region of a few atomic spacings around the line of dislocation. Outside this region, the displacement field $\mathbf{u}(\mathbf{x})$ is a smooth but multiple valued function. The change in the displacement field along a closed loop around the line of dislocation, $\Delta\mathbf{u} = \int_C dx_\alpha \partial\mathbf{u}/\partial x_\alpha = \mathbf{b}$, is known as the Burgers vector; it equals one of the Bravais lattice vectors. On account of this multiple-valuedness, a wave packet of incident wave vector $\mathbf{k}$ taken around the line of dislocation acquires a Berry phase

$$\Gamma = \oint_C d\mathbf{x}_c \cdot \left\langle u \middle| i \frac{\partial u}{\partial \mathbf{x}_c} \right\rangle = \oint_C d\mathbf{u} \cdot \mathbf{f}(\mathbf{k}_c) \approx \mathbf{b} \cdot \mathbf{f}(\mathbf{k}), \tag{4.19}$$

where we have assumed $\langle u | i \partial u/\partial \mathbf{k} \rangle$ to be zero[48] and the corrections arising from the changes in the wave vector to be negligible. In other words, the action integral of the last term of Eq. (4.13) around a dislocation gives us a Berry phase that is proportional to the Burgers vector.

Note that this Berry phase is independent of the path as long as it encloses the dislocation line. What we have is a situation similar to the Aharonov-Bohm effect,[49] with the dislocation playing the role of the solenoid, and the Berry curvature $\mathbf{\Omega_{xx}}$ the role of the magnetic field. Just as in the case of the solenoidal field, $\mathbf{\Omega_{xx}} = 0$ everywhere except for the core region where it should be taken to be singular.

The Berry phase (4.19) affects the scattering of electrons by a dislocation,[50] and our result can be used to compute the shift in the scattering fringe pattern due the Berry phase. The intensity distribution has interference terms of the form $\cos(\theta+\Gamma)$ due to each pair of paths along the two sides of the dislocation, where θ is given by the path length difference per wave length of the incident beam. The Berry phase and hence the shift are maximal when the incident wave vector $\mathbf{k}$ is such that $\mathbf{f}(\mathbf{k}) = m\mathbf{v} - \hbar\mathbf{k}$ is parallel to the Burgers vector $\mathbf{b}$. To fix ideas, let us make the assumption that $\mathbf{f} \| \mathbf{k}$. For an edge dislocation, where $\mathbf{b}$ lies in the normal plane of the dislocation axis, we expect that maximal effect of the Berry phase is seen when the direction of the incident beam is perpendicular to the axis and coincide with the direction of $\mathbf{b}$. For a screw dislocation, the maximal Berry phase occurs when $\mathbf{k}$ is parallel to the axis along which $\mathbf{b}$ lies. However, since the beam must pass the dislocation in order to produce the interference pattern, the maximal Berry-phase effect should actually occur when $\mathbf{k}$ is along some finite angle away from the axis.

The Berry phase can also affect the electron diffraction pattern of a deformed crystal with or without a dislocation. When an electron beam of wave vector $\mathbf{k}$ is sent through a crystal, it propagates as Bloch waves in different bands of the crystal, all with the same Bloch wave vector, which is equal to $\mathbf{k}$ modulo a reciprocal lattice vector. Because of the energy differences of the bands, the Bloch waves grow out of phase from one another as they propagate. Therefore, when they exit the crystal, they recombine to produce not only the incident beam but also the diffracted beams. For a deformed crystal, the phase change of a Bloch wave is given by the time integral of the Lagrangian (4.13). The contribution from the $\dot{\mathbf{x}}_c \cdot \mathbf{k}_c$ term may be dropped, because it is independent of the band index. For weak strains, we may also neglect the deformation potential and the third term in Eq. (4.13). The dominant correction to the dynamical phase arises from the last term: $\Delta\mathbf{u} \cdot \mathbf{f}(\mathbf{k})$, where $\Delta\mathbf{u}$ is the change in the displacement field over the path of propagation of the Bloch waves. To show the soundness of these general ideas, we have calculated the diffraction pattern from a thin slab of crystal containing a screw dislocation, correctly reproducing earlier experimental and theoretical results.[51]

V. SUMMARY

We provide a unified framework for wave-packet dynamics of electrons in slowly perturbed crystals, which consists of constructing a wave packet using the Bloch states belonging to a single band of the local periodic Hamiltonian, obtained by replacing the perturbations by their value at the center of the wave packet, and deriving its dynamics in a general form, based on the time-dependent variational principle. We derive the wave-packet energy up to first order in the gradient of the perturbations and all kinds of Berry-phase corrections to the semiclassical dynamics and the quantization rule. Also, we give a discussion of a formal quantization procedure through the Hamiltonian formalism with the semiclassical dynamics as the starting point.

We illustrate our framework with two cases of perturbations. For electromagnetic fields, previous results of orbital magnetization and anomalous velocity are obtained purely from a single-band point of view. For deformations in crystals, we obtain a Berry-phase term in the Lagrangian due to lattice tracking, which gives to the new terms of tracking velocity and force in the equations of motion of the wave packet. For multiple-valued displacement fields in the presence of dislocations, this term manifests as a Berry phase, which we show to be proportional to the Burgers vector around each dislocation. Also, we relate the deformation correction to the wave-packet energy to the shift in band energy under uniform strain, which turns out to be the same as the deformation potential for electron-phonon interaction at long wavelengths.

The combined effects of electromagnetic and deformational perturbations are yet to be studied. Given that the perturbed Hamiltonian is of the form Eq. (3.1), the equations of motion for the wave-packet dynamics can be completely determined in terms of the properties of the unperturbed crystal and the fields of perturbations. Such a theory will provide a basis for electron transport in deformed crystals and should be pursued in the near future.

ACKNOWLEDGMENTS

The authors wish to thank M. C. Chang, R. Diener, E. Demircan, S. Fishman, D. Gavenda, G. A. Georgakis, L. Kleinman, M. Marder, F. Nori, R. Resta, E. C. G. Sudarshan, Bala Sundaram, and J. Zak for many insightful discussions. This work was supported by the NSF (Grants Nos. DMR 9705406 and PHY 9722610), and by the R. A. Welch Foundation.

APPENDIX A: THE GRADIENT CORRECTION $\Delta\mathcal{E}$

In the derivation below, the band indices for the Bloch states and the energy bands have been restored.

We begin with the matrix elements of the position operator,[10]

$$\langle \psi_{n\mathbf{q}}|\hat{\mathbf{x}}|\psi_{n'\mathbf{q}'}\rangle=\left[i\frac{\partial}{\partial\mathbf{q}}\delta_{nn'}+\left\langle u_n\left| i\frac{\partial u_{n'}}{\partial\mathbf{q}}\right\rangle\right.\right]\delta(\mathbf{q}'-\mathbf{q}), \tag{A1}$$

and the identity

$$\begin{aligned}\left\langle \psi_{n\mathbf{q}}\left|\frac{\partial\hat{H}_c}{\partial\mathbf{x}_c}\right|\psi_{n'\mathbf{q}'}\right\rangle &= \delta(\mathbf{q}-\mathbf{q}')\left\langle u_n\left|\frac{\partial\hat{H}_c}{\partial\mathbf{x}_c}\right|u_{n'}\right\rangle \\ &= \delta(\mathbf{q}-\mathbf{q}')\left[(\mathcal{E}_{cn}-\mathcal{E}_{cn'})\left\langle\frac{\partial u_{n\mathbf{q}}}{\partial\mathbf{x}_c}\right|u_{n'\mathbf{q}}\right\rangle \\ &\quad +\frac{\partial\mathcal{E}_{cn}}{\partial\mathbf{x}_c}\delta_{nn'}\right],\end{aligned} \tag{A2}$$

which are easily verified.

From Eqs. (A1), (A2), and the completeness relation

$$\sum_n\int d^3q|\psi_{n\mathbf{q}}\rangle\langle\psi_{n\mathbf{q}}|=\hat{\mathbb{1}}, \tag{A3}$$

we can show that

$$\begin{aligned}&\left\langle\psi_{n\mathbf{q}}\left|\frac{\partial\hat{H}_c}{\partial\mathbf{x}_c}\cdot\hat{\mathbf{x}}\right|\psi_{n\mathbf{q}'}\right\rangle \\ &\quad=\frac{\partial\mathcal{E}_{cn}}{\partial\mathbf{x}_c}\cdot\langle\psi_{n\mathbf{q}}|\hat{\mathbf{x}}|\psi_{n\mathbf{q}'}\rangle \\ &\qquad+i\left\langle\frac{\partial u_{n\mathbf{q}}}{\partial\mathbf{x}_c}\right|\cdot(\mathcal{E}_{cn}-\hat{H}_c)\left|\frac{\partial u_{n\mathbf{q}}}{\partial\mathbf{q}}\right\rangle\delta(\mathbf{q}-\mathbf{q}').\end{aligned} \tag{A4}$$

If we assume that the wave packet is constructed from the Bloch states of the nth band, we have

$$\left\langle\Psi\left|\frac{\partial\hat{H}_c}{\partial\mathbf{x}_c}\right|\Psi\right\rangle=\int d^3q|a|^2\frac{\partial\mathcal{E}_{cn}}{\partial\mathbf{x}_c}=\left.\frac{\partial\mathcal{E}_{cn}}{\partial\mathbf{x}_c}\right|_{\mathbf{q}=\mathbf{q}_c}, \tag{A5}$$

as only the second term of Eq. (A2) contribute to the expectation value. By the same token, from Eqs. (A5) and (A4), we obtain

$$\left\langle\Psi\left|\frac{\partial\hat{H}_c}{\partial\mathbf{x}_c}\cdot(\hat{\mathbf{x}}-\mathbf{x}_c)\right|\Psi\right\rangle=i\left\langle\frac{\partial u_{n\mathbf{q}}}{\partial\mathbf{x}_c}\right|\bullet(\mathcal{E}_{cn}-\hat{H}_c)\left|\frac{\partial u_{n\mathbf{q}}}{\partial\mathbf{q}}\right\rangle\Bigg|_{\mathbf{q}=\mathbf{q}_c}. \tag{A6}$$

Hence, the expectation value (2.17) of Eq. (2.15) is just half of the sum of (A6) and its complex conjugate.

APPENDIX B: THE DEFORMED CRYSTAL POTENTIAL

Given the atomic displacements $\{\mathbf{u}_l\}$, which could be due to either strain or rotations, let us denote the deformed crystal potential regarded as a function of the coordinates of the electron and the equilibrium atomic positions by $V(\mathbf{x};\{\mathbf{R}_l+\mathbf{u}_l\})$. If the displacements are small, we can expand the potential in powers of $\{\mathbf{u}_l\}$ and do away with the perturbation theory. When they are large, we have to adopt a different technique. For this purpose, we introduce a smooth displacement field $\mathbf{u}(\mathbf{x})$ such that $\mathbf{u}(\mathbf{R}_l+\mathbf{u}_l)=\mathbf{u}_l$, and write the potential as

$$V[\mathbf{x}-\mathbf{u}(\mathbf{x});\{\mathbf{R}_l+\mathbf{u}_l-\mathbf{u}(\mathbf{x})\}], \tag{B1}$$

where we have used the invariance property of a potential under a simultaneous translation of electronic and atomic positions. We may now expand the potential in powers of $\mathbf{u}_l-\mathbf{u}(\mathbf{x})$ as

$$V_0[\mathbf{x}-\mathbf{u}(\mathbf{x})]+\sum_l [\mathbf{u}_l-\mathbf{u}(\mathbf{x})]_\alpha V_{l\alpha}+\cdots. \quad \text{(B2)}$$

where $V_0(\mathbf{x}-\mathbf{u})\equiv V(\mathbf{x}-\mathbf{u};\{\mathbf{R}_l\})$ is the potential used in the deformable ion model in which the approximated potential at $\mathbf{x}$ equals the undeformed crystal potential at the undeformed electron coordinate $\mathbf{x}-\mathbf{u}(\mathbf{x})$, and

$$V_{l\alpha}\equiv\frac{\partial V[\mathbf{x}-\mathbf{u}(\mathbf{x});\{\mathbf{R}_l\}]}{\partial R_{l\alpha}}=V_{l\alpha}[\mathbf{x}-\mathbf{u}(\mathbf{x})-\mathbf{R}_l]. \quad \text{(B3)}$$

The equality in the last equation is meant to suggest that the center of fall off of $V_{l\alpha}$ is at the zero of the expression $\mathbf{x}-\mathbf{u}(\mathbf{x})-\mathbf{R}_l$, viz., $\mathbf{x}=\mathbf{u}_l+\mathbf{R}_l$.

The expansion (B2) is meaningful only if $V_{l\alpha}$ decreases sufficiently rapidly with increasing $|\mathbf{x}-\mathbf{u}(\mathbf{x})-\mathbf{R}_l|$. This condition holds for metals because of Coulomb screening; it has been argued that $V_{l\alpha}$ is short ranged[52] also for nonpolar semiconductors and insulators.

Under such a condition, we may write

$$\begin{aligned} u_{l\alpha}&=u_\alpha(\mathbf{x}+\mathbf{R}_l+\mathbf{u}_l-\mathbf{x})\\ &\approx u_\alpha(\mathbf{x})+(\mathbf{R}_l+\mathbf{u}_l-\mathbf{x})_\beta s_{\alpha\beta}(\mathbf{x})\approx u_\alpha(\mathbf{x})\\ &\quad+[\mathbf{R}_l+\mathbf{u}(\mathbf{x})-\mathbf{x}]_\beta s_{\alpha\beta}(\mathbf{x}), \end{aligned} \quad \text{(B4)}$$

whence the summation in Eq. (B2) can be put into the form $s_{\alpha\beta}\mathcal{V}_{\alpha\beta}$ with

$$\mathcal{V}_{\alpha\beta}[\mathbf{x}-\mathbf{u}(\mathbf{x})]=\sum_l [\mathbf{R}_l+\mathbf{u}(\mathbf{x})-\mathbf{x}]_\beta V_{l\alpha}. \quad \text{(B5)}$$

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