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Semi-classical wave packet dynamics in non-uniform electric fields

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We study the semi-classical theory of wave packet dynamics in crystalline solids extended to include the effects of a non-uniform electric field. In particular, we derive a correction to the semi-classical equations of motion (EOMs) for the dynamics of the wave packet center that depends on the gradient of the electric field and on the quantum metric (also called the Fubini-Study, Bures, or Bloch metric) on the Brillouin zone. We show that the physical origin of this term is a contribution to the total energy of the wave packet that depends on its electric quadrupole moment and on the electric field gradient. We also derive an equation relating the electric quadrupole moment of a sharply-peaked wave packet to the quantum metric evaluated at the wave packet center in reciprocal space. Finally, we explore the physical consequences of this correction to the semi-classical EOMs. We show that in a metal with broken time-reversal and inversion symmetry, an electric field gradient can generate a longitudinal current which is linear in the electric field gradient, and which depends on the quantum metric at the Fermi surface. We then give two examples of concrete lattice models in which this effect occurs. Our results show that non-uniform electric fields can be used to probe the quantum geometry of the electronic bands in metals and open the door to further studies of the effects of non-uniform electric fields in solids.

Electron wave packets in a solid placed in an applied electric field experience an anomalous contribution to their velocity which has its origin in the *Berry curvature* of the electronic bands. This anomalous velocity is responsible for the quantized Hall conductivity of Chern insulators, and the intrinsic contribution to the anomalous Hall effect in metals, among other things, and these effects can all be understood within a framework based on the semi-classical equations of motion (EOMs) for electron wave packets in solids^{1–8} (see also the review⁹). Combining the semi-classical EOMs with a Boltzmann equation approach to transport is particularly useful in the search for novel physical consequences of band geometry and topology^{5,6,10–13}.

One issue which is not addressed by the current semiclassical framework is the effect of a non-uniform electric field on wave packet motion. However, it is known that nonuniform electric fields probe some of the most subtle and interesting effects in condensed matter systems, for example the Hall viscosity in quantum Hall systems^{14,15} and electrical multipole moments in insulators^{16–18}. In addition, it is likely that non-uniform electric fields can have significant effects in metals where the partially filled conduction band can respond quickly to an applied field. These expectations motivate a systematic study of the semi-classical EOMs in an expansion in *spatial derivatives* of the external electric field.

In this article we initiate this study by considering the semiclassical dynamics of electron wave packets in the presence of a constant electric field *gradient*. We derive a correction to the usual semi-classical EOM for the time derivative of the wave packet center in real space. This correction depends on the *gradient* of the electric field, and on the *quantum metric*¹⁹ on the Brillouin zone (BZ) for the electronic band whose states are used in the construction of the wave packet. The quantum metric (also called the Fubini-Study metric, Bures metric, Bloch metric, etc.) has previously been studied in the context of band theory and the semi-classical EOMs in Refs. 20–36.

The correction to the semi-classical EOMs that we derive depends on the *derivative* of the quantum metric. As a consequence, we show that this correction does not affect transport in insulators. On the other hand, we show one direct effect of this correction on transport in metals where it can lead to a longitudinal current proportional to the electric field gradient and to the quantum metric at the Fermi surface. Thus, our result shows that the quantum geometry of bands in metals can be probed by a transport experiment using a non-uniform electric field. We now turn to an explanation of our results.

Setup: We study the dynamics of electrons of charge Q = -e in a crystal and in the presence of a *time-independent* electric field $\mathbf{E}(\mathbf{x})$. Let $\hat{x}^{\mu}, \hat{p}_{\nu}, \mu, \nu = 1, \dots, D$, denote the position and momentum operators for a single electron in D spatial dimensions, with $[\hat{x}^{\mu}, \hat{p}_{\nu}] = i\hbar \delta^{\mu}_{\nu}$. The single particle Hamiltonian is

$$\hat{H} = \hat{H}_0 + Q\varphi(\hat{\mathbf{x}}) , \qquad (1)$$

where \hat{H}_0 is a Hamiltonian for an electron in a periodic potential $V(\hat{\mathbf{x}})$, for example the standard non-relativistic Hamiltonian $\hat{H}_0 = \frac{1}{2m} \delta^{\mu\nu} \hat{p}_{\mu} \hat{p}_{\nu} + V(\hat{\mathbf{x}})$ for particles of mass m. In fact, our only requirement for \hat{H}_0 is that it be subject to Bloch's theorem. The second term in \hat{H} captures the coupling to the electric field $\mathbf{E}(\mathbf{x})$, which is determined by the potential $\varphi(\mathbf{x})$ as $E_{\mu}(\mathbf{x}) = -\frac{\partial \varphi(\mathbf{x})}{\partial x^{\mu}}$.

Bloch's theorem implies that \hat{H}_0 has a basis of eigenstates ("Bloch waves") $|\psi_{n,\mathbf{q}}\rangle$ which are labeled by a band index nand a wavevector \mathbf{q} (in the first BZ) and obey $\hat{H}_0|\psi_{n,\mathbf{q}}\rangle = \mathcal{E}_n(\mathbf{q})|\psi_{n,\mathbf{q}}\rangle$, where $\mathcal{E}_n(\mathbf{q})$ are the energy eigenvalues. In addition, we can write $|\psi_{n,\mathbf{q}}\rangle = e^{iq_\mu \hat{x}^\mu}|u_{n,\mathbf{q}}\rangle$ where the function $u_{n,\mathbf{q}}(\mathbf{x}) := \langle \mathbf{x}|u_{n,\mathbf{q}}\rangle$ has the periodicity of the crystal lattice. Note that the Bloch states are time-independent since we have made the simplifying assumption that our Hamiltonian is time-independent. We normalize the Bloch states so that $\langle \psi_{n,\mathbf{q}}|\psi_{n',\mathbf{q}'}\rangle = \delta_{n,n'}\delta^{(D)}(\mathbf{q}-\mathbf{q}')$, which implies that $\langle u_{n,\mathbf{q}}|u_{n',\mathbf{q}}\rangle = \delta_{n,n'}$. Here, the the inner product of the $|u_{n,\mathbf{q}}\rangle$ is defined as independent over the real space unit cell times a factor of $\frac{(2\pi)^D}{v_c}$, where v_c is the volume of the real space unit cell³⁷. We also introduce a crystal momentum operator \hat{q}_{μ} which is diagonal in the basis of Bloch states and satisfies $\hat{q}_{\mu}|\psi_{n,\mathbf{q}}\rangle = q_{\mu}|\psi_{n,\mathbf{q}}\rangle$.

We are interested in the leading corrections to the semiclassical EOMs due to a non-zero electric field gradient, and so we choose a potential of the form $\varphi(\mathbf{x}) = -E_{\mu}^{(0)}x^{\mu} - \frac{1}{2}E_{\mu\nu}^{(0)}x^{\mu}x^{\nu}$, where $E_{\mu}^{(0)}$ and $E_{\mu\nu}^{(0)}$ (with $E_{\mu\nu}^{(0)} = E_{\nu\mu}^{(0)}$) are two sets of constant parameters. The components of the electric field are then $E_{\mu}(\mathbf{x}) = E_{\mu}^{(0)} + E_{\mu\nu}^{(0)}x^{\nu}$. We see that $E_{\mu\nu}^{(0)}$ specify the uniform part of the electric field, while $E_{\mu\nu}^{(0)}$ specify the electric field gradient.

Wave packets and their first moments: We study the timeevolution (using the full Hamiltonian \hat{H}) of a wave packet $|\Psi(t)\rangle$ constructed from the Bloch states $|\psi_{n,\mathbf{q}}\rangle$. We assume that the wave packet is constructed from states within a single band, and so we drop the band index n from the notation. We define this wave packet state as $|\Psi(t)\rangle = \int d^D \mathbf{q} \, a(\mathbf{q},t) |\psi_{\mathbf{q}}\rangle$, where $a(\mathbf{q},t)$ is a complex amplitude which must satisfy the normalization condition $\int d^D \mathbf{q} \, |a(\mathbf{q},t)|^2 = 1$ (\mathbf{q} integrals run over the first BZ). By plugging into the Schrodinger equation $i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$, one can show that $a(\mathbf{q},t)$ satisfies

$$i\hbar\dot{a}(\mathbf{q},t) = a(\mathbf{q},t)\mathcal{E}(\mathbf{q}) + Q \int d^{D}\mathbf{q}' \ a(\mathbf{q}',t)\langle\psi_{\mathbf{q}}|\varphi(\hat{\mathbf{x}})|\psi_{\mathbf{q}'}\rangle ,$$
(2)

where the dot denotes a time derivative.

The semi-classical EOMs for wave packet dynamics in solids can be derived by studying the dynamics of the first moments $X^{\mu}(t)$ and $K_{\mu}(t)$ of the wave packet in position and reciprocal space, respectively. These are defined by $X^{\mu}(t) = \langle \Psi(t) | \hat{x}^{\mu} | \Psi(t) \rangle$ and $K_{\mu}(t) = \langle \Psi(t) | \hat{q}_{\mu} | \Psi(t) \rangle = \int d^{D} \mathbf{q} q_{\mu} | a(\mathbf{q},t) |^{2}$. We derive the semi-classical EOMs for $X^{\mu}(t)$ and $K_{\mu}(t)$ by first computing the exact expressions for $\dot{X}^{\mu}(t)$ and $\dot{K}_{\mu}(t)$, and then truncating these expressions using the assumption that the wave packet is sharply-peaked about the locations $X^{\mu}(t)$ and $K_{\mu}(t)$ in position and reciprocal space. To derive the equations for $\dot{X}^{\mu}(t)$ and $\dot{K}_{\mu}(t)$ we simply differentiate the expressions for $X^{\mu}(t)$ and $K_{\mu}(t)$ with respect to time, and then we substitute in for $\dot{a}(\mathbf{q}, t)$ and $\dot{a}(\mathbf{q}, t)$ using Eq. (2) and its complex conjugate.

After a tedious but straightforward calculation, we find that the equation for $\dot{X}^{\mu}(t)$ takes the form

$$\dot{X}^{\mu}(t) = \frac{1}{\hbar} \Big\langle \frac{\partial \mathcal{E}(\hat{\mathbf{q}})}{\partial q_{\mu}} \Big\rangle_{t} - \frac{1}{\hbar} Q E_{\nu}^{(0)} \Big\langle \Omega^{\mu\nu}(\hat{\mathbf{q}}) \Big\rangle_{t} - \frac{1}{2\hbar} Q E_{\nu\lambda}^{(0)} \Big\langle \{\hat{x}^{\lambda}, \Omega^{\mu\nu}(\hat{\mathbf{q}})\} \Big\rangle_{t} - \frac{1}{2\hbar} Q E_{\nu\lambda}^{(0)} \Big\langle \frac{\partial g^{\nu\lambda}(\hat{\mathbf{q}})}{\partial q_{\mu}} \Big\rangle_{t},$$
(3)

where $\langle \cdot \rangle_t$ denotes an expectation value in the state $|\Psi(t)\rangle$, and $\{\cdot, \cdot\}$ denotes an anti-commutator (third term on the righthand side). In this equation $\Omega^{\mu\nu}(\mathbf{q})$ is the Berry curvature, which is expressed in terms of the Berry connection $\mathcal{A}^{\mu}(\mathbf{q}) =$ $i \langle u_{\mathbf{q}} | \frac{\partial u_{\mathbf{q}}}{\partial q_{\mu}} \rangle$ as $\Omega^{\mu\nu}(\mathbf{q}) = \frac{\partial \mathcal{A}^{\nu}(\mathbf{q})}{\partial q_{\mu}} - \frac{\partial \mathcal{A}^{\mu}(\mathbf{q})}{\partial q_{\nu}}$. The quantity $g^{\mu\nu}(\mathbf{q})$ is the quantum metric on the BZ, and is defined as

$$g^{\mu\nu}(\mathbf{q}) = \frac{1}{2} \left(\left\langle \frac{\partial u_{\mathbf{q}}}{\partial q_{\mu}} \middle| \frac{\partial u_{\mathbf{q}}}{\partial q_{\nu}} \right\rangle - \left\langle \frac{\partial u_{\mathbf{q}}}{\partial q_{\mu}} \middle| u_{\mathbf{q}} \right\rangle \left\langle u_{\mathbf{q}} \middle| \frac{\partial u_{\mathbf{q}}}{\partial q_{\nu}} \right\rangle + (\mu \leftrightarrow \nu) \right).$$
(4)

Both $\Omega^{\mu\nu}(\mathbf{q})$ and $g^{\mu\nu}(\mathbf{q})$ are invariant under a gauge transformation $|u_{\mathbf{q}}\rangle \rightarrow e^{-if(\mathbf{q})}|u_{\mathbf{q}}\rangle$ for any function $f(\mathbf{q})$. The equation for $\dot{K}_{\mu}(t)$ is much simpler, and it takes the form

$$\dot{K}_{\mu}(t) = \frac{1}{\hbar} Q E_{\mu}(\mathbf{X}(t)) , \qquad (5)$$

where $E_{\mu}(\mathbf{X}(t)) = E_{\mu}^{(0)} + E_{\mu\nu}^{(0)} X^{\nu}(t)$ is the electric field at the location of the first moment $X^{\mu}(t)$.

To derive these equations, it is necessary to use explicit expressions for the matrix elements $\langle \psi_{\mathbf{q}} | \hat{x}^{\mu} | \psi_{\mathbf{q}'} \rangle$ and

 $\langle \psi_{\mathbf{q}} | \hat{x}^{\mu} \hat{x}^{\nu} | \psi_{\mathbf{q}'} \rangle$ of the position operator in the Bloch states. We record these expressions in Eqs. (3) and (4) of the Supplemental Material³⁸. In the derivation we also used several integrations by parts in integrals over the BZ, and we neglected boundary terms. If the amplitudes $a(\mathbf{q}, t)$ or the Berry connection $\mathcal{A}^{\mu}(\mathbf{q})$ are not single-valued, then there could be some interesting, subtle additions to these modified EOMs. In the Supplemental Material we show that by a suitable choice of gauge for the Bloch states $|\psi_{\mathbf{q}}\rangle$, we can make $a(\mathbf{q}, t)$ single-valued for all t. In that case the only possible source of boundary corrections arise, and we leave a detailed discussion of any alternatives to future work.

To obtain the semi-classical EOMs for $X^{\mu}(t)$ and $K_{\mu}(t)$ we make the substitutions $\hat{x}^{\mu} \to X^{\mu}(t)$ and $\hat{q}_{\mu} \to K_{\mu}(t)$ in all expectation values in Eq. (3) and Eq. (5). Our result, which is one of the main results of this article, is that the semi-classical EOMs take the form

$$\dot{X}^{\mu} = \frac{1}{\hbar} \frac{\partial \mathcal{E}(\mathbf{K})}{\partial K_{\mu}} - \Omega^{\mu\nu}(\mathbf{K}) \dot{K}_{\nu} - \frac{1}{2\hbar} Q E_{\nu\lambda}^{(0)} \frac{\partial g^{\nu\lambda}(\mathbf{K})}{\partial K_{\mu}} \quad (6a)$$
$$\dot{K}_{\mu} = \frac{1}{\hbar} Q E_{\mu}(\mathbf{X}) , \qquad (6b)$$

where we also used the second equation to rewrite part of

the $\dot{X}^{\mu}(t)$ equation in terms of $\dot{K}_{\mu}(t)$. The main difference compared to the usual semi-classical EOMs is the term $-\frac{1}{2\hbar}QE^{(0)}_{\nu\lambda}\frac{\partial g^{\nu\lambda}(\mathbf{K})}{\partial K_{\mu}}$. This new term depends on the gradient of the electric field, since it depends on $E^{(0)}_{\nu\lambda}$ but not $E^{(0)}_{\mu}$, and it also probes the geometry of the band structure since it involves the quantum metric $g^{\nu\lambda}(\mathbf{K})$.

Interpretation: We now show that the new term in (6) arises from an electric field-induced correction to the energy of the wave packet. In the absence of an electric field we have $\langle \Psi(t) | \hat{H}_0 | \Psi(t) \rangle = \int d^D \mathbf{q} |a(\mathbf{q}, t)|^2 \mathcal{E}(\mathbf{q}) \approx \mathcal{E}(\mathbf{K})$, where $\mathbf{K}(t)$ is the wave packet center. In the presence of the electric field, we show in the Supplemental Material that the wave packet energy takes the form

$$\langle \Psi(t)|\hat{H}|\Psi(t)\rangle \approx \mathcal{E}(\mathbf{K}) - QE^{(0)}_{\mu}X^{\mu} - \frac{1}{2}QE^{(0)}_{\mu\nu}\left(X^{\mu}X^{\nu} + g^{\mu\nu}(\mathbf{K})\right)$$
(7)

$$\equiv \mathcal{E}_{eff}(\mathbf{X}, \mathbf{K}) . \tag{8}$$

As a result, the corrected semi-classical EOM for $\dot{X}^{\mu}(t)$ can be rewritten as

$$\dot{X}^{\mu} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_{eff}(\mathbf{X}, \mathbf{K})}{\partial K_{\mu}} - \Omega^{\mu\nu}(\mathbf{K}) \dot{K}_{\nu} .$$
(9)

We can also rewrite the equation for $\dot{K}_{\mu}(t)$ as $\dot{K}_{\mu} = -\frac{1}{\hbar} \frac{\partial \mathcal{E}_{eff}(\mathbf{X}, \mathbf{K})}{\partial X^{\mu}}$.

In this form, the correction to the $\dot{X}^{\mu}(t)$ and $\dot{K}_{\mu}(t)$ equations closely resembles a similar correction which occurs for electrons in a magnetic field. In that case the correction to the wave packet energy arises from the magnetic moment of the wave packet⁶. In the present case of a non-uniform electric field, the corrections to the energy depend on the dipole moment $X^{\mu}(t)$ of the wave packet (the term proportional to $E_{\mu\nu}^{(0)}$), and on the *quadrupole* moment of the wave packet (the term proportional to $E_{\mu\nu}^{(0)}$). Indeed, in the Supplemental Material we show that for a wave packet $|\Psi(t)\rangle$ sharply peaked at position **K** in reciprocal space, the quadrupole moment is given by

$$\langle \Psi(t)|\hat{x}^{\mu}\hat{x}^{\nu}|\Psi(t)\rangle \approx X^{\mu}X^{\nu} + g^{\mu\nu}(\mathbf{K})$$
 (10)

The correction due to the dipole moment is already present in the case of a uniform electric field, and it does not alter the semi-classical EOMs. On the other hand, the correction proportional to the quadrupole moment is only present in a non-uniform field, and it does alter the semi-classical EOMs. We also note that to find the $g^{\mu\nu}(\mathbf{K})$ term in $\mathcal{E}_{eff}(\mathbf{X}, \mathbf{K})$, we need to expand $Q\langle \Psi(t)|\varphi(\hat{\mathbf{x}})|\Psi(t)\rangle$ to second order about the wave packet center in real space, and so this term cannot be found using the first order expansion of Ref. 7.

Physical consequences: We now discuss physical consequences of the new term in Eq. (6) for transport in solids. Within the semi-classical approach, the current density $j^{\mu}(\mathbf{r})$ at position \mathbf{r} in the material is given by $j^{\mu}(\mathbf{r}) = Q \int d^D \mathbf{X} \frac{d^D \mathbf{K}}{(2\pi)^D} f(\mathbf{X}, \mathbf{K}, t) \dot{X}^{\mu} \delta^{(D)}(\mathbf{X}-\mathbf{r})$, where $f(\mathbf{X}, \mathbf{K}, t)$

is the non-equilibrium distribution function which specifies the occupation, at time t, of the volume element $d^D \mathbf{X} \frac{d^D \mathbf{K}}{(2\pi)^D}$ at position (\mathbf{X}, \mathbf{K}) in phase space. The full distribution function can be obtained by solving the Boltzmann equation. In the relaxation time approximation, with relaxation time τ , $f(\mathbf{X}, \mathbf{K}, t)$ takes the form of a power series in τ , $f(\mathbf{X}, \mathbf{K}, t) = f_0(\mathbf{K}) + O(\tau)$, where $f_0(\mathbf{K})$ is the equilibrium distribution function specifying the occupied states in reciprocal space at temperature $T^{5,6,10-13}$. In what follows, we will be interested in the currents which come from this zeroth order contribution, which captures the intrinsic part of the linear response of the system to the applied electric field. The zeroth order contribution to the current is then $j_0^{\mu}(\mathbf{r}) = Q \int \frac{d^D \mathbf{K}}{(2\pi)^D} f_0(\mathbf{K}) \dot{X}^{\mu} \Big|_{\mathbf{X}=\mathbf{r}}$. In D = 2, for example, $j_0^{\mu}(\mathbf{r})$ contains the intrinsic contribution to the anomalous Hall effect. Using Eq. (6), we find that $j_0^{\mu}(\mathbf{r})$ contains the additional term

$$j_{\text{geom.}}^{\mu}(\mathbf{r}) = -\frac{Q^2}{2\hbar} \int \frac{d^D \mathbf{K}}{(2\pi)^D} f_0(\mathbf{K}) E_{\nu\lambda}^{(0)} \frac{\partial g^{\nu\lambda}(\mathbf{K})}{\partial K_{\mu}} , \quad (11)$$

which involves the electric field gradient and the quantum metric. We will refer to $j_{geom.}^{\mu}$ as the *geometric* current.

The geometric current is easiest to understand in the case of a metal in D = 1 dimension (so $\mu, \nu = 1$ in all equations). Recall that we considered wave packets constructed from states in a single band. We assume a partial filling of this band such that the Fermi level \mathcal{E}_F crosses the band at the set of wave numbers $\{k_{I,+}, k_{I,-}\}_{I \in \{1,...,n_F\}}$ for some integer n_F (so $2n_F$ is the total number of Fermi points). Our notation means that $\frac{\partial \mathcal{E}(K_1)}{\partial K_1}$ is positive at a + Fermi point and negative at a - Fermi point (we assume that \mathcal{E}_F is chosen so that there is no Fermi point where $\frac{\partial \mathcal{E}(K_1)}{\partial K_1}$ vanishes). At temperature T = 0 the distribution function $f_0(K_1)$ is equal to 1 if $\mathcal{E}(K_1) \leq \mathcal{E}_F$ and zero otherwise. After an integration by parts, and using $\frac{\partial f_0(K_1)}{\partial K_1} = \sum_{I=1}^{n_F} [\delta(K_1 - K_{I,-}) - \delta(K_1 - K_{I,+})]$, we find that $(h = 2\pi\hbar)$

$$j_{\text{geom.}}^{1} = -\frac{1}{2} \frac{Q^{2}}{h} E_{11}^{(0)} \sum_{I=1}^{n_{F}} \left[g^{11}(K_{I,+}) - g^{11}(K_{I,-}) \right] , \quad (12)$$

which is non-zero if the sum does not equal zero.

Next, we consider a similar example for a metal in D = 2. To illustrate the nontrivial response we compute $j_{\text{geom.}}^1$ as an example. We again consider a single band and we assume the Fermi surface consists of a single closed contour C. For simplicity, we assume further that the parts of C to the left and right of the K_2 axis can be specified by single-valued functions $h_L(K_2)$, $h_R(K_2)$, such that $K_1 = h_L(K_2)$ defines the part of C to the left of the K_2 axis, and $K_1 = h_R(K_2)$ defines the part of C to the right (note that for a generic C the functions $h_{R/L}(K_2)$ would not be single-valued). Let $K_{2,+} > 0$ and $K_{2,-} < 0$ be the two points where C intersects the K_2 axis. This situation is illustrated in Fig. 1. At T = 0 the distribution function for this metal is $f_0(\mathbf{K}) = 1$ for \mathbf{K} inside C, and zero otherwise. We then have $\frac{\partial f_0(\mathbf{K})}{\partial K_1} =$

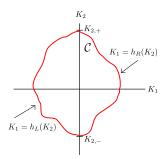


FIG. 1. A Fermi surface C (red contour), whose segments to the left and right of the K_2 axis are defined by the relations $K_1 = h_L(K_2)$, $K_1 = h_R(K_2)$, respectively, where $h_{R/L}(K_2)$ are single-valued functions of K_2 .

$$\delta(K_{1} - h_{L}(K_{2})) - \delta(K_{1} - h_{R}(K_{2})), \text{ and so}$$

$$j_{\text{geom.}}^{1} = -\frac{Q^{2}}{2h} \frac{E_{\nu\lambda}^{(0)}}{2\pi} \left(\int_{K_{2,-}}^{K_{2,+}} dK_{2} g^{\nu\lambda}(\mathbf{K}) \Big|_{K_{1} = h_{R}(K_{2})} - \int_{K_{2,-}}^{K_{2,+}} dK_{2} g^{\nu\lambda}(\mathbf{K}) \Big|_{K_{1} = h_{L}(K_{2})} \right).$$
(13)

Since $j_{\text{geom.}}^1$ involves an integral of $g^{\mu\nu}(\mathbf{K})$ only on \mathcal{C} , we see that this current is a Fermi surface property, like the intrinsic contribution to the anomalous Hall effect⁸, and it vanishes in insulators (which have a full band, $f_0(\mathbf{K}) = 1 \forall \mathbf{K}$).

Symmetry analysis: In systems with time-reversal symmetry we have $\mathcal{E}(\mathbf{K}) = \mathcal{E}(-\mathbf{K})$ and $g^{\mu\nu}(\mathbf{K}) = g^{\mu\nu}(-\mathbf{K})$, and identical conditions hold in the case of inversion symmetry. These conditions imply that $j^{\mu}_{\text{geom.}} = 0$. To prove this we use these conditions to first replace $g^{\mu\nu}(\mathbf{K})$ in Eq. (11) with $g^{\mu\nu}(-\mathbf{K})$. Next, we use the fact that $f_0(\mathbf{K}) = f_0(-\mathbf{K})$ if $f_0(\mathbf{K})$ is a function of $\mathcal{E}(\mathbf{K})$ only (as it would be in thermal equilibrium or at T = 0). Finally, we change integration variables from \mathbf{K} to $-\mathbf{K}$ to find that time-reversal or inversion symmetry imply that $j^{\mu}_{\text{geom.}} = -j^{\mu}_{\text{geom.}}$, and so $j^{\mu}_{\text{geom.}} = 0$. Therefore we must break these symmetries to obtain $j^{\mu}_{\text{geom.}} \neq 0$.

Examples in D = 1 *and* D = 2: We now discuss two examples of lattice models of metals in D = 1 and D = 2 which yield a non-zero geometric current. We present the detailed results for the geometric current in these models in the Supplemental Material. In D = 1 we consider the two-band model with Bloch Hamiltonian

$$H_{1D}(k) = A\sin(k)\mathbb{I} + \sin(k)\sigma^{x} + (m+1-\cos(k))\sigma^{z}$$
, (14)

where \mathbb{I} is the 2×2 identity matrix and $\sigma^{x,y,z}$ are the Pauli matrices. In D = 2 we consider the two-band model with Bloch Hamiltonian

$$H_{2D}(\mathbf{k}) = A\sin(k_1)\mathbb{I} + \sin(k_1)\sigma^x + \sin(k_2)\sigma^y + (m+2-\cos(k_1)-\cos(k_2))\sigma^z .$$
(15)

In both cases we choose the parameters m and A so that there is an energy gap between the two bands of the model. We then

fill the lower band and partially fill the upper band to a Fermi energy \mathcal{E}_F to obtain a model of a metal. In the Supplemental Material we show that under these conditions, and when the parameter $A \neq 0$, both of these models display a nontrivial geometric current in the presence of a non-uniform electric field in the X^1 direction (i.e., $E_{11}^{(0)} \neq 0$). In both cases the condition $A \neq 0$ is required to break inversion and/or time-reversal symmetry, which then allows for a non-zero $j_{\text{geom.}}^{\mu}$ according to our previous discussion.

Discussion: A natural question to ask is how one can distinguish the geometric current of Eq. (12) from a more typical longitudinal current of the Drude form. The Drude contribution has the form

$$j_{\text{Drude}}^{1}(r^{1}) = \tau \frac{Q^{2}}{h} E_{1}(r^{1}) \sum_{I=1}^{n_{F}} \left[v(k_{I,+}) - v(k_{I,-}) \right] , \quad (16)$$

where τ is the relaxation time and $v(k) = \frac{\partial \mathcal{E}(k)}{\partial k}$. To distinguish this from Eq. (12) we choose an electric field which is a pure gradient around an origin, $E_1(r^1) = E_{11}^{(0)}r^1$. We then compute the average of the current over a spatial region centered at that origin $r^1 \in [-\frac{L}{2}, \frac{L}{2}]$. We find that $\int_{-\frac{L}{2}}^{\frac{L}{2}} dr^1 j_{\text{Drude}}^1(r^1) = 0$, while

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} dr^{1} j_{\text{geom.}}^{1}(r^{1}) = -\frac{LQ^{2}E_{11}^{(0)}}{2h} \sum_{I=1}^{n_{F}} \left[g^{11}(K_{I,+}) - g^{11}(K_{I,-})\right]$$
(17)

Thus, a spatial average of the current about the origin can distinguish between these two kinds of responses when the electric field is a pure gradient ("pure" refers to the fact that $E_1(0) = 0$ and $E_1(r^1)$ is linear near $r^1 = 0$).

Eq. (17) shows that information about the quantum metric at the Fermi points can be extracted from a transport experiment using an electric field which is a pure gradient. By averaging the current over a spatial region which is symmetric about the origin, any Drude contribution to the current will be canceled. Then, since L (the length of the spatial region), Q, $E_{11}^{(0)}$, and h are known to the experimenter, the signed sum $\sum_{I=1}^{n_F} \left[g^{11}(K_{I,+}) - g^{11}(K_{I,-})\right]$ can be extracted from this transport data.

A second natural question concerns the conditions under which the electric field gradient term is expected to significantly alter the semi-classical dynamics. After all, if the electric field varies slowly over the width of the wave packet, then it should be reasonable to neglect the gradient term. To understand the relevant scales we use Eq. (10), which implies that the squared spread $\langle \Psi(t) | \hat{x}^{\mu} \hat{x}^{\nu} | \Psi(t) \rangle - X^{\mu} X^{\nu}$ of a wave packet sharply peaked at **K** in reciprocal space is equal to $g^{\mu\nu}(\mathbf{K})$. For simplicity, consider the case of D = 1. Then the width of the wave packet is $\sqrt{g^{11}(\mathbf{K})}$ and so the change of the electric field over the width of the wave packet is $\Delta E_1 \approx E_{11}^{(0)} \sqrt{g^{11}(\mathbf{K})}$. If $\Delta E_1 \ll E_1^{(0)}$ (the uniform part of the electric field), then we can neglect the gradient term. On the other hand, we must include this gradient term if ΔE_1 is comparable to or larger than $E_1^{(0)}$.

Conclusion: In this article we extended the semi-classical theory of electron wave packet motion in solids to incorporate the effects of a non-uniform electric field. In particular, we systematically calculated corrections to the semi-classical EOMs in an expansion in derivatives of the electric field, and we obtained the correction proportional to the first derivative of the electric field. Our main result, shown in Eqs. (6), is a correction to the semi-classical EOM for the wave packet center in real space which depends on the electric field gra*dient*, and on the quantum metric $g^{\mu\nu}(\mathbf{q})$ on the BZ. We then gave a physical interpretation of this new term as arising from the energy associated with the electric quadrupole moment of the wave packet in the presence of the non-uniform electric field. We also showed that this correction to the semi-classical EOMs does not affect transport in insulators, but does lead to a nontrivial transport signature in metals with broken timereversal and inversion symmetry. Specifically, we showed that in such metals an electric field gradient can generate a longitudinal current which is proportional to the electric field gradient and to the quantum metric at the Fermi surface. Since the current depends only on the quantum metric at the Fermi surface, we expect that it will be robust to the inclusion of interaction or disorder effects, as in the case of the anomalous Hall effect in metals⁸.

We envision at least two possible directions for future

work. The first would be to understand the corrections to the semi-classical EOMs (6) which involve higher derivatives of the electric field. The correction proportional to the second derivative would be particularly interesting as it should allow for a derivation of an analog of the formula of Hoyos and Son¹⁴, which relates the finite wave vector Hall conductivity of a quantum Hall system to the Hall viscosity, but in the context of Chern insulators (where there is no magnetic field) instead of Landau levels. A second direction would be to derive semi-classical EOMs for the higher moments of the wave packet, for example the second moments $X^{\mu\nu}(t) :=$ $\langle \Psi(t)|\hat{x}^{\mu}\hat{x}^{\nu}|\Psi(t)\rangle$ and $K_{\mu\nu}(t):=\langle \Psi(t)|\hat{q}_{\mu}\hat{q}_{\nu}|\Psi(t)\rangle$ in position and reciprocal space, respectively. In particular, it would be interesting to understand how these second moments respond to non-uniform electric fields. We leave these topics for future work.

Note added: After this work was completed we became aware of Ref. 39, which obtained many of the same results as part of a study of *nonreciprocal directional dichroism* in crystalline solids.

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- ¹ R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).
- ² W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957).
- ³ J. M. Luttinger, Phys. Rev. **112**, 739 (1958).
- ⁴ E. Adams and E. Blount, J. Phys. Chem. Solids **10**, 286 (1959).
- ⁵ M.-C. Chang and Q. Niu, Phys. Rev. Lett. **75**, 1348 (1995).
- ⁶ M.-C. Chang and Q. Niu, Phys. Rev. B **53**, 7010 (1996).
- ⁷ G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999).
- ⁸ F. D. M. Haldane, Phys. Rev. Lett. **93**, 206602 (2004).
- ⁹ D. Xiao, M.-C. Chang, and Q. Niu, Rev. Mod. Phys. 82, 1959 (2010).
- ¹⁰ J. E. Moore and J. Orenstein, Phys. Rev. Lett. **105**, 026805 (2010).
- ¹¹ J. Orenstein and J. E. Moore, Phys. Rev. B 87, 165110 (2013).
- ¹² S. Zhong, J. Orenstein, and J. E. Moore, Phys. Rev. Lett. **115**, 117403 (2015).
- ¹³ I. Sodemann and L. Fu, Phys. Rev. Lett. **115**, 216806 (2015).
- ¹⁴ C. Hoyos and D. T. Son, Phys. Rev. Lett. **108**, 066805 (2012).
- ¹⁵ B. Bradlyn, M. Goldstein, and N. Read, Phys. Rev. B 86, 245309 (2012).
- ¹⁶ W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science **357**, 61 (2017).
- ¹⁷ W. A. Wheeler, L. K. Wagner, and T. L. Hughes, arXiv preprint:1812.06990 (2018).
- ¹⁸ B. Kang, K. Shiozaki, and G. Y. Cho, arXiv preprint: 1812.06999 (2018).
- ¹⁹ J. P. Provost and G. Vallee, Commun. Math. Phys. **76**, 289 (1980).
- ²⁰ N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997).

- ²¹ S. Matsuura and S. Ryu, Phys. Rev. B **82**, 245113 (2010).
- ²² T. Neupert, C. Chamon, and C. Mudry, Phys. Rev. B 87, 245103 (2013).
- ²³ M. Kolodrubetz, V. Gritsev, and A. Polkovnikov, Phys. Rev. B 88, 064304 (2013).
- ²⁴ M. Legner and T. Neupert, Phys. Rev. B 88, 115114 (2013).
- ²⁵ Y.-Q. Ma, Phys. Rev. E **90**, 042133 (2014).
- ²⁶ Y. Gao, S. A. Yang, and Q. Niu, Phys. Rev. Lett. **112**, 166601 (2014).
- ²⁷ Y. Gao, S. A. Yang, and Q. Niu, Phys. Rev. B **91**, 214405 (2015).
- ²⁸ A. Srivastava and A. Imamoğlu, Phys. Rev. Lett. **115**, 166802 (2015).
- ²⁹ F. Piéchon, A. Raoux, J.-N. Fuchs, and G. Montambaux, Phys. Rev. B **94**, 134423 (2016).
- ³⁰ F. Freimuth, S. Blügel, and Y. Mokrousov, Phys. Rev. B **95**, 184428 (2017).
- ³¹ L. Liang, S. Peotta, A. Harju, and P. Törmä, Phys. Rev. B 96, 064511 (2017).
- ³² T. Ozawa, Phys. Rev. B **97**, 041108 (2018).
- ³³ M. Iskin, Phys. Rev. A **97**, 033625 (2018).
- ³⁴ T. Ozawa and N. Goldman, Phys. Rev. B **97**, 201117 (2018).
- ³⁵ O. Bleu, G. Malpuech, Y. Gao, and D. D. Solnyshkov, Phys. Rev. Lett. **121**, 020401 (2018).
- ³⁶ M. Iskin, Phys. Rev. A **97**, 063625 (2018).
- ³⁷ E. I. Blount, in *Solid state physics*, Vol. 13 (Elsevier, 1962) pp. 305–373.
- ³⁸ M. F. Lapa and T. L. Hughes, Supplemental material for "Semiclassical wave packet dynamics in non-uniform electric fields".
- ³⁹ Y. Gao and D. Xiao, arXiv:1810.02728 (2018).