Coordinate shift in the semiclassical Boltzmann equation and the anomalous Hall effect

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Electrons in a crystal generically experience an anomalous coordinate shift (a side jump) when they scatter off a defect. We propose a gauge invariant expression for the side jump associated with scattering between particular Bloch states. Our expression for the side jump follows from the Born series expansion for the scattering T matrix in powers of the strength of the scattering potential. Given our gauge invariant side jump expression, it is possible to construct a semiclassical Boltzmann theory of the anomalous Hall effect which expresses all previously identified contributions in terms of gauge invariant quantities and does not refer explicitly to off-diagonal terms in the density-matrix response.

I. INTRODUCTION

The near-equilibrium dynamics of a uniform system of classical charged particles in a weak electric field **E** is described by the classical Boltzmann equation

$$\frac{\partial f_l}{\partial t} + e\mathbf{E}\frac{\partial f_l}{\partial \mathbf{k}} = -\sum_{l'} \omega_{ll'}(f_l - f_{l'}), \qquad (1)$$

where $l=(\mu,\mathbf{k})$ is a combined index with **k** the momentum and μ the label for some discrete internal degrees of freedom, and $\omega_{ll'}$ is the scattering rate between unit momentum space volumes. The momentum distribution function f_l can be written as the sum of its equilibrium value $f_0(\epsilon_l)$, where ϵ_l is the energy dispersion, and a nonequilibrium correction g_l, i.e., $f_l=f_0(\epsilon_l)+g_l$. Equation (1) can also be applied successfully to quantum systems in many instances. In the semiclassical theory of electronic transport in a crystal for example, μ becomes the Bloch band index, f_l can be interpreted as a probability density in phase space that has been coarse grained by constructing wave packets, and $f_0(\epsilon_l)$ is the Fermi distribution function.

In spite of the classical form of Eq. (1) the scattering rate $\omega_{ll'}$ often has to be calculated purely quantum mechanically and is given by the golden rule expression in terms of the T matrix, which can in turn be written as a Born series in powers of disorder strength.

The semiclassical Eq. (1) is very powerful since it automatically takes care of the summation of various infinite series of Feynman diagrams that appear in quantum linear response theory, and it keeps the physical meaning of all terms transparent. However, since the only role of the electric field in Eq. (1) is to accelerate wave packets constructed from states within a single band, and the only role of impurities is to produce incoherent instantaneous scatterings, it appears clear that this approach must be often insufficient. The best known example where Eq. (1) apparently fails is in evaluating the anomalous Hall effect (AHE) in spin-orbit coupled ferromagnetic metals, which can be dominated by an interband coherence response.

The rigorous quantum mechanical theory of the anomalous Hall effect in this case has been constructed by Kohn and Luttinger,[1,2] who considered the equation of motion of the density matrix in momentum space. They found that elements of the density matrix that are off diagonal in the band index (interband coherence contributions) are induced both by an external electric field and by disorder. These couple to off diagonal elements of the velocity operator, thus contributing to the Hall current in addition to the skew scattering contribution,[3,4] that can be completely explained in the framework of Eq. (1).

The renewed semiclassical theory, based on wave packet equations,[5] provided a simple explanation of those contributions. In this theory the Berry phase changes the velocity of wave packets and leads to the so called intrinsic contribution[5–11] to the AHE. Another ingredient in the semiclassical theory is to consider the charge transport not only between collisions with impurities but also the transport during collisions, namely, the so-called side jump effect.[12]

The side jump is the coordinate shift acquired by a particle during the scattering event. Recently, it was shown that for a smooth impurity potential it can be found by integrating wave packet equations over the scattering time.[10] After the gauge invariant expression for the side jump is found, one can calculate the related drift velocity and the anomalous contribution to the distribution function, which in addition to the solution of the Eq. (1) are sufficient to calculate the Hall current.[10]

The advantage of the semiclassical approach is in its simplicity. It operates only with gauge invariant quantities, such as the side jump, the scattering rate, anomalous and usual velocities and the distribution function. All of them have a clear physical meaning. In contrast, the approach by Kohn and Luttinger is rather obscure. The main reason is that the off-diagonal elements of the density matrix or velocity operator are not gauge invariant. Many of the individual contributions to the Hall effect in the Kohn-Luttinger approach are expressed in terms of gauge-dependent quantities which cannot have separate physical meaning. This may be one reason why many authors cite this article, but try to invent their own way to calculate the Hall current.[13–16] Another alternative approach can be found in work by Adams and Blount,[14] and Nozieres[15] and proceeds by projecting all operators to a single band of interest, or in the case of band-degeneracies in semiconductors, to a subsystem of two de-

generate bands.[15] For electrons in the conduction band of common semiconductors, the disorder potential then acquires form $V(\mathbf{r}) \rightarrow V' = V(\mathbf{r}) + \alpha\sigma \cdot \mathbf{k} \times \nabla V(\mathbf{r})$. Projection to the subsystem also modifies the coordinate operator $\mathbf{r} \rightarrow i\partial/\partial\mathbf{k} + \mathbf{A}$, where $\mathbf{A}$ is the Berry connection of the band(s) (see Refs. 17 and 18 for reviews). One then can define gauge-dependent side-jump velocities $-i[i\partial/\partial\mathbf{k}, V']$ and $-i[\mathbf{A}, V']$. Although such a technique can lead to the correct answer it is framed in terms of noncommuting coordinates, and gauge-dependent velocities. The projected theory is in practice useful only for semiconductors with sufficiently smooth disorder potential. Hence its applicability is strongly restricted.

Unfortunately, the gauge invariant approach to calculate the anomalous shift proposed in Ref. 10 is also restricted only to very smooth disorder potentials; it is not even obvious whether it is equivalent to the Born approximation in the weak potential limit, because the Born and the adiabatic approximations often have very different domains of validity. Hence it would be valuable to find an alternative approach that applies to weak disorder potentials of arbitrary range.

In the present work we propose a gauge invariant expression for the side jump for an arbitrary type of a scattering that can be treated in the Born approximation. This allows one to evaluate all the major contributions to the anomalous Hall effect that have been identified in work by Kohn and Luttinger, but now using only classical concepts, without explicit reference to elements of the density matrix or Green functions that are off diagonal in band index or to noncommuting coordinates.

II. GAUGE INVARIANT COORDINATE SHIFT

To define the coordinate shift (side jump) in terms of well defined quantities that can be evaluated using scattering theory, we assume that a long time before the scattering event the center-of-mass of the wave packet moves freely according to the law $\mathbf{r_c}(t)_{t \rightarrow -\infty} = \delta\mathbf{r}_{-\infty} + \mathbf{v_k}t$ where $\mathbf{v_k}$ is the velocity of the free wave packet and t is time. Suppose the wave packet scatters from an impurity with the center at $\mathbf{r}_0 = 0$. Then, if the momentum changes to $\mathbf{k}'$, a long time after the scattering event the coordinate of the outgoing state center-of-mass should behave for $t \rightarrow +\infty$ as $\mathbf{r_c}(t)_{t \rightarrow +\infty} = \delta\mathbf{r}_{+\infty} + \mathbf{v_{k'}}t$. We define the scattering-induced coordinate shift as

$$\delta\mathbf{r}_{\mathbf{k}',\mathbf{k}} = \delta\mathbf{r}_{+\infty} - \delta\mathbf{r}_{-\infty}. \quad (2)$$

The naive treatment of the Boltzmann equation (1) based only on the scattering rate disregards this coordinate shift. Below we construct the theory that enables us to calculate the coordinate shift in the lowest nonzero Born approximation and add it to the contributions to the Hall conductance captured by calculations based on Eq. (1). For simplicity, we will consider first transport in a single band and later generalize results to the multiple band situation. Let $\psi_\mathbf{k}(\mathbf{r}, t) = [1/(2\pi)^{D/2}]e^{i\mathbf{k}\cdot\mathbf{r} - i\epsilon(\mathbf{k})t}|u_\mathbf{k}\rangle$ be the Bloch state with a momentum-dependent periodic spinor $|u_\mathbf{k}\rangle$. The naive expression for the coordinate shift, $\delta\mathbf{r}_{\mathbf{k}',\mathbf{k}} = \langle u_\mathbf{k}'|i(\partial/\partial\mathbf{k}')|u_\mathbf{k}'\rangle - \langle u_\mathbf{k}|i(\partial/\partial\mathbf{k})|u_\mathbf{k}\rangle$ is gauge dependent, i.e., it changes under an

arbitrary momentum-dependent phase change for the periodic spinors $|u_\mathbf{k}\rangle$, and cannot be correct in general. We derive the correct form for this expression in the weak potential scattering limit. To find the correct expression, we prepare the wave packet that approaches the impurity. The wave function of the wave packet is a superposition of eigenstates of the unperturbed Hamiltonian $\psi_\mathbf{k}(\mathbf{r}, t)$ with the real-valued Gaussian envelope factor $w(\mathbf{k} - \mathbf{k}_0)$, centered near the average momentum $\mathbf{k}_0$:

$$\Psi_{\mathbf{k}_0}(\mathbf{r}, t) = \int d\mathbf{k}\, w(\mathbf{k} - \mathbf{k}_0)\psi_\mathbf{k}(\mathbf{r}, t). \quad (3)$$

We assume a vanishing width of the wave packet in momentum space in the usual way. Hence, when multiplied by a smooth function of momentum the envelope function $w(\mathbf{k} - \mathbf{k}_0)$ can be treated as a δ-function. However, when multiplied by a true δ function, it is considered smooth, reflecting the finite width of the wave packet. Correspondingly, in coordinate space, the wave packet should be considered as large in comparison with a lattice constant, but small compared to other length scales. We can evaluate its charge center as follows:

$$\mathbf{r}_c(\mathbf{k}_0) = \int d\mathbf{r}\,\Psi_{\mathbf{k}_0}(\mathbf{r}, t)^*\mathbf{r}\Psi_{\mathbf{k}_0}(\mathbf{r}, t). \quad (4)$$

We substitute Eq. (3) into Eq. (4), then notice that $\mathbf{r}e^{i\mathbf{k}\cdot\mathbf{r}} = -i[(\partial/\partial\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}]$ and integrate by parts. Using the orthogonality of plane waves $[\Omega_0/(2\pi)^D]\Sigma_{\vec{R}}e^{i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}} = \delta(\mathbf{k}_1 - \mathbf{k}_2)$, and assuming that the periodic functions are normalized, $\langle u_\mathbf{k}|u_\mathbf{k}\rangle = 1$, and then the δ-function-like properties of envelope functions we finally find that, before scattering, the center of mass of such an unperturbed wave packet moves according to the law

$$\mathbf{r}_c(\mathbf{k}_0, t)_{t \rightarrow -\infty} = \mathbf{v}_{\mathbf{k}_0}t + \delta\mathbf{r}_{-\infty} = \frac{\partial\epsilon(\mathbf{k}_0)}{\partial\mathbf{k}_0}t + \left\langle u_{\mathbf{k}_0}\left|i\frac{\partial}{\partial\mathbf{k}_0}u_{\mathbf{k}_0}\right.\right\rangle. \quad (5)$$

(Ω_0 is the unit cell volume and $\Sigma_{\vec{R}}$ is a sum over lattice vectors.) Now consider how the state which initially coincides with the Bloch state $\psi_\mathbf{k}(\mathbf{r}, t)$ moves under the influence of a weak potential of an impurity $V(\mathbf{r})$. The solution of the Schrödinger equation can be written in terms of the eigenvectors of the unperturbed Hamiltonian $\psi_{\mathbf{k}'}(\mathbf{r}, t)$ as

$$\psi_\mathbf{k}^{out}(\mathbf{r}, t) = \int d\mathbf{k}'\, C(\mathbf{k}', t)\psi_{\mathbf{k}'}(\mathbf{r}, t). \quad (6)$$

To lowest order in the strength of the potential, perturbation theory leads to the following expression for time-dependent coefficients $C(\mathbf{k}', t)$ [see, for example, Eq. (19.9) in Ref. 19]:

$$C(\mathbf{k}', t) = -iV_{\mathbf{k}',\mathbf{k}}\int_{-\infty}^t e^{i[\epsilon(\mathbf{k}')-\epsilon(\mathbf{k})]t'}dt' + \delta(\mathbf{k}' - \mathbf{k}), \quad (7)$$

where $V_{\mathbf{k}',\mathbf{k}} = \langle\psi_{\mathbf{k}'}(\mathbf{r})|\hat{V}|\psi_\mathbf{k}(\mathbf{r})\rangle$ is the matrix element of the disorder potential between two eigenstates of the unperturbed Hamiltonian. Higher order terms can be incorporated into the above formula by substituting the T matrix instead of

the disorder potential matrix elements [see, for example, Eq. (19.10) in Ref. 19]

$$C(\mathbf{k}',t) = -iT_{\mathbf{k}',\mathbf{k}}\int_{-\infty}^{t} e^{i[\epsilon(\mathbf{k}')-\epsilon(\mathbf{k})]t'}dt' + \delta(\mathbf{k}'-\mathbf{k}). \quad (8)$$

The time integral in Eq. (7) is formally divergent, reflecting the fact that for infinite interaction time the initial state is completely destroyed. We add a regularizing factor in the exponent $e^{i[\epsilon(\mathbf{k}')-\epsilon(\mathbf{k})]t'} \rightarrow e^{i[\epsilon(\mathbf{k}')-\epsilon(\mathbf{k})]t'-[\eta \, \text{sgn}(t')]t'}$ to limit the effective finite time of interaction. Performing the integration in Eq. (7) taking the limit $\eta \rightarrow 0$ after $t \rightarrow +\infty$ we thus find that at large positive time [see, for example, Eq. (19.60) in Ref. 19]

$$C(\mathbf{k}', +\infty) = c(\mathbf{k}',\mathbf{k}) + \delta(\mathbf{k}'-\mathbf{k}), \quad (9)$$

where

$$c(\mathbf{k}',\mathbf{k}) = -2\pi i T_{\mathbf{k}',\mathbf{k}}\delta[\epsilon(\mathbf{k}')-\epsilon(\mathbf{k})]. \quad (10)$$

For $\mathbf{k}' \neq \mathbf{k}$ the square of the amplitude $|c(\mathbf{k}',\mathbf{k})|^2$ is the scattering probability from the state with momentum $\mathbf{k}$ into the one with momentum $\mathbf{k}'$. Due to the δ function in Eq. (10), the expression $|c(\mathbf{k}',\mathbf{k})|^2$, should be understood in the regularized sense, i.e., assuming that η is small but finite. Given these standard results from time-dependent perturbation theory, we can reconstruct the state of the wave packet after scattering

$$\Psi^{\text{out}}(\mathbf{r},t) = \int d\mathbf{k}\, w(\mathbf{k}-\mathbf{k}_0)\psi_{\mathbf{k}}^{\text{out}}(\mathbf{r},t), \quad (11)$$

where $\psi_{\mathbf{k}}^{\text{out}}(\mathbf{r},t)$ is given in Eq. (6). The average coordinate of the center-of-mass of the final state can be calculated by the same steps as used for the ingoing wave packet. We find that

$$\mathbf{r_c}(t)_{t \rightarrow +\infty} = \int d\mathbf{r}[\Psi^{\text{out}}(\mathbf{r},+\infty)]^* \mathbf{r}\Psi^{\text{out}}(\mathbf{r},+\infty) = \mathbf{r}_{+\infty}^{\text{I}} + \mathbf{r}_{+\infty}^{\text{II}}$$
$$+ \mathbf{r}_{+\infty}^{\text{III}}, \quad (12)$$

where

$$\mathbf{r}_{+\infty}^{\text{I}} = \int d\mathbf{k}'|C(\mathbf{k}',+\infty)|^2\left(\mathbf{v}_{\mathbf{k}'}t + \left\langle u_{\mathbf{k}'} \left| i\frac{\partial}{\partial\mathbf{k}'}u_{\mathbf{k}'}\right\rangle\right),$$
$$(13)$$

$$\mathbf{r}_{+\infty}^{\text{II}} = \int d\mathbf{k}'[c(\mathbf{k}',\mathbf{k}_0)]^* i\frac{\partial}{\partial\mathbf{k}'}c(\mathbf{k}',\mathbf{k}_0), \quad (14)$$

$$\mathbf{r}_{+\infty}^{\text{III}} = \lim_{\mathbf{k}_1,\mathbf{k}_2 \rightarrow \mathbf{k}_0}\left(i\frac{\partial}{\partial\mathbf{k}_1}c(\mathbf{k}_1,\mathbf{k}_2) - i\frac{\partial}{\partial\mathbf{k}_2}c^*(\mathbf{k}_2,\mathbf{k}_1)\right). \quad (15)$$

$\mathbf{r}_{+\infty}^{\text{III}}$ originates from the δ function in Eq. (8). In what follows, we will restrict our calculations to the lowest nonzero order in the potential $V_{\mathbf{k}',\mathbf{k}}$.

The perturbation expansion of the T matrix is well known

$$T_{\mathbf{k}',\mathbf{k}} = V_{\mathbf{k}',\mathbf{k}} + \sum_{\mathbf{k}''}\frac{V_{\mathbf{k}',\mathbf{k}''}V_{\mathbf{k}'',\mathbf{k}}}{\epsilon(\mathbf{k}'')-\epsilon(\mathbf{k})+i\eta} + \cdots. \quad (16)$$

It will be useful to represent the disorder potential matrix elements in the form

$$V_{\mathbf{k}',\mathbf{k}} = |V_{\mathbf{k}',\mathbf{k}}|e^{i\,\text{arg}(V_{\mathbf{k}',\mathbf{k}})}. \quad (17)$$

Then, taking into account that $\int d\mathbf{k}'(\partial/\partial\mathbf{k}')|c(\mathbf{k}',\mathbf{k}_0)|^2 = 0$, the Eq. (14) can be rewritten as

$$\mathbf{r}_{+\infty}^{\text{II}} = -\int d\mathbf{k}'|c(\mathbf{k}',\mathbf{k}_0)|^2\frac{\partial}{\partial\mathbf{k}'}\,\text{arg}(V_{\mathbf{k}',\mathbf{k}_0}). \quad (18)$$

Substituting Eq. (16) into Eq. (15) and noting that $-2\pi iV_{\mathbf{k}',\mathbf{k}}\delta[\epsilon(\mathbf{k}')-\epsilon(\mathbf{k})] \approx c(\mathbf{k}',\mathbf{k})$ we find to the second order in $V_{\mathbf{k}',\mathbf{k}}$ that

$$\mathbf{r}_{+\infty}^{\text{III}} = -\int d\mathbf{k}'|c(\mathbf{k}',\mathbf{k}_0)|^2\frac{\partial}{\partial\mathbf{k}_0}\,\text{arg}(V_{\mathbf{k}',\mathbf{k}_0}) + f(\mathbf{k}_0)\mathbf{v}_{\mathbf{k}_0},$$
$$(19)$$

where $f(\mathbf{k}_0)$ is some function, whose exact expression will not be needed. The last term in Eq. (19) does not break any symmetry and can be interpreted as renormalizing the normal velocity of the part of wave packet that did not change the direction of motion after interacting with impurity. In what follows, we will ignore it as it has no influence on the Hall current at the leading order of perturbation theory. Combining the remaining nontrivial terms from Eqs. (13), (18), and (19) we find the coordinate of the wave packet center-of-mass is

$$\mathbf{r_c}(t)_{t \rightarrow +\infty} = \int d\mathbf{k}'|C(\mathbf{k}',+\infty)|^2[\mathbf{v}_{\mathbf{k}'}t + \langle u_{\mathbf{k}'}|i(\partial/\partial\mathbf{k}')u_{\mathbf{k}'}\rangle$$
$$- \hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}_0}\,\text{arg}(V_{\mathbf{k}',\mathbf{k}_0})], \quad (20)$$

where $\hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}_0} = \partial/\partial\mathbf{k}' + \partial/\partial\mathbf{k}_0$ The coefficient $|C(\mathbf{k}',+\infty)|^2$ can be interpreted as the scattering probability into state $\mathbf{k}'$ from the initial state $\mathbf{k}_0$. Thus Eq. (20) has a semiclassical meaning such that the average final coordinate is the sum over probabilities of final states multiplied the corresponding coordinate shifts. Combining this result with the expression for initial coordinate of the wave packet (5) one can read the expression for the total anomalous shift corresponding to the scattering of the wave packet from the state with average momentum $\mathbf{k}$ into the one with $\mathbf{k}'$ in the lowest nonzero Born approximation:

$$\delta\mathbf{r}_{\mathbf{k}',\mathbf{k}} = \left\langle u_{\mathbf{k}'}\left|i\frac{\partial}{\partial\mathbf{k}'}u_{\mathbf{k}'}\right\rangle - \left\langle u_{\mathbf{k}}\left|i\frac{\partial}{\partial\mathbf{k}}u_{\mathbf{k}}\right\rangle - \hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}}\,\text{arg}(V_{\mathbf{k}',\mathbf{k}}). \quad (21)$$

Generalization to the multiple band case is simple. One should introduce the combined index $l = (\mu,\mathbf{k})$ in Eqs. (6), (7), and (16), and so on. Repeating the analogous steps we find that the expression for the anomalous coordinate shift after scattering from the state l into the state l' is

$$\delta \mathbf{r}_{l'l} = \left\langle u_{l'} \left| i\frac{\partial}{\partial \mathbf{k}'} u_{l'} \right\rangle - \left\langle u_l \left| i\frac{\partial}{\partial \mathbf{k}} u_l \right\rangle - \hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}} \arg(V_{l',l}). \right.$$

(22)

Equation (22) is the main result of this work. It provides a gauge invariant expression for the wave packet coordinate shift (side jump) which has a clear semiclassical interpretation and is valid for an arbitrary impurity potential that can be treated in the Born approximation.

III. RELATION TO PANCHARATNAM PHASE

Under the gauge transformation $|u_l\rangle \rightarrow \exp[i\phi_\mu(\mathbf{k})]|u_l\rangle$ the argument of the potential operator matrix element in Eq. (22) changes as $\arg(V_{l',l}) \rightarrow \arg(V_{l',l}) + \phi_\mu(\mathbf{k}) - \phi_{\mu'}(\mathbf{k}')$, which compensates noninvariance of other two terms. To make more incite in symmetries and gauge invariance of the side jump expression we consider the case when the periodic part of the Bloch function is only momentum dependent. For simplicity we consider scatterings in the same band only, from radial spin-independent impurity potential. Then matrix elements of the potential become $V_{\mathbf{k}',\mathbf{k}} = V^0(\mathbf{k}' - \mathbf{k})\langle u_{\mathbf{k}'}|u_{\mathbf{k}}\rangle$, where $V^0(\mathbf{k}' - \mathbf{k}) \sim \int d\mathbf{r} \exp[-i(\mathbf{k}' - \mathbf{k})\mathbf{r}]V(\mathbf{r})$ and for radial impurity $\hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}} \arg[V^0(\mathbf{k}' - \mathbf{k})] = 0$. Thus Eq. (21) simplifies

$$\delta \mathbf{r}_{\mathbf{k}',\mathbf{k}} = \left\langle u_{\mathbf{k}'} \left| i\frac{\partial}{\partial \mathbf{k}'} u_{\mathbf{k}'} \right\rangle - \left\langle u_{\mathbf{k}} \left| i\frac{\partial}{\partial \mathbf{k}} u_{\mathbf{k}} \right\rangle \right. \right.$$
$$- \hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}} \arg(\langle u_{\mathbf{k}'}|u_{\mathbf{k}}\rangle).$$

(23)

Interestingly, in this case the side jump does not depend on the form of the scattering potential explicitly. In the case of a very small scattering angle[20] ($|\mathbf{k}' - \mathbf{k}| \ll |\mathbf{k}|$) one can (for nondegenerate bands) disregard interband scattering and make additional approximations valid up to the first order in the small parameter $|\mathbf{k}' - \mathbf{k}|$, for example $|u_{\mathbf{k}'}\rangle \approx |u_{\mathbf{k}}\rangle + (\mathbf{k}' - \mathbf{k})|(\partial u_{\mathbf{k}}/\partial \mathbf{k})\rangle$ and $|\langle u_{\mathbf{k}'}|u_{\mathbf{k}}\rangle| \approx 1$. Substituting this in Eq. (23) we find that up to first order in $|\mathbf{k}' - \mathbf{k}|$ the anomalous shift is

$$\delta \mathbf{r}_{\mathbf{k}'\mathbf{k}} \approx \mathbf{F} \times (\mathbf{k}' - \mathbf{k}),$$

(24)

where $F_k = \epsilon_{ijk}\text{Im}(\langle \partial u_{\mathbf{k}}/\partial k_j | \partial u_{\mathbf{k}}/\partial k_i \rangle)$. By definition, $\mathbf{F}$ is the gauge invariant momentum space Berry curvature of the Bloch band. The result for the anomalous shift (24) coincides with the one derived in Ref. 10 in the adiabatic approximation. In the smooth potential limit the adiabatic and Born approximation results coincide.

One can check that Eq. (23) is related to the gauge invariant Pancharatnam phase $\Phi_{\mathbf{k}'',\mathbf{k},\mathbf{k}'}$

$$\delta \mathbf{r}_{\mathbf{k}',\mathbf{k}} = -\left(\frac{\partial \Phi_{\mathbf{k}'',\mathbf{k},\mathbf{k}'}}{\partial \mathbf{k}''}\right)_{\mathbf{k}'' \rightarrow \mathbf{k}} - \left(\frac{\partial \Phi_{\mathbf{k}'',\mathbf{k},\mathbf{k}'}}{\partial \mathbf{k}''}\right)_{\mathbf{k}'' \rightarrow \mathbf{k}'},$$

(25)

where

$$\Phi_{\mathbf{k}'',\mathbf{k},\mathbf{k}'} = \arg(\langle u_{\mathbf{k}''}|u_{\mathbf{k}}\rangle \langle u_{\mathbf{k}}|u_{\mathbf{k}'}\rangle \langle u_{\mathbf{k}'}|u_{\mathbf{k}''}\rangle).$$

(26)

The Pancharatnam phase $\Phi_{\mathbf{k}'',\mathbf{k},\mathbf{k}'}$ is the phase that would appear after the hopping over the closed path in the momen-
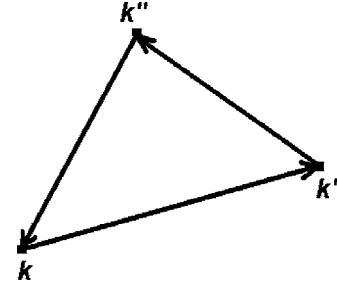

FIG. 1. Closed path in the momentum space representing the hopping amplitude of Eq. (26).

tum space over the contour $\mathbf{k}'' \rightarrow \mathbf{k} \rightarrow \mathbf{k}' \rightarrow \mathbf{k}''$ shown in Fig. 1. One can demonstrate that the phase (26) is also responsible for the skew scattering contribution. Taking the expression for T matrix (16) and calculating the scattering rate via the golden rule $\omega_{\mathbf{k}',\mathbf{k}} = 2\pi |T_{\mathbf{k}',\mathbf{k}}|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})$, we find for its asymmetric part the following expression (see Ref. 1 for the detailed derivation):

$$\omega_{\mathbf{k},\mathbf{k}'}^{(3a)} = -(2\pi)^2 \sum_{\mathbf{k}''} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}''})\delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})\text{Im}(V_{\mathbf{k},\mathbf{k}'}V_{\mathbf{k}',\mathbf{k}''}V_{\mathbf{k}'',\mathbf{k}}),$$

(27)

where the superscript $(3a)$ means that this is the antisymmetric part of the scattering rate calculated up to the order V^3 in the disorder potential. The nonzero value of the phase (26) is crucial to make the product of three potential matrix elements in Eq. (27) nonzero:

$$\text{Im}(V_{\mathbf{k},\mathbf{k}'}V_{\mathbf{k}',\mathbf{k}''}V_{\mathbf{k}'',\mathbf{k}}) \sim \text{Im}(\langle u_{\mathbf{k}}|u_{\mathbf{k}'}\rangle \langle u_{\mathbf{k}'}|u_{\mathbf{k}''}\rangle \langle u_{\mathbf{k}''}|u_{\mathbf{k}}\rangle).$$

(28)

IV. APPLICATION TO THE AHE

We now apply the side-jump expression (22) to the AHE using ideas that have their roots in earlier work that started from adiabatic approximations.[10,15] The average side-jump velocity can be expressed in terms of the rate of transitions and the side-jump associated with a particular transition

$$\mathbf{v}_l^{sj} = \sum_{l'} \omega_{l'l}\delta\mathbf{r}_{l'l} = \sum_{l'} 2\pi N \delta(\epsilon_l - \epsilon_{l'}) \left[|V_{ll'}|^2 \left(\left\langle u_{l'} \left| i\frac{\partial}{\partial \mathbf{k}'} u_{l'} \right\rangle \right. \right. \right.$$
$$\left. \left. - \left\langle u_l \left| i\frac{\partial}{\partial \mathbf{k}} u_l \right\rangle \right) - \text{Im}(V_{ll'}\hat{\mathbf{D}}_{\mathbf{k}'\mathbf{k}}V_{l'l}) \right].$$

(29)

Here we have used lowest Born approximation expression $\omega_{l'l} = 2\pi N \delta(\epsilon_l - \epsilon_{l'})|V_{l'l}|^2$, where N is the impurity concentration. A similar expression can be found in the second part of Eq. (2.38) in Ref. 1. Luttinger called this velocity the off-diagonal velocity because its calculation involved interband matrix elements of the velocity operator. Our result (29) is more general because we did not assume, as in Ref. 1, that Bloch bands are nondegenerate and that disorder potential is spin independent.

The side-jump velocity does not produce any contribution to the total current from the equilibrium distribution, but in

an external electric field a nonequilibrium correction to the distribution function appears. This correction is well known[1,21] $g_l = (-\partial f_0/\partial \epsilon_l) eE_x |v_l| \tau_\mu^\parallel \cos(\phi)$, where $\tau_\mu^\parallel$ is the transport life time defined as $1/\tau_\mu^\parallel = \Sigma_{l'} \omega_{ll'}[1 - (|v_{l'}|/|v_l|)\cos(\phi - \phi')]$ and ϕ is the angle between the velocity and the $\hat{x}$ direction, which we chose to be along the electric field. With this correction to the distribution, the side jump velocity leads to the current

$$\mathbf{J}^{sj} = e \sum_l g_l \mathbf{v}_l^{sj}. \tag{30}$$

A second effect follows from the change of energy of the scattered particle under side jump in the presence of an external electric field. Since total energy is conserved, the scattered particle acquires additional kinetic energy $\Delta \epsilon_{l'l} = \epsilon_{l'} - \epsilon_l = e\mathbf{E} \cdot \delta \mathbf{r}_{l'l}$ in order to compensate the change in the potential energy in the electric field. The equilibrium distribution would then become unstable

$$\frac{\partial f_l}{\partial t} = -\sum_{l'} \omega_{ll'}[f_0(\epsilon_l) - f_0(\epsilon_{l'})] = -\sum_{l'} \omega_{ll'}[-(\partial f_0/\partial \epsilon)\Delta \epsilon_{l'l}]$$
$$\neq 0, \tag{31}$$

unless compensated by an additional anomalous correction g_l^a to the distribution function. Substituting in the collision term $f_l = f_0 + g_l^a$ instead of f_0, in the stationary state we find the equation that determines g_l^a

$$\sum_{l'} \omega_{ll'}\left(g_l^a - g_{l'}^a + \frac{-\partial f_0}{\partial \epsilon} e\mathbf{E} \cdot \delta \mathbf{r}_{l'l}\right) = 0. \tag{32}$$

As in the case of the side jump velocity, we can find an analog of this equation in Luttinger's classic paper,[1] however, Luttinger split the correction g_l^a into nongauge invariant parts. One find that Eqs. (3.21), (3.22), (3.23), and (3.16) of his work are equivalent to Eq. (32).

In 2D the self-consistent approach to calculate g_l^a from Eq. (32) is to look for a solution in the form[22] $g_l^a(\phi) = \Sigma_n (g_l^a)^{(n)} e^{in\phi}$. For the case of isotropic bands and isotropic scatterers one may calculate the Hall current at zero temperature without finding the expression for the full distribution function. Multiplying Eq. (32) by $ev_\mu \sin(\phi)$, where v_μ is the Fermi velocity in the μth band and summing over $\mathbf{k}$, then taking into account that the Hall current contribution from the band μ is $I_\mu = e\Sigma_\mathbf{k} g_l^a v_\mu \sin(\phi)$, we arrive at the set of algebraic equations

$$I_\mu/\tau_\mu - \sum_{\mu'} I_{\mu'}/\tau_{\mu,\mu'}^c + i_\mu = 0, \tag{33}$$

where $1/\tau_\mu \equiv \Sigma_{l'} \omega_{ll'}$, $1/\tau_{\mu,\mu'}^c \equiv \Sigma_\mathbf{k} \omega_{ll'} \cos(\phi - \phi') v_\mu/v_{\mu'}$, and $i_\mu \equiv \Sigma_\mathbf{k} (-\partial f_0/\partial \epsilon_l) e^2 v_\mu \sin(\phi) \Sigma_{l'} \omega_{ll'} \mathbf{E} \cdot \delta \mathbf{r}_{l'l}$. The final Hall current from the anomalous distribution is $J_y^{adist} = \Sigma_\mu I_\mu$. The above result can be simplified if direct transitions between different bands are for some reasons forbidden, i.e., $\omega_{ll'} = \delta_{\mu\mu'} \omega_{\mathbf{k},\mathbf{k'}}^\mu$. Then, employing the symmetry of the problem one can derive a simple result

$$J_y^{adist} = J_y^{sj}, \tag{34}$$

where J_y^{sj} is found in Eq. (30). This equality has already been noticed in a less general context in Ref. 10.

In the semiclassical theory of the AHE the side jump effect is not the only disorder effect contributing to the Hall current. In the weak disorder limit, the dominant contribution to the anomalous Hall effect is rather due to skew scattering[3,4] which appears in the semiclassical Boltzmann equation through[1,2,4] the antisymmetric part of the Boltzmann equation collision term kernel $\omega_{l'l} - \omega_{ll'}$. The first nonzero contribution to the asymmetric part of $\omega_{ll'}$ appears from the golden rule already in the order V,[3] however, that contribution is parametrically very different from others and one should prolong to calculate the asymmetric parts of $\omega_{ll'}$ up to V,[4] including the localization correction, since corrections to Hall current due to $\omega_{ll'}$ in this order are parametrically similar with the side-jump contributions. The technique of such calculations is well known.[1] The asymmetric scattering leads to the asymmetric correction to the distribution function g_l^ω. One can find it from a standard selfconsistent procedure, described in details, for example, in Ref. 21 and the corresponding current contribution is $J_y^\omega = e\Sigma_l g_l^\omega |v_l| \sin(\phi)$. Thus skew scattering can be totally understood and calculated with the semiclassical Boltzmann equation.

Finally the important contribution to the AHE is the Berry-phase contribution.[5-11] This contribution is completely independent of scatterers and is now often referred to as the intrinsic contribution to the anomalous Hall effect. The intrinsic anomalous Hall effect has been evaluated explicitly in recent years for a variety of different ferromagnetic materials using relativistic first principles electronic-structure methods.[23-25] It can be nonperturbative in character because of band crossings, a property that partially explains the fact that it is often quantitatively important. Although it is really an interband coherence effect, it can be captured in a semiclassical theory by working with modified Bloch bands[5] that include band mixing by the electric field to leading order. The end result in this approach is the appearance of an anomalous velocity proportional to $|\mathbf{E}|$ in addition to the usual velocity $\mathbf{v}_l = \partial \epsilon_l/\partial \mathbf{k}$. The anomalous velocity $\mathbf{v}_l^{(a)} = \mathbf{F}_l \times e\mathbf{E}$ captures changes in the speed at which a wave packet moves between scattering events under the influence of the external electric field only. $\mathbf{F}_l$ is the Berry curvature of the band.[5] The corresponding correction to the current is $\mathbf{J}^{intrinsic} = e\Sigma_l f_l \mathbf{v}_l^{(a)}$.

Finally the total Hall current in the transverse to the electric field y direction is

$$J_y^{total} = J_y^{intrinsic} + J_y^{sj} + J_y^{adist} + J_y^\omega. \tag{35}$$

V. CONCLUSIONS

In this work we demonstrated the importance of the coordinate shift at a scattering event. We found the general gauge invariant expression for this shift and related it to the phases of the scattering T-matrix elements. We demonstrated that when equipped with this expression, the semiclassical Boltzmann equation correctly reproduces all contributions to the

AHE, that have been derived by Luttinger with a purely quantum mechanical approach. The existing alternative techniques inevitably have to deal either with adiabatic approximations or with nongauge invariant quantities such as nondiagonal density matrix elements. Instead, the golden rule with our gauge invariant expression for the side jump and the semiclassical Boltzmann equation are sufficient to derive the Hall current for arbitrary type of disorder. Such calculations, though tedious, usually can be well automated with scientific software packages.

Our conclusions about the role of the coordinate shift in the semiclassical Boltzmann equation are rather general and might be important beyond the physics of the anomalous Hall effect. Recently, Coulomb interactions and interactions with phonons and magnetic fields beyond conventional approximations have been discussed in the context of the Boltzmann equation.[26–28] It would be interesting to trace the role of the coordinate shift in similar interacting systems.

[1] J. M. Luttinger, Phys. Rev. **112**, 739 (1958).

[2] W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957).

[3] N. F. Mott, Proc. R. Soc. London, Ser. A **124**, 425 (1929).

[4] J. Smit, Physica (Amsterdam) **21**, 877 (1955); Phys. Rev. B **8**, 2349 (1973).

[5] G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999). For a simplified explanation see also the Appendix of Ref. 10.

[6] R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).

[7] T. Jungwirth, Qian Niu, and A. H. MacDonald, Phys. Rev. Lett. **88**, 207208 (2002).

[8] M. Onoda and N. Nagaosa, J. Phys. Soc. Jpn. **71**, 19 (2002); Z. Fang et al., Science **302**, 5642 (2003).

[9] Yugui Yao et al., Phys. Rev. Lett. **92**, 037204 (2004).

[10] N. A. Sinitsyn, Qian Niu, Jairo Sinova, and K. Nomura, Phys. Rev. B **72**, 045346 (2005).

[11] Wei-Li Lee, Satoshi Watauchi, V. L. Miller, R. J. Cava, and N. P. Ong, Science **303**, 1647 (2004); Wei-Li Lee et al., Phys. Rev. Lett. **93**, 226601 (2004); N. Manyala et al., Nat. Mater. **3**, 255 (2004).

[12] L. Berger, Phys. Rev. B **2**, 4559 (1970).

[13] V. K. Dugaev, P. Bruno, M. Taillefumier, B. Canals, and C. Lacroix, Phys. Rev. B **71**, 224423 (2005); cond-mat/0502386 (unpublished).

[14] E. N. Adams and E. I. Blount, J. Phys. Chem. Solids **10**, 286 (1959).

[15] P. Nozieres and C. Lewiner, J. Phys. (France) **34**, 901 (1973).

[16] A. Cre'pieux and P. Bruno, Phys. Rev. B **64**, 014416 (2001).

[17] K. Y. Bliokh and Y. P. Bliokh, Ann. Phys. (N.Y.) **319**, 13 (2005).

[18] E. I. Blount, Solid State Physics (Academic Press, New York, 1962), Vol. 13, pp. 305–373.

[19] E. Merzbacher, Quantum Mechanics (Wiley, New York, 1970).

[20] M. G. Vavilov and I. L. Aleiner, Phys. Rev. B **69**, 035303 (2004).

[21] J. Schliemann and D. Loss, Phys. Rev. B **68**, 165311 (2003).

[22] I. A. Dmitriev, A. D. Mirlin, and D. G. Polyakov, Phys. Rev. B **70**, 165305 (2004).

[23] H. Ebert, Rep. Prog. Phys. **59**, 1665 (1996).

[24] A. Perlova et al., J. Magn. Magn. Mater. **272-276**, 523 (2004).

[25] Helmut Rathgen, Mikhail I. Katsnelson, Olle Eriksson, and G. Zwicknagl1, Phys. Rev. B **72**, 014451 (2005).

[26] W. C. Kerr, M. J. Rave, and L. A. Turski, Phys. Rev. Lett. **94**, 176403 (2005).

[27] E. Ciancio, R. C. Iotti, and F. Rossi, Phys. Rev. B **69**, 165319 (2004).

[28] M. M. Glazov and E. Ya. Sherman, Phys. Rev. B **71**, 241312(R) (2005).