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Theoretical treatment of the Rashba effect in angle-resolved magnetoresistance of a two-dimensional oxide layer

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The Rashba interaction is known to yield unusual effects in two-dimensional electron solids. One of these is the magnetotransport under the combined influence of an in-plane electric field and a magnetic field. The result is an anisotropic magnetoresistance that characterizes the band propagation concomitant with the spintronic influence of the Rashba coupling and the Zeeman interaction with the applied magnetic field. With the recent experimental results in mind, we present here a fully microscopic treatment of the underlying relaxation behavior using the methods of dissipative quantum statistical mechanics. The employed Kubo formula for the conductivity helps to make connection with particle diffusivity of the two-dimensional electronic solid and also under certain limits, with the semiclassical Boltzmann transport equation for the conductivity. The presented theory is in good agreement with recent data.

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I. INTRODUCTION

Emmanuel I Rashba had pioneered a new field of research during the 1960s to the 1980s by delving into the various ramifications of the well-known spin-orbit interaction when it comes to two-dimensional electron solids [1]. The work has had such a far-reaching impact on contemporary solid-state physics, for example in carbon-based systems, topological insulators, geometric phase problems, spintronics, etc., that *Physical Review B*, in its December 2022 issue, had decided to honor Rashba on his 95th birthday by launching a series of Rashba effect-related contributions [2]. The present paper is one such tributary attempt wherein we present results on how the effect influences transport phenomena under a weak electric field in a two-dimensional oxide layer, being further probed by an in-plane magnetic field.

The focus here is then on anisotropic magnetoresistance (AMR) and planar Hall effect (PHE) as can be measured through the conductivity tensor which is calculated in linear response theory (LRT) with the aid of the Kubo formula [3]. The specific system of theoretical interest is an interface of $LaV0_3$ and $KTa0_3$ (LVO-KTO) that has recently received much active attention in our experimental group [4]. The observed "negative longitudinal magneto resistance (NLMR)" and the "chiral anomaly" had so far been believed to be the hallmark of topological Dirac and Weyl semimetals [5–15]. However, what our oxide material, endowed with a strong Rashba coupling, has provided is believed to be a paradigm shift for certain unusual signatures of NLMR that may lead to possible engineering of nonmagnetic materials for magnetic sensors [4].

The classical Kubo formula for the nontransient conductivity tensor reads [16]

$$\sigma_{\mu\gamma} = \beta \int_0^\infty dt \langle j_\mu(0) j_\gamma(t) \rangle_0, \tag{1}$$

where β equals $(k_B T)^{-1}$, k_B being the Boltzmann constant and T the temperature and the j's are the current density components. The variable t is the time elapsed from its initial value of zero, on which the current density depends in view of its dynamic evolution. The indices μ and γ are x or y in the present case of a 2DEG (two-dimensional electron gas) chosen in the XY plane, in which the electric field is applied along the μ direction. Finally, the angular brackets denote a statistical mechanical average with the aid of an underlying density operator, with the suffix 0 indicating that the average is to be calculated in LRT in the absence of the applied electric field. We undertake to provide in the text a critical reappraisal of Eq. (1) based on a minimal model that incorporates the Rashba interaction within a band picture in the tight-binding (TB) approximation [17].

When it comes to low temperature dissipative quantum transport of an electron there are several directions in which Eq. (1) has to be generalized: (a) The prefactor in conjunction with the statistical weight provided by the density operator has to incorporate the Fermi distribution of electrons, (b) the current density which in turn is related to velocity has to be regarded as a quantum operator the eigenvalue of which is a group velocity that arises from the bands split by the Rashba coupling (see below) in an underlying Bloch lattice, and (c) *most topically*, the dynamics of the velocity operator has to be viewed in light of contemporary approaches to dissipation in quantum systems [18,19].

As far as points (a) and (b) are concerned, there have been recent advances in terms of a semiclassical Boltzmann transport equation that brings out the omnipresent Fermi

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distribution and the band splitting of the group velocity operator. That formula reads [20–22]

$$\sigma_{\mu\gamma} = \left(e^2\tau/m\right)\sum_{\mathbf{k},\mathbf{B}}\left(-\partial f^{\mathrm{B}}_{\mathrm{st}}/\partial\varepsilon^{\mathrm{B}}_{\mathbf{k}}\right)v^{\mathrm{B}}_{\mu}(\mathbf{k})v^{\mathrm{B}}_{\gamma}(\mathbf{k}). \qquad (2)$$

Here e is the electron's charge, m is its (effective) mass, f is the Fermi distribution (with a subscript indicating its "stationary" form) given by

$$f^{\mathrm{B}}_{\mathrm{st}} = \left[1+\exp\beta\left(\varepsilon^{\mathrm{B}}_{\mathbf{k}} - \in_{\mathrm{F}}\right)\right]^{-1}, T \to o, \qquad (3)$$

with $\in_{\mathrm{F}}$ being the Fermi energy. The derivative of $f^{\mathrm{B}}_{\mathrm{st}}$ is calculated with respect to the band energy $\varepsilon^{\mathrm{B}}_{\mathbf{k}}$, and the v's are band velocity eigenvalues. The index $\mathbf{k}$ which is summed over is the wave number in the Bloch reciprocal space of the TB lattice, the magnitude of which is nearly k_{F}, the Fermi momentum, because as $T \to 0$,

$$(-\partial f/\partial \in) \approx \delta(\varepsilon - \in_{\mathrm{F}}). \qquad (4)$$

The additional summation over the band index B runs over two values $+1$ and -1 of the electron's spin that occurs in the Rashba coupling. The crucial simplifying input in this semiclassical theory is the "relaxation time approximation" in which the velocity correlation is a single exponential in τ that appears as a featureless parameter. It is this last step which needs a much closer look in terms of the dependence of the relaxation time τ on the band index $\mathbf{k}$ if any, the temperature T, and other parameters of the external heat bath that is responsible in the first place in triggering relaxation (or dissipation) in the system. We will make a critical examination of Eq. (2) and *interalia* provide a microscopic theory for τ based on a system-plus-bath approach of nonequilibrium statistical mechanics [18,19].

Given this background the paper is organized as follows. In Sec. II A, we introduce the Hamiltonian for the system of our focus which is split into three components: (1) for the underlying 2DEG in a TB description, (2) for the Rashba interaction, and (3) for the Zeeman coupling due to the in-plane external magnetic field **B**. It is pertinent here to point out that although our system Hamiltonian resembles that of much-studied graphene in the so-called Dirac limit, the spin here is that of an itinerant electron while that in graphene is a pseudospin representing the occupation of an unpaired electron in a honeycomb lattice [23–25]. The system Hamiltonian given by (1)–(3) can be exactly diagonalized within the 2 × 2 Hilbert space of the electronic spin, thus yielding the band velocities. In Sec. II B, we revisit the Kubo formula and indicate how the Fermi distribution occurs naturally via the initial density operator in thermal equilibrium over which the expectation in Eq. (1) is to be computed. With this modified Kubo formula at hand, we turn our attention in Sec. II C, to elucidate the parameter range that is of interest in the experimental system of our focus [22]. As it turns out, the Rashba, the Zeeman, and the thermal energy are all of the same order at, say $T \sim 10$ K, whereas the tunneling energy Δ is ~5000 K. Therefore, as far as the heat bath-induced dissipative dynamics is concerned, only the TB Hamiltonian matters. The same is true for the equilibrium density matrix. Thus, while the influence of the Rashba and the Zeeman interactions is crucial in calculating the band velocities, they can be ignored in the relaxational dynamics. With this proviso we next present our central result in Sec. III which hinges on relating the velocity correlation in the Kubo formula to electron diffusivity in the TB lattice. This enables a microscopic analysis for the relaxation time τ from a system-plus-heat bath formulation [26,27]. With the analytically derived results for the conductivity tensor and hence the resistivity tensor at our disposal, we provide in Sec. IV a comparison with the experimental results. Finally, Sec. V concludes with a summary of our principal results.

II. SYSTEM HAMILTONIAN

A. Hamiltonian and band velocities

As stated in the Introduction, our system of interest is a 2DEG described by a nearest-neighbor TB model under the additional influence of a Rashba spin-orbit coupling and a Zeeman term due to a **B** field that is taken in an arbitrary direction in the XY plane at an angle of φ with the x axis. The system Hamiltonian is then

$$H_{\mathrm{s}} = H_{\mathrm{o}} + H_{\mathrm{R}} + H_{\mathrm{Z}}, \qquad (5)$$

where

$$\begin{aligned} H_{\mathrm{o}} &= -\Delta\left(Q^{+}_{\mathrm{x}} + Q^{+}_{\mathrm{y}}\right), Q^{+}_{\mathrm{x,y}} = K_{\mathrm{x,y}} + \mathrm{H.a.},\\ K_{\mathrm{x}} &= \sum_{\mathrm{nx,ny}} |n_{\mathrm{x}}, n_{\mathrm{y}}\rangle\langle n_{\mathrm{x}} + d,\ n_{\mathrm{y}}|,\\ K_{\mathrm{y}} &= \sum_{\mathrm{nx,ny}} |n_{\mathrm{x}}, n_{\mathrm{y}}\rangle\langle n_{\mathrm{x}},\ n_{\mathrm{y}} + d|, \end{aligned} \qquad (6)$$

with Δ being the frequency (in units of Planck constant $\hbar = 1$) with which the electron tunnels from one site to its nearest neighbor site and d is the lattice parameter for the underlying square lattice. The summation is over indices characterized by two coordinates n_{x} and n_{y}. The translation operator K_{x} puts the electron one lattice site ahead in the x direction and its Hermitian adjoint (denoted by H.a.) does the opposite move. The operator K_{y} performs the same in the y direction.

We next come to discuss the Rashba Hamiltonian H_{R}. For this we need to define the velocity operator (distinct from the band velocity) which is the time derivative of the position operator given by

$$N = \mathbf{i}N_{\mathrm{x}} + \mathbf{j}N_{\mathrm{y}},\ N_{\mathrm{x}} = \Sigma n_{\mathrm{x}}|n_{\mathrm{x}},\ n_{\mathrm{y}}\rangle, \qquad (7)$$

and similarly for N_{y}. Here **i** and **j** are unit vectors along the x and y axes. The time derivatives are given by the respective commutators with H_{o} yielding for the velocity operators

$$v_{\mathrm{x,y}} = -id\Delta Q^{-}_{\mathrm{x,y}}, Q^{-}_{\mathrm{x,y}} = K_{\mathrm{x,y}} - \mathrm{H.a.} \qquad (8)$$

The Rashba Hamiltonian can then be constructed as

$$H_{\mathrm{R}} = -id\Delta\Lambda(\sigma_{\mathrm{x}}Q^{-}_{\mathrm{y}} - \sigma_{\mathrm{y}}Q^{-}_{\mathrm{x}}), \qquad (9)$$

where the constant Λ that characterizes the strength of the Rashba coupling subsumes the internal electric field that is created by the materials preparation of the oxide layers.

Finally, the piece that augments the system Hamiltonian is the Zeeman coupling with the applied field:

$$H_{z} = -B(\sigma_{\mathrm{x}}\ \cos\varphi + \sigma_{\mathrm{y}}\ \sin\varphi), \qquad (10)$$

where the amplitude B is taken to absorb constants like the Bohr magneton and the g factor.

It is evident that the presence of the Rashba effect intertwines the dynamics along the x and y directions. Furthermore, the effect helps entangle the spin with the electron motion leading to "spintronics." What the Rashba coupling also does is to split the bands into two. However, the saving grace is that all the translation operators and their Hermitian adjoints commute with each other and hence the Bloch wave number $\mathbf{k}$ remains a good quantum number [28]. Therefore, the system Hamiltonian H_{s}, while being off-diagonal in the 2×2 Hilbert space of the electron's spin, remains diagonal in the Bloch $|\mathbf{k}\rangle$ space. The four relevant matrix elements of H_{s} are

$$\begin{aligned}\langle \mathbf{k},+|H_{\mathrm{s}}|\mathbf{k},+\rangle &= \langle \mathbf{k},-|H_{\mathrm{s}}|\mathbf{k},-\rangle\\ &= -\Delta\langle \mathbf{k}|(Q_{\mathrm{x}}^{+}+Q_{\mathrm{y}}^{+})|k\rangle\\ &= -2\Delta(\cos dk_{\mathrm{x}}+\cos dk_{\mathrm{y}}),\end{aligned} \quad (11)$$

$$\begin{aligned}\langle \mathbf{k},+|H_{\mathrm{s}}|\mathbf{k},-\rangle &= \langle \mathbf{k},-|H_{\mathrm{s}}|\mathbf{k},+\rangle^{*}\\ &= -id\Delta\Lambda\langle \mathbf{k}|(Q_{\mathrm{y}}^{-}+iQ_{\mathrm{x}}^{-})|\mathbf{k}\rangle - B\,e^{-\mathrm{i}\varphi}\\ &= 2d\Delta\Lambda(\sin dk_{\mathrm{y}} - i\sin dk_{\mathrm{x}}) - B\,e^{-\mathrm{i}\varphi}.\end{aligned} \quad (12)$$

The corresponding 2×2 matrix can be easily diagonalized yielding for the band energy two eigenvalues [22]:

$$\begin{aligned}\varepsilon_{\mathbf{k}}^{+,-} &= -2\Delta(\cos\, dk_{\mathrm{x}}+\cos dk_{y})(+,-)\sqrt{S_{\mathbf{k}}},\\ S_{\mathbf{k}} &= B^{2}+2B\lambda(\sin dk_{\mathrm{x}}\sin\varphi-\sin dk_{\mathrm{y}}\cos\varphi)\\ &\quad +\lambda^{2}(\sin^{2}dk_{\mathrm{x}}+\sin^{2}dk_{\mathrm{y}}),\ \lambda=2d\Delta\Lambda,\end{aligned} \quad (13)$$

from which the band velocities can be derived from the relation

$$v(\mathbf{k})^{+,-} = (\partial\varepsilon_{\mathbf{k}}^{+,-}/\partial\mathbf{k}). \quad (14)$$

B. Kubo formula revisited

In this subsection we first provide a brief overview of the quantum mechanical interpretation of the Kubo formula. The aim is to justify the occurrence of the Fermi distribution function (or more accurately, its derivative with respect to energy) as in the semiclassical theory embodied in Eq. (2).

We first expand the meaning of the correlation function in Eq. (1) in the canonical ensemble of statistical mechanics [29]:

$$\beta\langle j_{\alpha}(0)j_{\gamma}(t)\rangle_{0} = \beta\mathrm{Tr}\{\rho(t=o)j_{\alpha}(0)e^{\mathrm{i}H\mathrm{t}}j_{\gamma}(o)\,e^{-\mathrm{iHt}}\}, \quad (15)$$

where

$$\rho(t=o)=\exp(-\beta H_{\mathrm{s}})\exp(-\beta H_{\mathrm{b}})/Z_{\mathrm{s}}Z_{\mathrm{b}}, \quad (16)$$

with H_{s} being the system Hamiltonian given by Eq. (3) onwards, H_{b} is the Hamiltonian for the bath, (to be specified below)and Z's are the corresponding partition functions. As is customary in the analysis of quantum dissipative systems [18,19] the bath is taken as a large system of noninteracting quantum harmonic oscillators, coupled linearly with H_{s} in terms of the displacement coordinates of the oscillators. Viewed as a collection of elementary quantum excitations, the bath could represent either phonons or electrons other than the one of interest in band propagation. The spectral densities of these elementary excitations determine whether the concerned bath is a phononic or an electronic one [18,19].

The time evolution of the current density operator, on the other hand, is governed by the full Hamiltonian H embracing the system, the bath and their interaction:

$$H = H_{\mathrm{s}}+H_{\mathrm{I}}+H_{\mathrm{b}}, \quad (17)$$

wherein the model for H_{I}, assumed linear in the bath coordinate as implied above, in the spirit of the spin-boson Hamiltonian of dissipative quantum systems [30], will be indicated in detail below, in Sec. III C.

The scenario is that at time $t=o$, the system of interest is taken to have come to equilibrium at the temperature T of the bath in line with the Gibbsian canonical ensemble picture of equilibrium statistical mechanics. Hence the initial density matrix has the factorized form of Eq. (16). Having set our time at $t=o$ we imagine the system's equilibrium to be disturbed by the application of a weak electric field that is applied, say, in the x direction. Relaxation processes induced by H_{I} then set in, as the electric field causes energy absorption by the system with corresponding transitions in the bath in order to balance the net energy. The electric field would cause a current, not only along the x axis, but also a Hall current along the y axis as well, because of the presence of the magnetic field [embodied by H_{z} in Eq. (5)] in conjunction with the Rashba interaction H_{R}. The Kubo idea is to examine the asymptotic steady-state limit of the time-integrated correlation function in Eq. (1).

Because the current density is a system operator that commutes with the bath Hamiltonian, Eq. (15) can be further rearranged as

$$\beta\langle j_{\alpha}(0)j_{\gamma}(t)\rangle_{0}=\beta\mathrm{Tr}_{\mathrm{s}}[\exp(-\beta H_{\mathrm{s}})/Z_{\mathrm{s}}]j_{\alpha}(0)[(U(t))_{\mathrm{av}}j_{\gamma}(o)], \quad (18)$$

where the bath-averaged time-evolution operator in the Liouville space is given by [19]

$$(U(t))_{\mathrm{av}} = \sum_{b,b'}\langle b|\rho_{b}|b\rangle(b,\ b|U(t)|b',\ b'). \quad (19)$$

A comment is in order regarding the definition indicated in Eq. (19). What has been achieved in $(\ldots)_{\mathrm{av}}$ is the "tracing-out" of the degrees of freedom of the heat bath, weighted by its own density matrix ρ_{b}. In the path integral formulation of the time evolution of the density operator $\boldsymbol{\rho}\,(t)$ in the Schrödinger picture, this step is tantamount to rewriting the system observables in terms of the so-called *influence functional* [31]. While the latter is a formal step, an explicit modeling of the bath such as in terms of quantum harmonic oscillators with specific spectral properties yields useful, tractable expressions for the influence functional.

The next step is to take the prefactor β inside the trace and rewrite the statistical weight in Eq. (18) as

$$\beta\exp(-\beta H_{\mathrm{s}}) = \{-[\partial/\partial H_{\mathrm{s}}]\exp(-\beta H_{\mathrm{s}})\}. \quad (20)$$

At this stage we specialize to the model at hand and recognize that the system Hamiltonian H_{s} is diagonal in the Bloch space of the TB lattice and moreover the current density or the band velocity operator is also diagonal in this representation. Furthermore, in order to account for the Pauli exclusion principle for electrons at low temperatures we transit to the grand canonical ensemble from the canonical ensemble. Accordingly, the trace over the states of H_s would yield from Eq. (18)

$$\beta\langle j_\alpha(0)\, j_\gamma(t)\rangle_0 = \sum_{\mathrm{B},\mathbf{k},\mathbf{k}'}\Big\{ -\left(\partial \mathrm{f}^{\mathrm{B}}_{\mathbf{k}}/\partial\varepsilon^{\mathrm{B}}_{\mathbf{k}}\right) v^{\mathrm{B}}_{\mathbf{k},\alpha} \times (\mathbf{k},\,\mathbf{k};B,B|(U(t))_{\mathrm{av}}|\mathbf{k}',\ \mathbf{k}';B,\ B)\, v^{\mathrm{B}}_{\mathbf{k}'\gamma}\Big\}. \tag{21}$$

The problem then boils down to computing the matrix elements of the averaged time-evolution operator.

C. Parameter range of interest

In the experimental system under consideration, the Fermi energy $\epsilon_\mathrm{F} = -1.42\Delta$, corresponding to a filling factor of 1/2 electron per site implying "half filling," on average [22]. Thus, the tunneling energy is of the same order as the Fermi energy whereas both are nearly 500 times larger than the Rashba energy H_R, the Zeeman energy H_Z, and the thermal energy $k_\mathrm{B}T$. In fact, for $T = 10$ K, the magnetic field $B \sim 13$ T and the Rashba constant $\lambda \sim 15$ K, the estimated value of the tunneling energy is $\Delta \sim 0.5$ eV which is of the order of 5000 K while the Fermi energy is of the same order. The upshot is that the overwhelmingly dominant term in the system Hamiltonian is the tunneling energy in the underlying tight-binding model which leads to significant simplification in the analysis of the experiment. Thus, while the presence of the Rashba and the Zeeman couplings is crucial for the band velocities and therefore in the AMR and PHE measurements, their influence on both the Fermi distribution (providing the statistical weight to the velocity correlation) and the time evolution of the band velocity operator (leading to relaxational or dissipative dynamics) can be largely ignored.

Given the above consideration, the band index B occasioned by the Rashba spin splitting can be omitted in the Fermi function as well as in the time-development operator. Consequently, the Kubo formula for the electric conductivity tensor can be rewritten from Eq. (1) and subsequent analyses embodied in Eqs. (18)–(21) as

$$\sigma_{\alpha\gamma} = \int_0^\infty dt\ \Sigma_{\mathrm{B},\,\mathbf{k},\,\mathbf{k}'}[-(\partial \mathrm{f}_\mathbf{k}/\partial\varepsilon_\mathbf{k})]v^{\mathrm{B}}_{\mathbf{k},\,\alpha} \times (\mathbf{k},\mathbf{k}|(U(t))_{\mathrm{av}}|\mathbf{k}',\mathbf{k}')v^{\mathrm{B}}_{\mathbf{k}'\mathrm{y}}, \tag{22}$$

where the band energy $\varepsilon_\mathbf{k}$ appearing above can be approximated as [cf. Eq. (11a)]

$$\varepsilon_\mathbf{k} = -2\Delta(\cos dk_\mathrm{x} + \cos dk_\mathrm{y}). \tag{23}$$

The relevant components of the conductivity tensor from which the resistivities ρ_xx (for AMR) and ρ_xy (for PHE) can be obtained by inverting a 2 × 2 matrix, are given by $\alpha = \gamma = x$ and $\alpha = x, \gamma; = y$, respectively. The problem then is reduced to a detailed analysis of the bath-averaged time evolution operator which is the crux of the present work and is presented in the next section.

III. RELAXATIONAL DYNAMICS

A. A stochastic framework

In order to motivate our calculation of the averaged time-evolution operator we first put forward a stochastic model picture. The physical scenario in interpreting the expression in the integrand of Eq. (22) is the following. In the reciprocal Bloch space, we start from a band velocity $v^{\mathrm{B}}_{\mathrm{k},\alpha}$ at time $t = o$. As time progresses the velocity of the electron undergoes multiple scattering processes due to defects or phonons or other electrons, etc., as in the Drude model [20]. We assume the scattering to be a Markov process for which only the initial and the final steps matter. The interpretation of $(U(t))_{\mathrm{av}}$ is that it is a *conditional probability* of, given that the initial velocity is $v^{\mathrm{B}}_{\mathbf{k},\alpha}$, finding the velocity as $v^{\mathrm{B}}_{\mathbf{k},\gamma}$ at time t. For a stationary Markov process

$$(U(t))_{\mathrm{av}} = \exp{(Wt)}, \tag{24}$$

where W is the (time-independent) "relaxation matrix" or the "rate matrix."

One familiar approach in gas phase spectroscopy, adequate for our motivational purpose, is to imagine "strong collisions" for the underlying scattering processes in which W is assumed to have the form [32,29]

$$W = \nu\,(T - I), \tag{25}$$

where ν is a mean rate of collisions, T is a collision matrix, and I is the unit matrix. The strong collision model assumes

$$(\mathbf{k},\ \mathbf{k}|T|\mathbf{k}',\ \mathbf{k}') = p(\mathbf{k}'), \tag{26}$$

independent of the initial momentum state $|\mathbf{k}\rangle$, $p(\mathbf{k}')$ being the *a priori* probability of landing into the momentum state $|\mathbf{k}'\rangle$. Evidently, the form of T is consistent with detailed balance of transitions, which further yields

$$(U(t))_{\mathrm{av}} = \exp(-\nu t)\,\delta_{\mathbf{k},\mathbf{k}'} + [1 - \exp(-\nu t)]\,p(\mathbf{k}'). \tag{27}$$

When we substitute Eq. (27) into Eq. (22) only the diagonal term—the first term on the right in Eq. (27)—survives the independent summation over $\mathbf{k}$ and $\mathbf{k}'$; it corresponds to the decaying velocity correlation from its initial value in a given $\mathbf{k}$th state. On the other hand, the second square-bracketed term describes the decay of the mean velocity which is related to the time derivative of the mean position. Because the latter is zero in the absence of a forcing field, we are led to the Boltzmann kinetic theory formula of Eq. (2), upon carrying out the time integral in Eq. (27), provided we identify the inverse of ν as the Drude relaxation time τ. The purpose of this section is to present below a microscopic justification for this Markov scenario.

B. Connection with particle diffusion

Before we embark on our system-plus-bath analysis (in Sec. III C below) we make a further preliminary discussion on how to connect the conductivity to particle diffusivity. To do this, we take note of the parameter range of our attention, as amplified in Sec. II C. It is clear that once the band velocities are specified in accordance with Eq. (14) viz., $v_\mathrm{x}(\mathbf{k}) = \partial\varepsilon_\mathbf{k}/\partial k_\mathrm{x}$ and $v_\mathrm{y}(\mathbf{k}) = \partial\varepsilon_\mathbf{k}/\partial k_\mathrm{y}$, the time evolution (*sans* the Rashba and Zeeman interactions) proceeds independently along the x and y axes. Thus, as far as the relaxation dynamics are concerned, we may look at the simpler one-dimensional problem in computing the correlation function

$$C_{\mathrm{xx}}(t) = \langle v_{\mathrm{x}}(o) v_{\mathrm{x}}(t)\rangle,\ v_{\mathrm{x}}(t) = [(U(t))_{\mathrm{av}}\, v_{\mathrm{x}}(o)], \tag{28}$$

and employ a stratagem to relate $C(t)$ to the particle diffusivity. For this, it is to be noted that the position operator from which the velocity operator is derived is

$$X(t) = X(o) + \int_o^t dt'\, v_{\mathrm{x}}(t'), \tag{29}$$

and hence the variance is given by

$$\begin{aligned}\langle [X(t) - X(o)]^2\rangle &= \int_o^t dt' \int_o^t dt' \langle v_x(t'') v_x(t')\rangle \\ &= 2\int_o^t dt'(t - t')C(t'),\end{aligned} \tag{30}$$

where, in the last step, we brought in a prefactor 2 by first changing the upper limit of the second integral over t'' to t' instead of t, used stationarity of the velocity correlation, did one partial integration over t'', and, finally, employed the definition of $C(t)$ as in Eq. (28). The procedure is standard in the theory of diffusion processes [31]. From Eq. (30) we then immediately have a relation between the electrical conductivity σ_{xx} and particle diffusivity D_{xx}, because

$$\begin{aligned}D_{\mathrm{xx}} &= \mathrm{Lim}\,(t \to \infty)\,[(d/dt)\langle (X(t) - X(o))^2\rangle] \\ &= \int_{\mathrm{o}}^{\infty} dt\, C_{\mathrm{xx}}(t).\end{aligned} \tag{31}$$

The above scenario can be immediately adapted to the one-dimensional version of the TB model at hand for which the position operator has the structure

$$X = dN_{\mathrm{x}} = d\Sigma n_{\mathrm{x}} |n_{\mathrm{x}}\rangle\langle n_{\mathrm{x}}|, \tag{32}$$

and the corresponding velocity operator is

$$v_{\mathrm{x}} = -\,i[H_{\mathrm{o}},\, N_{\mathrm{x}}], \tag{33}$$

where now [cf., Eq. (6)],

$$H_{\mathrm{o}} = -\Delta(K_{\mathrm{x}} + K_{\mathrm{x}}^{\dagger}),\ K_{\mathrm{x}} = \Sigma n_{\mathrm{x}} |n_{\mathrm{x}}\rangle\langle n_{\mathrm{x}} + d|. \tag{34}$$

Thus [cf. Eq. (8)]

$$v_{\mathrm{x}} = -id\,\Delta(K_{\mathrm{x}} - K_{\mathrm{x}}^{\dagger}). \tag{35}$$

In the preceding discussion, we have employed the commutation properties, special to the TB model [28]

$$[N_{\mathrm{x}},\, K_{\mathrm{x}}] = -K_{\mathrm{x}},\ [N_{\mathrm{x}},\, K_{\mathrm{x}}^{\dagger}] = K_{\mathrm{x}}^{\dagger}. \tag{36}$$

C. Spin-boson-like model for diffusivity

With the material in Secs. III A and III B at hand, our objective now is to relate our conductivity calculation to the particle diffusivity for a TB chain. The result for the diffusivity already exists in the literature [26,27,33] but, for the sake of contextuality and for consistency with notations employed in this paper, we outline the treatment based on the system-bath approach outlined above. We therefore spell out the form of the total Hamiltonian in Eq. (17) which now reads

$$\begin{aligned}&H = H_{\mathrm{o}} + H_{\mathrm{I}} + H_{\mathrm{B}},\ H_{\mathrm{o}} = -\Delta(K_{\mathrm{x}} + K_{\mathrm{x}}^{\dagger}), \\ &H_{\mathrm{I}} = dN_{\mathrm{x}}\Sigma g_{\mathbf{q}}(b_{\mathbf{q}} + b_{\mathbf{q}}^{\dagger}),\ H_{\mathrm{B}} = \Sigma\omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}.\end{aligned} \tag{37}$$

Relaxation occurs because H_{I} commutes with neither H_{o} nor H_{B}, causing energy transfer between the two otherwise independent systems. The Hamiltonian is spin-boson-like for dissipative tunneling in a symmetric double well wherein the tunneling term in H_{o} replaces $-\Delta\sigma_{\mathrm{x}}$ while the occupation operator N_{x} stands for σ_{z} [34–36].

In order that the coupling strength $g_{\mathbf{q}}$ may be treated to all orders in perturbation it is useful to make a "polaronic" transformation [37–41] on H with the aid of

$$S = \exp -N_{\mathrm{x}}\Sigma_{\mathbf{q}}(g_{\mathbf{q}}/2\omega_{\mathbf{q}})\,(b_{\mathbf{q}} - b_{\mathbf{q}}^{\dagger}). \tag{38}$$

Using the commutation relations in Eq. (36) the transformed Hamiltonian reads

$$\begin{aligned}&H' = SHS^{-1} = -\Delta(K_{\mathrm{x}}B_{+} + K_{\mathrm{x}}^{\dagger}B_{-}) + H_{\mathrm{B}}, \\ &B_{+} = \exp\,(g_{\mathbf{q}}/2\omega_{\mathbf{q}})\,(b_{\mathbf{q}} - b_{\mathbf{q}}^{\dagger}),\end{aligned} \tag{39}$$

where B_{-} is obtained by the Hermitian adjoint of B_{+}. The polaronic transformation then transfers the onus of the coupling to the tunneling term itself which further implies that any perturbation treatment would be tantamount to results up to the order Δ [2] though interaction with the bath is treated to all orders [42].

Unlike in the correlation function occurring in the Kubo formula, in which we work in the Heisenberg picture wherein the time dependence is assigned to the velocity operator, it is convenient to invoke the Schrödinger picture in which it is the density operator that is endowed with time dependence. Thus, the time variation of the mean-squared position is obtained from

$$(d/dt)\big\langle N_{\mathrm{x}}^2(t)\big\rangle = \mathrm{Tr}\big[(d/dt)\rho(t) N_{\mathrm{x}}^2(o)\big], \tag{40}$$

where

$$(d/dt)\rho(t) = -i\,[H,\ \rho(t)]. \tag{41}$$

Because the transformation under S leaves the number operator N_{x} invariant we may equivalently express Eq. (40) as

$$(d/dt)\big\langle N_{\mathrm{x}}^2(t)\big\rangle = \mathrm{Tr}\,\big[(d/dt)\rho'(t)\, N_{\mathrm{x}}^2(o)\big], \tag{42}$$

where $\rho'(t)$ is the polaron-transformed density operator that obeys the modified Liouville equation

$$(d/dt)\rho'(t) = -i\,[H',\, \rho'(t)], \tag{43}$$

the solution of which reads

$$\rho'(t) = e^{-\mathrm{i}\,\mathrm{H}'\,\mathrm{t}}\rho'(o)\, e^{\mathrm{i}\,\mathrm{H}'\,\mathrm{t}}. \tag{44}$$

Consistent with our relaxation theory approach the initial density matrix retains its factorized form, i.e.,

$$\rho'\,(o) = \rho(o) = \rho_{\mathrm{o}} \times \rho_{\mathrm{b}}. \tag{45}$$

The mathematical meaning of the step above is to choose that the electron is initially localized at a given site, the occupation operator of which commutes with S [26].

The next step, necessary for ascribing time dependence to the new bath operators B_+ and B_-, is to go to the *interaction picture*,

$$\begin{aligned} H_{\rm I}'(t) &= \exp(itH_{\rm b})H_{\rm I}' \exp(-itH_{\rm b}),\\ H_{\rm I}(t) &= -\Delta[K_{\rm x}B_+(t) + K_{\rm x}^{\dagger}B_-(t)],\\ B_+'(t) &= \exp(itH_{\rm b})\,B_+(o)\exp(-itH_{\rm b}). \end{aligned} \tag{46}$$

The polaron-transformed density operator in the interaction picture,

$$\rho_{\rm I}'(t) = \exp\,(-itH_{\rm b})\rho'(t)\exp\,(-itH_{\rm b}), \tag{47}$$

now obeys the equation

$$(d/dt)\rho_I'(t) = -i[H_I(t),\ \rho_I'(t)]. \tag{48}$$

Because $H_{\rm b}$, inherent in the interaction picture, commutes with $N_{\rm x}$, we may write the trace operation in Eq. (38) in a disjointed form,

$$(d/dt)\langle N_{\rm x}^2(t)\rangle = {\rm Tr}_{\rm s}\{[(d/dt)(U(t))_{\rm av}\rho_{\rm o}]N_{\rm x}^2(o)\}, \tag{49}$$

where ${\rm Tr}_{\rm s}\,\{\ldots\}$ denotes a restricted trace operation over the Hilbert space of $H_{\rm o}$ in Eq. (30) and $[U(t)]_{\rm av}$ is the bath-averaged time-evolution operator, given by Eq. (19).

Defining then a time-evolved density operator for the system alone, as

$$\rho_{\rm o}(t) = [(U(t))_{\rm av}\rho_{\rm I}'(t)], \tag{50}$$

it can be shown to obey a time-convolution-less master equation of the Gorini-Kossakowski-Sudarshan-Lindblad form [43],

$$\begin{aligned} (d/dt)\rho_{\rm o}(t) &= [(U(t))_{\rm av}\rho_{\rm o}(t)]\\ &= \int_{\rm o}^{\infty} dt'\,{\rm Tr}_{\rm b}[H_I(t'),\ [H_I(o),\ \rho_B\rho_o(t)]]. \end{aligned} \tag{51}$$

Our remaining task is to substitute Eq. (51) into Eq. (49) and compute the mean-squared displacement. This task has already been carried out in [26] although the authors had employed the time-convolution form of the master equation. It has been pointed out by the same authors however that the result for the mean-squared displacement is independent of whether one uses the time-convolution or time-convolution-less master equation [33].

The final expression for the time variation of the mean-squared displacement reads [26]

$$(d/dt)\langle[dN_{\rm x}(t)]^2\rangle = (d\Delta)^2\int_{\rm o}^{\rm t} dt'\langle\langle B_-(o)B_+(t')\rangle\rangle + {\rm c.c.}, \tag{52}$$

where the double angular brackets represent thermal average over the heat bath, and c.c. signifies the *complex conjugate.* We have [19]

$$\begin{aligned} \langle\langle B_-(o)B_+(t)\rangle\rangle &= \exp - \int_{\rm o}^{\infty} d\omega[J(\omega)/\omega^2][\coth\,(\beta\omega/2)\\ &\quad\times(1-\cos\omega t) + i\,\sin\omega t]\}, \end{aligned} \tag{53}$$

where we have gone to a continuum limit of the bosonic excitations of the bath and concomitantly have introduced a *spectral density* $J(\omega)$. Note that if the bath were absent $[J(\omega) = o]$ we would recover *ballistic motion* wherein

$$\langle[dN_{\rm x}(t)]^2\rangle \rightarrow (d\Delta t)^2, \tag{54}$$

which prompts us to define a *quantal velocity* as [28]

$$v_{\rm qu} = (d\Delta), \tag{55}$$

independent of the band index $\mathbf{k}$. Additionally when we switch on the bath, the averaged time-evolution operator, embodied under the integral over t in Eq. (52), remains independent of $\mathbf{k}$, which turns out to be in conformity with the assumption, which was stipulated at the outset in [22].

Goaded by the observation in the paragraph above, we can identify the matrix elements of the time-development operator as

$$(\mathbf{k},\ \mathbf{k}|(U(t))_{\rm av}|\mathbf{k}',\ \mathbf{k}') = \langle\langle B_-(o)B_+(t')\rangle\rangle + {\rm c.c.}\delta'_{\mathbf{k}\,\mathbf{k}}. \tag{56}$$

Interestingly, this form is already inherent in our earlier stochastic model considerations [cf. Eq. (27)]. Our final result for the conductivity tensor can then be written as

$$\begin{aligned} \sigma_{\alpha\gamma} &= (e^2/m)\int_0^{\infty} dt\,\Sigma_{\rm B,\,k}[-(\partial f_{\rm k}/\partial\varepsilon_{\rm k})]\ v_{\rm k,\,\alpha}^{\rm B}\,v_{\rm k,\,y}^{\rm B},\\ &\quad\times\exp\left\{-\int_{\rm o}^{\infty} d\omega[J\,(\omega)/\omega^2]\right.\\ &\quad\left.\times[\coth\,(\beta\omega/2)(1-\cos\omega t) + i\,\sin\omega t] + {\rm c.c.}\right\}. \end{aligned} \tag{57}$$

At first sight, the conductivity expression appears to have the Boltzmann kinetic theory form. However, what is noteworthy is that the relaxation time τ, though independent of $\mathbf{k}$, has a much richer structure given by

$$\begin{aligned} \tau &= \int_0^{\infty} dt\,\exp\left\{-\int_0^{\infty} d\omega[J(\omega)/\omega^2]\right.\\ &\quad\left.\times[\coth\,(\beta\omega/2)\,(1-\cos\omega t) + i\sin\omega t] + {\rm c.c.}\right\}. \end{aligned} \tag{58}$$

This expression for τ is quite general irrespective of whether we are dealing with a phononic or an electronic bath. The latter feature can be only unravelled when we make specific inputs about the spectral density $J(\omega)$. We shall make a further analysis of τ in the next section when we delve into the experimental results in light of Eq. (57).

IV. FREQUENCY SCALES AND COMPARISON WITH EXPERIMENT

As stressed earlier, the characteristics of the heat bath captured by the spectral density $J(\omega)$ naturally depend on whether the excitations are mediated by phonons or other electrons or impurities, leading to various levels of complexity [19]. However, and for illustrative purposes, we will present results for the much-used *Ohmic dissipation model*—an apt description of electron-hole excitations near the Fermi surface [44]—that is linear in ω for small ω and is governed by a cutoff frequency $\omega_{\rm c}$. For the case of the phononic bath the spectral density is a nonlinear function of ω, with the level of nonlinearity being dictated by whether the phonons are acoustic or optic

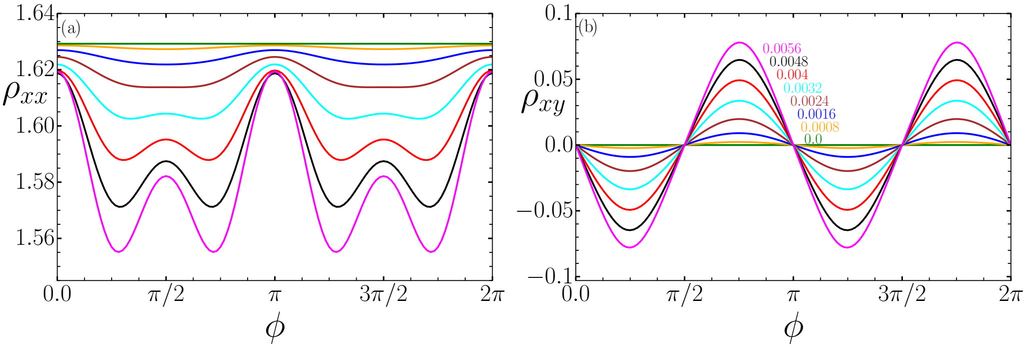

FIG. 1. (a) Plot of longitudinal resistivity ρ_{xx} as a function of in-plane angle φ of the applied magnetic field with respect to the electric field for different values of the magnetic field. (b) Variation of the Hall resistivity ρ_{xy} with respect to φ for different strengths of the magnetic field (after [22]).

[19]. While the phonon case can also be analyzed within the present formulation, we refrain from doing so for the sake of simplicity in our analytic treatment. Besides, the presently available experimental data do not warrant such an elaborate numerical analysis.

It is pertinent however, at this stage, to further amplify the meaning of Ohmic dissipation. It is well known in a path integral formulation of the density operator that the reduced density operator, after tracing out the bath coordinates, yields an *influence functional* of the Feynman-Vernon form [31]. This process is facilitated by the factorized form of the initial density matrix as in Eq. (45) or Eq. (16). What the explicit assumption of the nature of the bath in terms of quantum harmonic oscillators and the additional assumption of the Ohmic nature of the bath excitations does is to make the system obey, in the Heisenberg picture, a quantum Langevin equation with constant damping. Otherwise, we will end up with a Langevin equation endowed with a friction term in the structure of a memory kernel [31].

First, we discuss high temperature results within the Ohmic dissipation. By "high temperature" we do not mean such temperatures at which Kramers barrier activation [45] in the underlying TB lattice takes place, but simply that $k_{\mathrm{B}}T \gg \omega_{\mathrm{c}}$ upon restoring the Planck constant to the right. As it turns out, it is convenient to employ the so-called Drude cutoff for describing the high temperature results that assumes for $J(\omega)$ a Lorentzian form [26,33]

$$J(\omega) = 2\alpha\,\omega\left[\omega_{\mathrm{c}}^2/\left(\omega^2+\omega_{\mathrm{c}}^2\right)\right], \tag{59}$$

where α is the so-called *noise* parameter that yields the (dimensionless) strength of the heat bath coupling. We have then, from Eq. (58), in the notation of [26],

$$\tau = 2\int_0^\infty dt\ \cos[A_1(t)]\ \exp[-A_2(t)], \tag{60}$$

$$\begin{aligned} A_1(t) &= \pi\alpha[1-\exp(-\omega_{\mathrm{c}}t)],\\ A_2(t) &= -2\pi\alpha[\omega_{\mathrm{c}}t+\exp(-\omega_{\mathrm{c}}t)-1]/\omega_{\mathrm{c}}\beta. \end{aligned} \tag{61}$$

Further simplification ensues when we consider the long-time regime $\omega_{\mathrm{c}}t \gg 1$, which is quite appropriate as we are only interested in the asymptotic expression for the conductivity. In that situation the exponent acquires the form of a simple exponential and we recover the Drude τ for the semiclassical theory of Eq. (2) in which

$$\tau = \left[k_{\mathrm{B}}T/\pi\alpha\omega_{\mathrm{c}}^2\right]\cos(\pi\alpha). \tag{62}$$

In the experiments on the other hand, one is interested in the low temperature region below 10 K for which we must look into the opposite limit of $k_{\mathrm{B}}T \gg \omega_{\mathrm{c}}$, when the expressions for $A_1(t)$ and $A_2(t)$ in Eq. (60) have different and more complex forms:

$$\begin{aligned} A_1(t) &= 2\alpha\tan^{-1}(\omega_{\mathrm{c}}t),\\ A_2(t) &= \alpha\ln\left(1+\omega_{\mathrm{c}}^2\,t^2\right)+2\alpha\ln\{\beta\sinh(\pi t/\beta)/\pi t\}. \end{aligned} \tag{63}$$

Once again, we can simplify these expressions by going to the long-time limit $\omega_{\mathrm{c}}t \gg 1$, when

$$\begin{aligned} A_1(t) &= \pi\alpha,\\ A_2(t) &= 2\alpha\ln\{\beta\,\omega_{\mathrm{c}}\sin\,h(\pi t/\beta)/\pi\}. \end{aligned} \tag{64}$$

In this case, the Drude time has a much richer structure of

$$\tau = 2\cos(\pi\alpha)\int_{\mathrm{o}}^\infty dt\exp\{-2\alpha\ln[\beta\,\omega_{\mathrm{c}}\ \sin\,h(\pi t/\beta)/\pi]\}. \tag{65}$$

Finally, the relevant band velocities to be substituted into the conductivity expression in Eq. (57) are obtained by taking the derivatives of the band energy in Eq. (12) with respect to the appropriate wave vector components. We find [22]

$$\left(v_{\mathbf{k}}^{+,-}\right)_{\mathrm{x}} = -2d\Delta\ \sin\,dk_{\mathrm{x}}(+,-)\,(2\sqrt{S_{\mathbf{k}}})\,(\partial/\partial\mathbf{k}_{\mathrm{x}})\,S_{\mathbf{k}}. \tag{66}$$

A similar expression for $\left(v_{\mathbf{k}}^{+,-}\right)_{\mathrm{y}}$ holds by replacing $\mathbf{k}_{\mathrm{x}}$ by $\mathbf{k}_{\mathrm{y}}$. For the purpose of graphical illustration of our analytic results we rewrite Eq. (57) as

$$\begin{aligned} \sigma_{\mathrm{xx}} &= \tau(e^2/m)\,\Sigma_{\mathbf{k}}[(\partial f_{\mathbf{k}}/\partial\varepsilon_{\mathbf{k}}^+)(V_{\mathbf{k},\mathrm{x}}^+)^2+(\partial f_{\mathbf{k}}/\partial\varepsilon_{\mathbf{k}}^-)(V_{\mathbf{k},\mathrm{x}}^-)^2],\\ \sigma_{\mathrm{xy}} &= \tau(e^2/m)\,\Sigma_{\mathbf{k}}[(\partial f_{\mathbf{k}}/\partial\varepsilon_{\mathbf{k}}^+)\,V_{\mathbf{k},\mathrm{x}}^+\,V_{\mathbf{k},\mathrm{y}}^+ +(\partial f_{\mathbf{k}}/\partial\varepsilon_{\mathbf{k}}^-)V_{\mathbf{k},\mathrm{x}}^-V_{\mathbf{k},\mathrm{y}}^-]. \end{aligned} \tag{67}$$

Here, τ is given by Eq. (65) while the band velocities are to be read out from Eq. (66) supplemented by Eqs. (4) and (12). The corresponding resistivities can be calculated from

$$\rho_{\mathrm{xx}} = \sigma_{\mathrm{xx}}/\left(\sigma_{\mathrm{xx}}^2+\sigma_{\mathrm{xy}}^2\right),\qquad \rho_{\mathrm{xy}} = \sigma_{\mathrm{xy}}/\left(\sigma_{\mathrm{xx}}^2+\sigma_{\mathrm{xy}}^2\right). \tag{68}$$

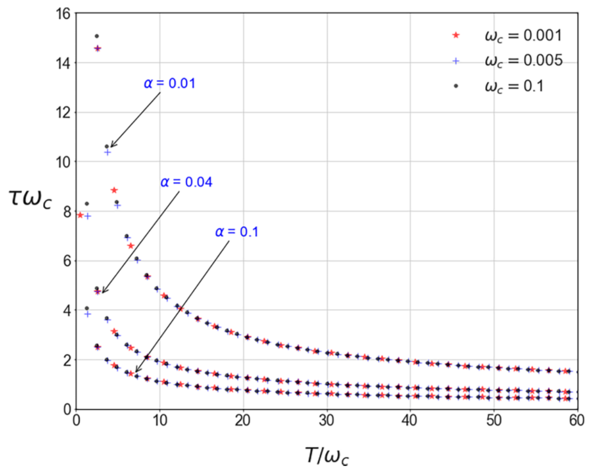

FIG. 2. Plot of dimensionless relaxation time $\tau\omega_c$ versus rescaled temperature T/ω_c for different values of the noise parameter and different values of the cut-off frequency ω_c.

It is evident that if we multiply the resistivities by τ, the angular variation of the rescaled resistivity will be governed by the φ dependence of the band velocities. This is demonstrated in Fig. 1(a) by plotting the longitudinal resistivity (AMR) ρ_{xx} as a function of the in-plane angle φ of the applied magnetic field with respect to the electric field, and in Fig. 1(b), the corresponding Hall resistivity (in PHE) ρ_{xy}, for different strengths of the magnetic field. The transition from a two-peak to a four-peak structure of the Hall resistivity is very much in conformity with experimental observations [22].

However, what was not measured so far in the experiments is the temperature dependence of the oscillation amplitudes, plotted in Fig. 1. This would need a separate calculation for the relaxation time τ as in Eq. (65) which is one of the main thrusts of the present paper. In addition to the temperature, τ depends on the noise parameter α and the bath cutoff frequency ω_c, both of which emerge from our microscopic treatment of the quantum heat bath. These results are presented in Fig. 2 which illustrate the temperature variation of the relaxation time τ for distinct values of α and ω_c. As would have been anticipated, τ monotonically decreases as the temperature increases towards the classical limit.

V. SUMMARY AND CONCLUDING REMARKS

We have presented here a comprehensive treatment of the Rashba coupling-dominated oxide layers in which planar resistivities have been earlier measured at low temperatures in the presence of an in-plane magnetic field. Three distinct kinds of interactions dominate the physics of this two-dimensional spintronic system. Of these, the band energy turns out to be more than three orders of magnitude larger than the competing effects of the Rashba energy arising from the intrinsic electric field normal to the oxide layer and the Zeeman energy due to the applied magnetic field. The experimental probe is a weak, time-independent electric field (or current), also applied in the plane. The corresponding linear response is governed by the Kubo conductivity tensors.

Our theoretical analysis is based on a fully quantum mechanical system-plus-bath approach in which ideas of dissipative quantum systems have been employed that make use of the familiar spin-boson Hamiltonian. Thus, we go beyond the extant semiclassical treatment that pivots around the classical Boltzmann transport equation. We show that the largeness of the band energy in comparison with the Rashba and the Zeeman couplings yields a simplified formalism in which the conductivity can be related to the particle-diffusivity in the manner of an Einstein kind of relation. As a result, the average time-development operator becomes independent of the band indices **k** and a Boltzmann equation-type conductivity formula emerges albeit the underlying relaxation time explicitly depends on the temperature and other bath parameters—features that are outside the realm of semiclassical methods. It is an interesting theoretical issue to relax the condition of the largeness of the band energy and treat it on the same footing as the Rashba and the Zeeman energies. The necessary framework is expected to need a more elaborate investigation of the master equation for the density operator. Such a treatment, beyond the scope of the present study, is left for future work.

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