Current response of nonequilibrium steady states in the Landau-Zener problem: Nonequilibrium Green's function approach

Sota Kitamura,[1] Naoto Nagaosa,[1,2] and Takahiro Morimoto[1,3]
[1]*Department of Applied Physics, The University of Tokyo, Hongo, Tokyo, 113-8656, Japan*
[2]*RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama, 351-0198, Japan*
[3]*JST, PRESTO, Kawaguchi, Saitama, 332-0012, Japan*

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The carrier generation in insulators subjected to strong electric fields is characterized by the Landau-Zener formula for the tunneling probability with a nonperturbative exponent. Despite its long history with diverse applications and extensions, study of nonequilibrium steady states and associated current response in the presence of the generated carriers has been mainly limited to numerical simulations so far. Here, we develop a framework to calculate the nonequilibrium Green's function of generic insulating systems under a DC electric field, in the presence of a fermionic reservoir. Using asymptotic expansion techniques, we derive a semiquantitative formula for the Green's function with nonperturbative contribution. This formalism enables us to calculate dissipative current response of the nonequilibrium steady state, which turns out to be not simply characterized by the intraband current proportional to the tunneling probability. We also apply the present formalism to noncentrosymmetric insulators, and propose nonreciprocal charge and spin transport peculiar to tunneling electrons.

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I. INTRODUCTION

Nonperturbative effects, which cannot be captured by order-by-order calculation, lead to a drastic change in the property of materials. The Landau-Zener tunneling [1,2] is a representative nonperturbative phenomenon, where application of an intense electric field to insulators leads to a rapid increase in the carrier generation rate.

Responses of quantum materials against external stimuli show a rich variety according to the symmetries of the underlying microscopic Hamiltonian. In particular, nonreciprocal transport is an important class of phenomena extensively explored both in linear and nonlinear regimes [3–10]. While the nonreciprocal response with a directional transport requires broken inversion symmetry, the presence of the time-reversal symmetry sometimes forbids the directionality, as typified in Onsager's reciprocal relation on generic linear responses [11].

Recent developments on the study of the nonlinear responses with a topological and geometric origin [12–17] suggest that the nonperturbative regime also hosts diverse novel phenomena including nonreciprocal transport and topological responses. Indeed, the nonreciprocity in the tunneling probability due to the geometric phase effect has been proposed recently [18,19].

Despite the potential importance, transport properties in the nonperturbative regime have not been explored so intensively. For the tunneling problems, quantitative estimation of the electric current associated with the tunneling carriers in the nonequilibrium states has been missing, except for several numerical studies in graphene [20–23] and correlated insulators [24–29], although the tunneling probability in the equilibrium (or in a mesoscopic environment) has been studied in a broad context [30–42]. The difficulty to do so stems from the far-from-equilibrium nature of the distribution of the excited electrons in the nonperturbative regime. To determine the nonequilibrium steady state, we have to deal with the Green's function or density matrix of the system in an open-dissipative setup. While such methods with the nonequilibrium ensemble are actively studied [43–50], it is still a nontrivial problem how to incorporate such nonequilibrium nature with the nonperturbative treatment of the tunneling process in the wave-function based theory.

In this paper, we consider a band insulator coupled to a fermionic particle reservoir under a DC electric field. The nonequilbirum steady state of this setup, schematically depicted in Fig. 1, is realized as a result of a balance between the nonperturbative excitation and relaxation due to the dissipation. We derive a concise formula for the nonequilibrium Green's function of the steady state, which includes a contribution from the nonperturbative tunneling process as well as the dissipative effect. This enables us to study the electric current due to the excited electrons, which exhibits nontrivial behaviors which cannot be deduced from the property of the tunneling probability. We clarify that there appears a competition between intraband and interband currents, which have different dependence on the electric field. We also apply the obtained formula to noncentrosymmetric insulators, in order to discuss the nonreciprocal transport. We reveal interesting phenomena, i.e., a crossover of the nonreciprocity ratio due to the competition mentioned above, and the nonreciprocal spin current due to the asymmetric band dispersion. Such nonreciprocal spin current of

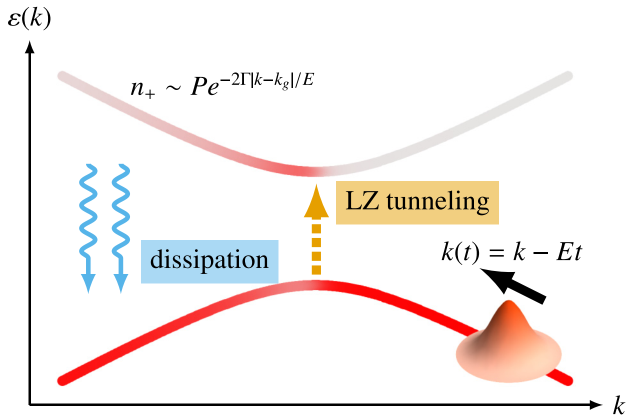

FIG. 1. Schematic picture of the nonequilibrium steady state for the open-dissipative Landau-Zener problem. The energy dispersion of a two-band insulator is colored in red, according to the occupation number $n_\pm$. Electrons driven by a static electric field E undergo the Landau-Zener tunneling with a probability P, when passing through the gap minimum. Excited electrons have a lifetime $t \sim 1/2\Gamma$ due to the coupling to the fermionic reservoir, which results in the exponential decay of the momentum distribution.

tunneling electrons may be related to chiral-induced spin selectivity (CISS) found in DNA molecules, where photoexcited electrons show spin accumulation through propagating in insulating DNA molecules [51,52].

This paper is organized as follows. In Sec. II, we develop a framework to calculate the nonequilibrium Green's function of the tunneling problem. We first review the calculation of the tunneling probability in isolated systems in Sec. II A. We introduce a key method, the adiabatic perturbation theory here. We extend this framework to open systems in Sec. II B, and construct the nonequilibrium Green's function using the solution of the equation of motion for the isolated system. We show the numerically calculated carrier density of the open system using the proposed framework in Sec. II C. We perform an asymptotic expansion for the nonequilibrium Green's function in Sec. III, in order to derive approximate analytic expressions. We summarize the main results in Sec. III A with a brief sketch of the derivation. We provide detail of the derivation with starting from the adiabatic limit in Sec. III B, where we find that the asymptotic evaluation reproduces the result of the Boltzmann equation with the relaxation-time approximation. We combine this with the method of the contour integral, to obtain the nonperturbative correction to the Green's function, in Sec. III C. We discuss the application of the obtained formula in Sec. IV. We discuss the nonperturbative electric current and associated nonreciprocity, as well as the extension of the formalism to lattice systems. Finally, we conclude the paper in Sec. V.

II. FORMULATION

A. Tunneling probability

We start with reviewing how the tunneling probability is described in isolated systems. The open-system formalism will be developed in the next subsection, based on the approach taken here.

In calculating the tunneling probability, the adiabatic perturbation theory [18,30–32,53], a series expansion with respect to a slowly changing parameter, plays a key role in capturing the nonperturbative nature. To see this, let us introduce a 2×2 Hamiltonian H in the momentum space (in the first-quantized form)

$$H(k)|u_{\pm,k}\rangle = \varepsilon_\pm(k)|u_{\pm,k}\rangle, \tag{1}$$

and consider its adiabatic time evolution. Here, $|u_{\alpha,k}\rangle$ is the Bloch wave function of the upper ($\alpha = +$) and lower ($\alpha = -$) bands with crystal momentum k and eigenenergy $\varepsilon_\alpha(k)$. In this study we consider a gapped case $\varepsilon_-(k) < \varepsilon_+(k)$.

We introduce a DC electric field E via the Peierls substitution $H(k) \to H(k - Et)$, where we set $e = \hbar = 1$ for simplicity. We consider the time evolution described by the time-dependent Schrödinger equation

$$i\partial_t|\Phi(t)\rangle = H(k - Et)|\Phi(t)\rangle. \tag{2}$$

We set the initial state at $t = t_i \to -\infty$ to be the eigenstate on the lower band, i.e., $|\Phi(t_i)\rangle = |\psi_{-,k}(t_i)\rangle \propto |u_{-,k-Et_i}\rangle$ [see Eq. (4) below].

It is well known as the adiabatic theorem that $|\langle u_{-,k-Et}|\Phi(t)\rangle|^2 \to 1$ in the weak field limit $E \to 0$. The tunneling probability, i.e., the probability to observe the state in the upper band (usually after a long time),

$$P = |\langle u_{+,k-Et}|\Phi(t)\rangle|^2 = 1 - |\langle u_{-,k-Et}|\Phi(t)\rangle|^2, \tag{3}$$

thus measures how much the adiabatic theorem is violated due to nonzero field strength $E \neq 0$. While this observation implies that it is convenient to expand $|\Phi(t)\rangle$ into the snapshot eigenstates $|u_{\pm,k-Et}\rangle$, we here introduce a suitable basis with an additional phase factor

$$|\psi_{\alpha,k}(t)\rangle = e^{-i\int_{t_0}^{t} dt'[\varepsilon_\alpha(k-Et')+EA_{\alpha\alpha}(k-Et')]}|u_{\alpha,k-Et}\rangle, \tag{4}$$

where $A_{\alpha\beta}(k) = i\langle u_{\alpha,k}|\partial_k|u_{\beta,k}\rangle$ is the Berry connection. Note that the lower limit of the t' integral is chosen to $t_0 := k/E \neq t_i$ for future convenience. Hereafter, we omit the arguments $k - Et$ when it is not confusing. While $|u_{\alpha,k-Et}\rangle$ is not necessarily smooth because of the arbitrariness of the phase factor (as a function of k), $|\psi_{\alpha,k}(t)\rangle$ does not depend on a gauge choice of $|u_{\alpha,k-Et}\rangle$ and is a smooth function of t,[1] thanks to the Berry phase factor. We call $|\psi_{\alpha,k}(t)\rangle$ the snapshot basis throughout this paper.

Now, by expanding $|\Phi(t)\rangle$ as

$$|\Phi(t)\rangle = \sum_{\alpha=\pm} a_\alpha(t)|\psi_{\alpha,k}(t)\rangle \tag{5}$$

[1]The gauge transformation we consider here is defined as $|u_{\alpha,k}\rangle \to |u_{\alpha,k}\rangle e^{i\Lambda_\alpha(k)}$ with an arbitrary real function Λ_α. Since the Berry connection is transformed as $A_{\alpha\alpha}(k) \to A_{\alpha\alpha}(k) - \partial_k\Lambda_\alpha(k)$, one can check that indeed the snapshot basis does not depend on the gauge choice of $|u_{\alpha,k}\rangle$ (except for the overall time-independent phase factor arising from the gauge choice at the initial time, i.e., $|\psi_{\alpha,k}(t)\rangle \to |\psi_{\alpha,k}(t)\rangle e^{i\Lambda_\alpha(k-Et_0)}$).

with $a_-(-\infty) = 1$ and $a_+(-\infty) = 0$, we obtain the equation of motion for $a_\pm(t)$ as

$$i\begin{pmatrix}\dot{a}_+(t)\\ \dot{a}_-(t)\end{pmatrix} = \begin{pmatrix}0 & W(t)\\ W^*(t) & 0\end{pmatrix}\begin{pmatrix}a_+(t)\\ a_-(t)\end{pmatrix}, \tag{6}$$

where

$$W(t) = EA_{+-}(k - Et)e^{i\int_{t_0}^{t}dt'[\varepsilon_+ - \varepsilon_- + E(A_{++} - A_{--})]}. \tag{7}$$

The adiabatic theorem immediately follows from the fact that $W(t) \to 0$ as $E \to 0$.

As $|W(t)| = o(|E|^0)$, we can regard $W(t)$ as a perturbation to the adiabatic time evolution. Within the first order, we obtain

$$a_+(t) \simeq -i\int_{-\infty}^{t} dt_1 W(t_1). \tag{8}$$

The formal full solution can also be obtained using the time-ordered exponential. The tunneling probability is now evaluated as $P = |a_+(t)|^2$.

As is well known as the Dykhne-Davis-Pechukas (DDP) method [30,31], in $t \to \infty$, one can evaluate Eq. (8) asymptotically by employing the contour integral in the complexified t_1 plane, which yields an essential singularity with respect to E. We discuss the asymptotic evaluation in terms of the contour integral for arbitrary t in Sec. III C.

We note that the difference of Berry connection $A_{++} - A_{--}$ that appears in Eq. (7) and seems gauge dependent can be rewritten by a gauge-invariant quantity, i.e., so-called "shift vector,"

$$R = A_{++} - A_{--} - \partial_k \arg A_{+-}. \tag{9}$$

This allows us to rewrite $W(t)$ as [18]

$$W(t) = E|A_{+-}(k - Et)|e^{i\int_{t_0}^{t}dt'(\varepsilon_+ - \varepsilon_- + ER) + i\arg A_{+-}(0)}. \tag{10}$$

This shift vector is known to appear in formulation of the second-order nonlinear optical response called "shift current" [12,13,15], and is a geometrical quantity that measures the real space shift between the centers of valence and conduction wave functions. As we show in Sec. IV B, shift vector also governs nonreciprocity in the tunneling current.

B. Nonequilibrium Green's function

Now, we introduce a particle reservoir (so-called Büttiker bath [44,46]) and consider a nonequilibrium steady state of the tunneling problem. We consider an open system described by

$$\hat{\mathcal{H}}(t) = \sum_k \hat{\mathcal{H}}_k(t), \tag{11}$$

$$\hat{\mathcal{H}}_k(t) = \sum_{\sigma\sigma'}\langle\sigma|H(k - Et)|\sigma'\rangle\hat{c}^\dagger_{k\sigma}(t)\hat{c}_{k\sigma'}(t) + \sum_{\sigma p}\omega_p\hat{b}^\dagger_{k\sigma p}(t)\hat{b}_{k\sigma p}(t) + \sum_{\sigma p}V_p\hat{b}^\dagger_{k\sigma p}(t)\hat{c}_{k\sigma}(t) + \text{H.c.} \tag{12}$$

Here, $H(k)$ is the Hamiltonian (1) defined in the previous subsection, and $\sigma = \uparrow, \downarrow$ is the pseudospin spanning the Hilbert space of 2×2 Hamiltonian $H(k)$ (corresponding to a sublattice, for instance). Note that we neglect the real spin of the electron here for simplicity. $\hat{c}_{k\sigma}(t)$ annihilates an electron with momentum k and pseudospin σ, while $\hat{b}_{k\sigma p}(t)$ annihilates an electron in a fermionic heat reservoir whose mode energy is ω_p. The second-quantized operators are represented in the Heisenberg representation, and denoted by hats. The spectral density of the fermionic reservoir is assumed to satisfy the broadband condition

$$\sum_p \pi|V_p|^2\delta(\omega - \omega_p) = \Gamma = \text{const}, \tag{13}$$

which makes the dissipative dynamics of electrons Markovian [see Eq. (A6)].

As we are interested in the tunneling process, it is natural to introduce the snapshot basis as in the isolated cases. Namely, we introduce an expansion of the field operator into the snapshot eigenstates as

$$\hat{c}_{k\sigma}(t) = \sum_\alpha \hat{\psi}_{\alpha,k}(t)\langle\sigma|\psi_{\alpha,k}(t)\rangle \tag{14}$$

$$= \sum_\alpha \hat{\psi}_{\alpha,k}(t)\langle\sigma|u_{\alpha,k-Et}\rangle e^{-i\int_{t_0}^{t}dt'(\varepsilon_\alpha + EA_{\alpha\alpha})}, \tag{15}$$

$$\hat{\psi}_{\alpha,k}(t) = \sum_\sigma\langle\psi_{\alpha,k}(t)|\sigma\rangle\hat{c}_{k\sigma}(t). \tag{16}$$

As the fermions in the reservoir are noninteracting, one can trace them out. As a result, they are embedded in a self-energy in terms of nonequilibrium Green's function. By inserting the above transformation to the snapshot basis into the well-known formula for the self energy (in the real-time representation with the original basis), we obtain [43,45]

$$G^R(t,t') = G^R_0(t,t')e^{-\Gamma(t-t')}, \tag{17}$$

$$G^A(t,t') = G^A_0(t,t')e^{-\Gamma(t'-t)}, \tag{18}$$

$$G^<(t,t') = (G^R * \Sigma^< * G^A)(t,t') \tag{19}$$

$$:= \int d\tau\, d\tau' G^R(t,\tau)\Sigma^<(\tau,\tau')G^A(\tau',t') \tag{20}$$

for the retarded, advanced, and lesser Green's functions, which are defined as $[G^R(t,t')]_{\alpha\beta} = [G^A(t',t)]^*_{\beta\alpha} = -i\langle\{\hat{\psi}_{\alpha,k}(t), \psi^\dagger_{\beta,k}(t')\}\rangle\Theta(t - t')$, $[G^<(t,t')]_{\alpha\beta} = i\langle\psi^\dagger_{\beta,k}(t')\hat{\psi}_{\alpha,k}(t)\rangle$ with $\Theta(t) = [1 + \text{sgn}(t)]/2$ being the step function. Here, $G^{R,A}_0$ denotes the Green's functions of the isolated system. The lesser Green's function $G^<$ is a particularly interesting quantity as it describes the electron occupation in the nonequilibrium states. The lesser component of the self-energy reads as

$$[\Sigma^<(\tau,\tau')]_{\alpha\beta} = i2\Gamma\int\frac{d\omega}{2\pi}e^{-i\omega(\tau-\tau')}f_D(\omega)\langle\psi_{\alpha,k}(\tau)|\psi_{\beta,k}(\tau')\rangle \tag{21}$$

with f_D being the Fermi-Dirac distribution function. We have omitted the interval of integration $(-\infty, \infty)$ for the τ, τ', ω integral. While this transformation is straightforward, we also provide a derivation using the Heisenberg equation in Appendix A for completeness.

To complete the framework, we need to specify the retarded Green's functions of the isolated system $G^R_0(t,t')$. As

$a_{\pm}(t)$ is the solution of the time-evolution equation (6), one can explicitly construct the retarded Green's function of the isolated system using a unitary matrix

$$U(t) = \begin{pmatrix} a_-^*(t) & a_+(t) \\ -a_+^*(t) & a_-(t) \end{pmatrix}, \tag{22}$$

which satisfies

$$i\dot{U}(t) = \begin{pmatrix} 0 & W(t) \\ W^*(t) & 0 \end{pmatrix} U(t). \tag{23}$$

One can easily check that $G_0^R(t,t')$ is represented as

$$G_0^R(t,t') = -iU(t)U^\dagger(t')\Theta(t-t'). \tag{24}$$

See also Appendix A.

To summarize, the nonequilibrium Green's function of the open system $G^<$ can be evaluated by (i) computing the time evolution of the isolated system (6) to obtain $a_\pm$ and construct G_0^R, and (ii) computing convolution of $\Sigma^<$ by performing τ, τ' and ω integrals in Eqs. (20) and (21). We provide analytic expressions for the outcome of this framework using various asymptotic methods in the next section.

Before closing the section, we remark that the nonequilibrium Green's function is time dependent, nevertheless, it represents a steady state. This is because we focus on a single electron with a particular momentum k (at $t = 0$), while the (steady) many-body state consists of electrons with various momenta. In other words, the Green's function we consider here is that for $\hat{\mathcal{H}}_k(t)$, while the physical system is given by $\hat{\mathcal{H}}(t) = \sum_k \hat{\mathcal{H}}_k(t)$ [see Eqs. (11) and (12)]. Many-body expectation values, which are given as a momentum average of single-electron expectation values, are indeed time independent since the direct relation between momentum and time, $k(t) = k - Et$, makes momentum average identical to time average.

C. Numerical calculation

Here we use the above framework for performing numerical calculations, and see the influence of the reservoir on the tunneling electrons. We calculate the carrier density $n_+(t)$ as a transient occupation of a single electron on the upper band,

$$n_+(t) = \langle \hat{\psi}_{+,k}^\dagger(t)\hat{\psi}_{+,k}(t)\rangle = \mathrm{Im}[G^<(t,t)]_{++}, \tag{25}$$

which can be translated into the momentum distribution of the excited electrons of the whole system. The carrier density $n_+(t)$ can be regarded as a counterpart of the (transient) tunneling probability in the case of isolated systems.

As a typical example, we consider the Landau-Zener model

$$H(k) = \begin{pmatrix} -vk & \delta \\ \delta & vk \end{pmatrix}, \tag{26}$$

whose time evolution (6) is known to be exactly solvable [2,53]. Let us discuss the properties of the isolated case first. The tunneling probability of the isolated case $P(t) = |a_+(t)|^2$ in the $t \to \infty$ limit is given as

$$P(t\to\infty) = e^{-E_{\rm th}/E} = \exp\left(-\frac{\pi\delta^2}{vE}\right), \tag{27}$$

which can also be exactly reproduced by the DDP method. The transient dynamics is also important for characterizing the tunneling process. We plot the tunneling probability $P(t) = |a_+(t)|^2$ as a function of t in Fig. 2, where we set $k(t=0) = 0$. It shows that the tunneling mainly occurs when the electron passes through the gap minimum ($t = 0$). In particular, the tunneling probability approaches to the step function $\Theta(t)$ asymptotically in the strong field limit. On the other hand, in the intermediate regime, the tunneling probability undergoes an overshoot behavior within the timescale of $\sim 1/\sqrt{vE}$, before converging to the final value.

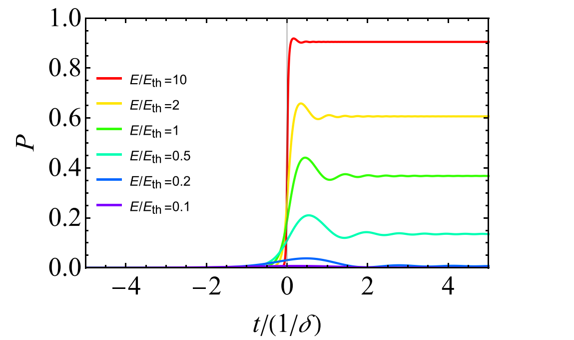

FIG. 2. Tunneling probability $P(t) = |a_+(t)|^2$ of the isolated system as a function of time t, for the Landau-Zener model. $E_{\rm th} = \pi\delta^2/v$.

Now, let us see how the carrier density (tunneling probability) is modified in the presence of the fermionic reservoir. We plot the numerically calculated transient occupation of a single electron on the upper band in the open system $n_+(t) = \mathrm{Im}[G^<(t,t)]_{++}$ in Fig. 3. Here, we set the temperature of the fermionic reservoir as $k_BT = 0.5\delta$, which is relatively high, and $\Gamma = 0.2\delta$. We can find two qualitatively different regimes. One is the low-field regime, where the tunneling amplitude in the isolated case is negligible compared with the thermal excitation. In this regime, the system should be well described by the perturbative treatment using the Boltzmann equation, where the distribution of the electron follows the equilibrium one with a drift of the momentum. On the other hand, as one increases the field strength, the nonperturbative tunneling process becomes dominant, and a jump in the carrier density evolves at $t = 0$. This generated carrier at the gap minimum gradually relaxes due to the coupling to the fermionic reservoir (see also Fig. 1).

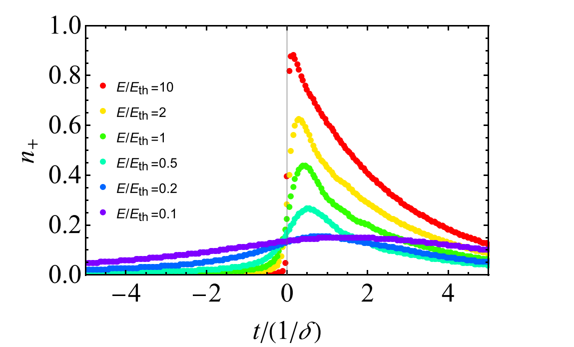

FIG. 3. Carrier density $n_+(t) = \mathrm{Im}[G^<(t,t)]_{++}$ of the open system as a function of time t, for the Landau-Zener model. $E_{\rm th} = \pi\delta^2/v$.

These features in the open system are expected to be universal in generic gapped systems, and to be captured qualitatively by analytic formulas using appropriate approximations, which we discuss in the next section.

III. ASYMPTOTIC EVALUATION

A. Overview

In this section, we evaluate the nonequilibrium Green's function (20) derived in the previous section, in an analytic manner using various approximations. Let us begin with a brief overview of our derivation of Green's functions, before going into the details of calculations presented in the next subsections. First, as a general remark, we note that the approximations we adopt are mainly based on asymptotic expansions, as in the DDP method in isolated systems. In contrast to usual Taylor series that has a finite convergence radius, these approximations are not necessarily improved by including the higher-order correction. Thus, we have to be careful on the condition when the approximation is justified.

We first consider the adiabatic limit and try to reproduce the low-field regime. Since the dynamics of the isolated system is trivial there, the central issue here is how to approximate τ, τ', and ω integrals in Eqs. (20) and (21). As we are considering the adiabatic limit, where the timescale associated with the change of the parameter is slow enough, we assume that it is also slower than the decay time $\sim 1/\Gamma$. We can perform the τ, τ' integrals in a form of an asymptotic series, which can be truncated in a low order if the above assumption holds. This corresponds to the gradient expansion known in the quantum kinetic theory [43], which is employed for deriving the quantum Boltzmann equation. Indeed, by performing ω integral in terms of the residue integral, we obtain

$$[G^<_{\rm ad}(t,t)]_{\pm\pm} \simeq i f_D(\varepsilon_\pm(t)) + i f_D'(\varepsilon_\pm(t))\partial_k\varepsilon_\pm(t)\frac{E}{2\Gamma} \tag{28}$$

at the leading order, which coincides with the result of the Boltzmann equation with the relaxation-time approximation. This is discussed in Sec. III B. We also show that the above approximation quantitatively deviates from the numerical result in an insulating system due to the nonperturbative contribution.

Next, we consider the tunneling contribution by extending the above result. As we need to construct the Green's function G_0^R, we have to calculate $a_+(t)$ at generic time t as opposed to the conventional tunneling problem where one considers only the $t \to \infty$ limit. According to the Lefschetz thimble approach recently proposed for the tunneling problem [54], the asymptotic form for the nonperturbative component should be given as

$$a_+(t) \simeq \sqrt{P_0}\,\Theta(t), \tag{29}$$

where P_0 is the tunneling probability of the isolated system in the $t \to \infty$ limit. While the discontinuity due to the step function is not present in the actual solution, this approximates the rapid increase at $t = 0$ that appeared in Fig. 2. With this correction we can approximate the nonequilibrium Green's function as

$$G^<(t,t) \simeq G^<_{\rm ad}(t,t) + i\begin{pmatrix} P_0 & \sqrt{P_0} \\ \sqrt{P_0} & -P_0 \end{pmatrix} \times [f_D(\varepsilon_-(0)) - f_D(\varepsilon_+(0))]e^{-2\Gamma t}\Theta(t), \tag{30}$$

where the second term describes the decay of the tunnel electron seen in Fig. 3. This is the key result of this study, which we discuss in Sec. III C.

B. Adiabatic limit

Let us consider a situation where the electric field is so weak that the nonperturbative contribution to the Green's function can be neglected. We consider the adiabatic limit $E \to 0$, where the isolated Green's function becomes trivial since $a_+(t) = 0$, $a_-(t) = 1$, and $U(t) = I_{2\times 2}$. In this limit, the lesser Green's function reads as

$$\left[G^<_{\rm ad}(t,t')\right]_{\alpha\beta} = i2\Gamma \int \frac{d\omega}{2\pi} f_D(\omega)e^{-i\omega(t-t')} \times \langle \mathcal{L}_\omega\psi_\alpha(t)|\mathcal{L}_\omega\psi_\beta(t')\rangle, \tag{31}$$

where $\mathcal{L}_\omega$ represents the Laplace transform (from τ to $\Gamma + i\omega$)

$$|\mathcal{L}_\omega\psi_\alpha(t)\rangle := \int_0^\infty d\tau |\psi_{\alpha,k}(t-\tau)\rangle e^{-(\Gamma+i\omega)\tau}. \tag{32}$$

In this section we try to construct an adiabatic perturbation expansion of the nonequilibrium Green's function. This can be done when the relaxation time $1/(2\Gamma)$ is sufficiently shorter than the typical timescale of adiabatic parameter change ($\propto 1/E$). In such a case, the Laplace transform (32) can be evaluated in an asymptotic series form as follows.

A straightforward and elementary approach to obtain an asymptotic expansion is successive use of integration by parts based on the relation

$$e^{-(\Gamma+i\omega)\tau - i\int_{t_0}^{t-\tau} dt'\varepsilon_\alpha} = -\frac{\partial_\tau\left(e^{-(\Gamma+i\omega)\tau - i\int_{t_0}^{t-\tau} dt'\varepsilon_\alpha}\right)}{\Gamma + i\omega - i\varepsilon_\alpha(t-\tau)}, \tag{33}$$

where we have introduced a shorthand notation $\varepsilon_\alpha(t-\tau) = \varepsilon_\alpha(k - E(t-\tau))$. Instead, here we use a more systematic approach in the following.

Since the integrand decays in the timescale of $1/\Gamma$, one can Taylor expand the slowly changing part of the integrand around $\tau = 0$ and perform the termwise Laplace transform, which yields the asymptotic series solution. However, as can be seen in the definition (4), the integrand $|\psi_{\alpha,k}(t-\tau)\rangle$ has two different timescales. One is the adiabatic timescale appearing via $k(t) = k - Et$, while another is the time dependence due to the dynamical phase factor $-i\int_{t_0}^{t} dt'\varepsilon_\alpha$. The latter should be separately treated in performing the Taylor expansion (at least at the leading order). To this end, we introduce the slow component at time t as

$$|\overline{\psi}_{\alpha,k}(t,\tau)\rangle = |\psi_{\alpha,k}(t-\tau)\rangle e^{-i\varepsilon_\alpha(t)\tau}, \tag{34}$$

where the additional phase factor cancels the dynamical phase around $\tau = 0$. One can easily check that $\partial_\tau|\overline{\psi}_{\alpha,k}(t,\tau)\rangle = O(E)$. Now, by expanding the slow component $|\overline{\psi}_{\alpha,k}(t,\tau)\rangle$, we obtain

$$|\mathcal{L}_\omega \psi_\alpha(t)\rangle = \int_0^\infty d\tau |\overline{\psi}_{\alpha,k}(t,\tau)\rangle e^{-[\Gamma+i\omega-i\varepsilon_\alpha(t)]\tau} \tag{35}$$

$$= \sum_{n=0}^\infty \frac{1}{n!}\frac{\partial^n}{\partial\tau^n}|\overline{\psi}_{\alpha,k}(t,\tau)\rangle\Big|_{\tau=0} \times \int_0^\infty d\tau\, \tau^n e^{-[\Gamma+i\omega-i\varepsilon_\alpha(t)]\tau} \tag{36}$$

$$= \sum_{n=0}^\infty \frac{\partial^n}{\partial\tau^n}\frac{|\overline{\psi}_{\alpha,k}(t,\tau)\rangle}{[\Gamma+i\omega-i\varepsilon_\alpha(t)]^{n+1}}\Big|_{\tau=0} \tag{37}$$

$$= \exp\left[-\frac{\partial}{\partial s}\frac{\partial}{\partial\tau}\right]\frac{|\overline{\psi}_{\alpha,k}(t,\tau)\rangle}{s+i\omega}\Big|_{s=\Gamma-i\varepsilon_\alpha(t),\tau=0}. \tag{38}$$

Equation (31) then reads as

$$[G^<_{\rm ad}(t,t')]_{\alpha\beta} = i2\Gamma \exp\left[-\frac{\partial}{\partial s}\frac{\partial}{\partial \tau} - \frac{\partial}{\partial s'}\frac{\partial}{\partial \tau'}\right] I(s,s')\langle\overline{\psi}_{\alpha,k}(t,\tau)|\overline{\psi}_{\beta,k}(t',\tau')\rangle\Big|_{s=\Gamma+i\varepsilon_\alpha(t),s'=\Gamma-i\varepsilon_\beta(t'),\tau=\tau'=0}, \tag{39}$$

where

$$I(s,s') = \int \frac{d\omega}{2\pi}\frac{f_D(\omega)e^{-i\omega(t-t')}}{(s-i\omega)(s'+i\omega)}. \tag{40}$$

Let us evaluate the ω integral $I(s,s')$. In this section, let us focus on the case $t=t'$. The integration can be performed using the residue integral as

$$I(s,s') = \frac{1}{s+s'}f_\Gamma(\mathrm{Im}s, -\mathrm{Im}s'), \tag{41}$$

by using $\mathrm{Re}s = \mathrm{Re}s' = \Gamma > 0$. Here, $f_\Gamma(\varepsilon_1,\varepsilon_2)$ is given by

$$f_\Gamma(\varepsilon_1,\varepsilon_2) = \frac{1}{2} - \frac{1}{2\pi i}\left[\Psi\left(\frac{1}{2}+\frac{\Gamma+i\varepsilon_1}{2\pi k_BT}\right) - \Psi\left(\frac{1}{2}+\frac{\Gamma-i\varepsilon_2}{2\pi k_BT}\right)\right], \tag{42}$$

with Ψ being the digamma function, which can be regarded as a "modified distribution function" reflecting the presence of the fermionic reservoir. We note that

$$\mathrm{Re}f_\Gamma(\varepsilon_1,\varepsilon_2) = \frac{1}{2}[f_\Gamma(\varepsilon_1,\varepsilon_1) + f_\Gamma(\varepsilon_2,\varepsilon_2)], \tag{43}$$

and $f_\Gamma(\varepsilon,\varepsilon)\to f_D(\varepsilon)$ as $\Gamma/k_BT\to 0$. Namely, the present bath behaves as an ideal bath when $\Gamma \ll k_BT$.

Having completed three integrations, we can obtain the expression for the lesser Green's function by evaluating $\exp[-\partial_s\partial_\tau - \partial_{s'}\partial_{\tau'}]$. While the s derivative of Eq. (41) consists of that of the distribution f_Γ and that of the denominator $(s+s')^{-1}$, the former should be smaller since it is higher order in Γ/k_BT. Thus, we truncate the former series at the first order:

$$e^{-\partial_s\partial_\tau-\partial_{s'}\partial_{\tau'}}I(s,s') = e^{i\partial_{\varepsilon_1}\partial_\tau - i\partial_{\varepsilon_2}\partial_{\tau'}}f_\Gamma e^{-\partial_s(\partial_\tau+\partial_{\tau'})}(s+s')^{-1} \tag{44}$$

$$\simeq [f_\Gamma + i(\partial_{\varepsilon_1}f_\Gamma\partial_\tau - \partial_{\varepsilon_2}f_\Gamma\partial_{\tau'})] \times e^{-\partial_s(\partial_\tau+\partial_{\tau'})}(s+s')^{-1}, \tag{45}$$

which leads to

$$[G^<_{\rm ad}(t,t)]_{\alpha\beta} \simeq if_\Gamma(\varepsilon_\alpha(t),\varepsilon_\alpha(t))\delta_{\alpha\beta} - 2\Gamma(\partial_{\varepsilon_\alpha}+\partial_{\varepsilon_\beta})f_\Gamma(\varepsilon_\alpha(t),\varepsilon_\beta(t)) \times e^{-\partial_\Gamma\partial_\tau/2}\frac{\langle\overline{\psi}_{\alpha,k}(t,\tau)|i\partial_\tau|\overline{\psi}_{\beta,k}(t,\tau)\rangle}{\varepsilon_\alpha(t)-\varepsilon_\beta(t)-i2\Gamma}\Big|_{\tau=0}. \tag{46}$$

The remaining τ derivative can be evaluated using

$$\langle\overline{\psi}_{\alpha,k}(t,\tau)|i\partial_\tau|\overline{\psi}_{\alpha,k}(t,\tau)\rangle = \varepsilon_\alpha(t) - \varepsilon_\alpha(t-\tau), \tag{47}$$

$$\langle\overline{\psi}_{+,k}(t,\tau)|i\partial_\tau|\overline{\psi}_{-,k}(t,\tau)\rangle = W(t-\tau)e^{i(\varepsilon_+(t)-\varepsilon_-(t))\tau}, \tag{48}$$

which results in, for the diagonal part,

$$[G^<_{\rm ad}(t,t)]_{\pm\pm} \simeq if_D(\varepsilon_\pm(t)) + if_D'(\varepsilon_\pm(t))\partial_k\varepsilon_\pm(t)\frac{E}{2\Gamma} \tag{49}$$

at the leading order, which reproduces the well-known result of the Boltzmann equation with the relaxation-time approximation. One can neglect the off-diagonal part

$$[G^<_{\rm ad}(t,t)]_{+-} \simeq -\frac{2\Gamma(\partial_{\varepsilon_+}+\partial_{\varepsilon_-})f_\Gamma(\varepsilon_+(t),\varepsilon_-(t))}{\varepsilon_+(t)-\varepsilon_-(t)-i2\Gamma}W(t), \tag{50}$$

which can be shown to be canceled with the perturbative correction to $U(t)$.

We examine the obtained formula by calculating the carrier density $n_+(t) = \mathrm{Im}[G^<(t,t)]_{++}$ in Fig. 4, where we set $\Gamma = 0.4\delta$, $k_BT=\delta$, and $E = 0.2(\pi\delta^2/v)$ for the Landau-Zener model. As can be seen in the numerical result plotted in Fig. 4(a), the results for the full expression of $G^<$, Eq. (20), and $G^<_{\rm ad}$ given by Eq. (31) agree well, which implies that the thermal excitation is the dominant mechanism for the carrier generation in this parameter regime. We plot the result using the asymptotic expansion (46) truncated at zeroth, first, and second derivatives with respect to τ. The first-order formula reproduces the numerical result semiquantitatively. The second-order correction makes the result worse, which is characteristic to the asymptotic expansion with vanishing convergent radius. One can also notice the overestimation of the height of the peak. This deviation is related to a nonperturbative effect peculiar to insulating systems, with which the agreement is substantially improved as can be seen in the green curve obtained with the saddle-point method. We discuss details of this effect in Appendix B.

C. Tunneling contribution

As one decreases the temperature or increases the field strength, the dominant mechanism for the carrier generation should switch from the thermal excitation to the quantum tunneling, which is not taken into account in the previous section. In this section, we consider the nonperturbative

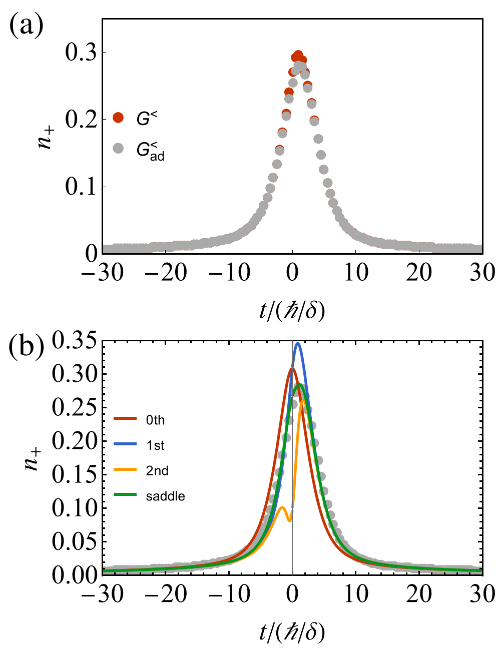

FIG. 4. Carrier density $n_+(t) = \mathrm{Im}[G^<(t,t)]_{++}$ of the Landau-Zener model as a function of time. $\Gamma = 0.4\delta$, $k_BT = \delta$, and $E = 0.2(\pi\delta^2/v)$. (a) Numerical calculation based on the full Green's function (20) (red) and based on the adiabatic component (31) (gray). (b) Comparison of the adiabatic component with the asymptotic expression (46). The Taylor expansion of $e^{-\partial_\Gamma\partial_\tau/2}$ is truncated at the nth order. The green line is the result of the saddle-point approximation (see Appendix B).

tunneling contribution. Since the Green's function includes such nonperturbative contribution in the time evolution of the isolated system $a_\pm(t)$, here we consider the first-order correction (8) in terms of the adiabatic perturbation.

The central issue here is that we have to compute $a_+(t)$ as a function of t, which is in contrast to the conventional tunneling problem discussing the $t \to \infty$ limit. We first discuss this using the Lefschetz thimble approach [54]. Then, we construct $G_0^R(t,t')$ with the tunneling correction and derive the formula for $G^<(t,t')$.

1. Thimble decomposition

As is also known in the DDP method, it is essential to regard the t_1 integral in Eq. (8) as a contour integral of a complexified variable ($k - Et_1 \to z_1$ here), in capturing the nonperturbative nature of the tunneling probability. The Lefschetz thimble method is a powerful tool in computing contour integral, which provides a systematic decomposition of the contour of integration C_0 [with $a_+(t) = \int_{C_0} dz_1 e^{f(z_1)}$] into a deformed contour C composed of the steepest descents of $\mathrm{Re} f(z_1)$ that extend from saddle points (and the end point of C_0). See Refs. [54,55] and Appendix C for details. Because the steepest descent of $\mathrm{Re} f(z_1)$ coincides with the isopleth of $\mathrm{Im} f(z_1)$ due to the Cauchy-Riemann relations, the integrand along the deformed contour has no oscillation (as opposed to the original one) and is easier to evaluate.

The saddle point is a special point where the steepest descent and ascent join, whose position is obtained by solving $\partial_{z_1} f(z_1) = 0$. In the present case, this equation reads as

$$\frac{\partial}{\partial z_1} \ln \tilde{A}_{+-} - i\frac{\Delta}{E} - iR = 0, \tag{51}$$

where $\tilde{A}_{+-}(z_1)$ is the analytic continuation of the dipole matrix element $|A_{+-}(k - Et_1)|$, $R = A_{++} - A_{--} - \partial_k \arg A_{+-}$ the shift vector, and $\Delta = \varepsilon_+ - \varepsilon_-$. As we show in Appendix C, when E is small enough, the solution $z_1 = k_s$ can be found in the vicinity of the gap-closing point $z_1 = k_c$ with $\Delta(k_c) = 0$ (i.e., where the second term vanishes). This can be seen in the plot of $\mathrm{Re} f(z_1)$ for the Landau-Zener model ($E > 0$) (Fig. 5), where the gap-closing points and saddle points are marked with black and red points, respectively.

According to the Lefschetz thimble method, the steepest descent attached to a given saddle point belongs to the deformed contour C, if its steepest ascent has an intersection with the original contour C_0, as exemplified in Figs. 5(a) and 5(b): The saddle point in the lower half-plane (marked with red dot) has a steepest ascent parallel to the imaginary axis (red dashed line), which crosses the real axis at $z = k - Et_g$ [the gap minimum point $\partial_k\Delta = 0$, represented by the blue dot in Fig. 5(b)]. As the original contour C_0 (blue line) runs from $+\infty$ to $k - Et$, the steepest descent has a contribution when $t > t_g$. Indeed, the deformed contour C drawn by red curves is composed of two pieces in Fig. 5(b) with $t > t_g$, in contrast to Fig. 5(a) with $t < t_g$. While there are also two saddle points in the upper half-plane (and more on another Riemann surface), they always have no contribution as their steepest ascents do not intersect with the real axis.

The saddle-point contribution present in $t > t_g$ can be evaluated approximately using Laplace's method, which results in

$$a_+(t) \simeq \sqrt{P_0}\Theta(t) = e^{\mathrm{Im}\int_0^{k_c} dk[\Delta/|E| + \mathrm{sgn}(E)R]}\Theta(t). \tag{52}$$

Here, for simplicity, we have set $t_g = 0$ by shifting the origin of time, and set $\arg A_{+-}(k=0)$ such that the tunneling amplitude becomes real [see Eq. (C23)]. We keep only the leading order in E for the prefactor. See Appendix C for details.

The discontinuous behavior $\Theta(t)$ roughly approximates the time profile shown in Fig. 2 if we neglect the overshoot behavior in $0 < t \lesssim 1/\sqrt{vE}$. The overshoot behavior is related to the last segment of the deformed contour C (steepest ascent toward the terminal point $z_1 = k - Et$), although we neglect it in this study. When E is small enough, perturbative evaluation of the last segment yields an $O(E\sqrt{P_0})$ term to the Green's function, which reproduces the overshoot behavior, although it cannot capture the suppression in the strong E regime. We note that its contribution to the electric current is higher order than the interband component (we derive below) with $O(\sqrt{P_0})$.

2. Green's function

Let us evaluate the influence of the tunneling contribution (52) on the nonequilibrium Green's function. With this contribution, the retarded Green's function of the isolated system reads as

$$G_0^R(t,t') \simeq -i\Theta(t-t')I_{2\times 2} + i\begin{pmatrix} P_0/2 & -\sqrt{P_0} \\ \sqrt{P_0} & P_0/2 \end{pmatrix}\Theta(t)\Theta(-t'), \tag{53}$$

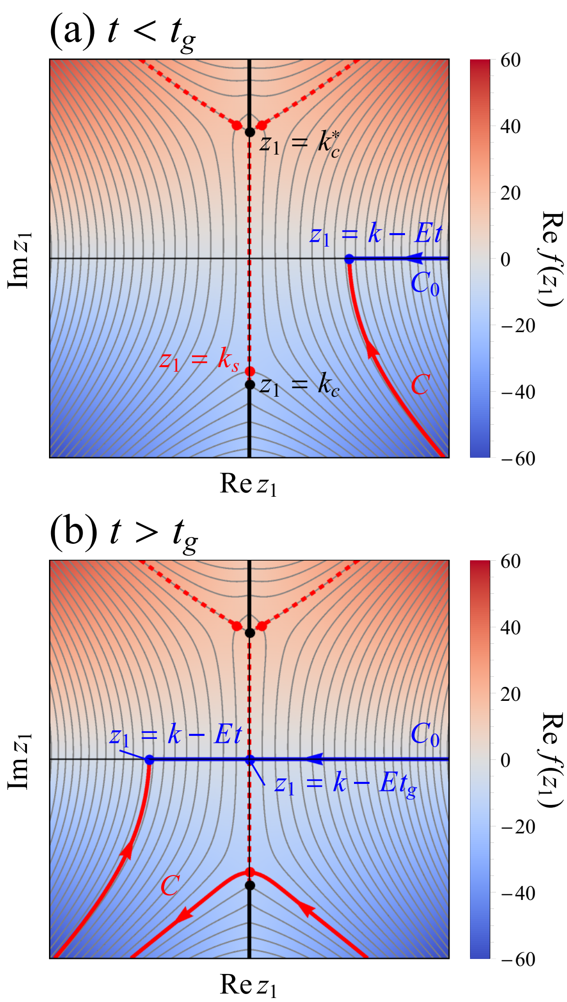

FIG. 5. Re$f(z_1)$ for $a_+(t) = \int_{C_0} dz_1 e^{f(z_1)}$ [see Eqs. (8) and (C1)] in the complexified momentum plane ($z_1 = k - Et_1$). Gray lines are the steepest descents. The gap-closing points $z_1 = k_c, k_c^*$ are indicated by black dots, from which the branch cut drawn by the black thick lines extends. The saddle points $z_1 = k_s$ are marked with red dots, while red dashed lines are associated steepest ascents. The original contour of integration C_0 indicated by blue line is deformed into C composed of the steepest descents attached to saddle points (and the terminal point of the C_0), drawn as red solid lines. t_g is defined via the crossing point $z_1 = k - Et_g$ between the real axis and the red dashed line (steepest ascent). $t \gtrless t_g$ (whether $z_1 = k - Et_g$ intersects with C_0 or not) determines whether the steepest descent attached to the saddle point ($z_1 = k_s$) belongs to C or not.

where the diagonal entries in the second term arise from the correction to $a_-(t)$ that keeps the norm conservation $|a_+|^2 + |a_-|^2 = 1$ up to $O(P_0)$.

Since the tunneling process is approximated to be instantaneous and represented by the step function within the present approximation, the second term can be rewritten in terms of $G^R_{0,\mathrm{ad}}(0,t') = -i\Theta(0-t')I_{2\times2}$. Then, $G^R(t,t') = G^R_0(t,t')e^{-\Gamma(t-t')}$ reads as

$$G^R(t,t') = G^R_{\mathrm{ad}}(t,t') + M(t)\Theta(t)G^R_{\mathrm{ad}}(0,t'), \tag{54}$$

where

$$M(t) = -\begin{pmatrix} P_0/2 & -\sqrt{P_0} \\ \sqrt{P_0} & P_0/2 \end{pmatrix} e^{-\Gamma t} \tag{55}$$

and $G^R_{\mathrm{ad}}(t,t') = G^R_{0,\mathrm{ad}}(t,t')e^{-\Gamma(t-t')}$.

By substituting this and $G^A(t,t') = [G^R(t',t)]^\dagger$ into Eq. (20), $G^< = G^R * \Sigma^< * G^A$, we obtain $G^<$ with the tunneling correction, in terms of $G^<_{\mathrm{ad}} = G^R_{\mathrm{ad}} * \Sigma^< * G^A_{\mathrm{ad}}$ (here the asterisk denotes convolution in time and matrix product in the band index). Namely, we can summarize the (equal-time) expression into

$$G^<(t,t) = G^<_{\mathrm{ad}}(t,t) + G^<_{\mathrm{LZ}}(t,t)\Theta(t) \tag{56}$$

with

$$G^<_{\mathrm{LZ}}(t,t) = M(t)G^<_{\mathrm{ad}}(0,0)M^\dagger(t) + M(t)G^<_{\mathrm{ad}}(0,t) + G^<_{\mathrm{ad}}(t,0)M^\dagger(t). \tag{57}$$

In particular, the diagonal component of the correction term $G^<_{\mathrm{LZ}}(t,t)$ reads as

$$[G^<_{\mathrm{LZ}}(t,t)]_{\pm\pm} = [G^<_{\mathrm{ad}}(0,0)]_{\mp\mp}P_0e^{-2\Gamma t} - i\,\mathrm{Im}[G^<_{\mathrm{ad}}(t,0)]_{\pm\pm}P_0e^{-\Gamma t} \pm 2i\,\mathrm{Im}[G^<_{\mathrm{ad}}(t,0)]_{\pm\mp}\sqrt{P_0}e^{-\Gamma t}. \tag{58}$$

Since we have evaluated the equal-time expression $G^<_{\mathrm{ad}}(t,t)$ in the previous section, we have to evaluate the adiabatic Green's function $G^<_{\mathrm{ad}}(t,t')$ with $t > t' = 0$ here. If we evaluate Eq. (40) with $t > t'$, we obtain

$$I(s,s') = \frac{f_D(-is)e^{-s(t-t')}}{s+s'} + \sum_{n=0}^{\infty} \frac{ik_BTe^{-\omega_n(t-t')}}{(s-\omega_n)(s'+\omega_n)}, \tag{59}$$

where $\omega_n = (2n+1)\pi k_BT$ is the Matsubara frequency. Since we are considering $k_BT \gg \Gamma = \mathrm{Re}s$, the second term is negligible for $t - t' \neq 0$. In addition to the s derivative of the distribution f_D and the denominator $(s+s')^{-1}$, we have that of $e^{-s(t-t')}$ in the evaluation of $e^{-\partial_s\partial_\tau - \partial_{s'}\partial_{\tau'}}I(s,s')$ in the present case. This contribution is problematic when $t - t'$ is large since

$$e^{-\partial_s\partial_\tau}e^{-s(t-t')} = e^{-s(t-t')}e^{-\partial_s\partial_\tau}e^{(t-t')\partial_\tau} \tag{60}$$

acts as a time-translation operator for τ. This leads to the breakdown of the assumption that τ is small, which is necessary for performing the gradient expansion (38). To cancel this time translation effect, we need to choose the slow component as

$$|\psi_{\alpha,k}(t-\tau)\rangle = |\overline{\psi}_{\alpha,k}(t',\tau-(t-t'))\rangle e^{i\varepsilon_\alpha(t')[\tau-(t-t')]}. \tag{61}$$

For details, see Appendix D. Then, as the remaining factors in $I(s,s')$ are the same as in the previous calculation, we arrive at a similar expression as Eq. (46):

$$[G^<_{\mathrm{ad}}(t,t')]_{\alpha\beta} \simeq if_D(\varepsilon_\alpha(t') - i\Gamma)e^{-\Gamma(t-t')}\delta_{\alpha\beta} - 2\Gamma f_D'(\varepsilon_\alpha(t') - i\Gamma)e^{-\Gamma(t-t')} \times e^{-\partial_\Gamma\partial_\tau/2}\frac{\langle\overline{\psi}_{\alpha,k}(t',\tau)|i\partial_\tau|\overline{\psi}_{\beta,k}(t',\tau)\rangle}{\varepsilon_\alpha(t') - \varepsilon_\beta(t') - 2i\Gamma}\bigg|_{\tau=0}. \tag{62}$$

As the drift correction $\propto f_D'$ is less relevant when E is increased (correction may make the asymptotic expansion worse), let us consider only the first term. The correction to the nonequilibrium Green's function reads as

$$[G^<_{\rm LZ}(t,t)]_{\pm\pm}\Theta(t) = \pm i[f_D(\varepsilon_-(0)) - f_D(\varepsilon_+(0))]P_0e^{-2\Gamma t}\Theta(t). \quad (63)$$

The physical meaning of this expression is apparent. The tunneling occurs at $t=0$ with probability P_0, which is instantaneous and governed by the quasiequilibrium distribution at $t=0$ (although this is an approximation). This contribution decays in the timescale of $1/(2\Gamma)$, as the excited electrons are relaxed due to the dissipation to the heat bath. This picture is schematically summarized in Fig. 1.

In the same way, one can calculate the off-diagonal part as

$$[G^<_{\rm LZ}(t,t)]_{+-} \simeq \big([G^<_{\rm ad}(0,t)]_{--} - [G^<_{\rm ad}(t,0)]_{++}\big)\sqrt{P_0}e^{-\Gamma t} \quad (64)$$

$$\simeq i[f_D(\varepsilon_-(0)) - f_D(\varepsilon_+(0))]\sqrt{P_0}e^{-2\Gamma t}, \quad (65)$$

where we have dropped $O(EP_0)$. It is worth noting that the off-diagonal component has a halved nonperturbative exponent, which implies that the interband current may be crucial for the transport property. We compare intraband and interband contributions for the electric current in Sec. IV A.

IV. APPLICATIONS

A. Nonperturbative electric transport in band insulators

We have derived a formula for the nonequilibrium Green's function with the nonperturbative correction in the previous section. The original motivation to calculate this is to obtain the nonequilibrium distribution of the electron and calculate physical observables, such as the electric current. Here, let us evaluate the nonperturbative electric current of the band insulators as an application of the present framework. The velocity operator in the snapshot basis is expressed as

$$\hat{v} = \sum_{\sigma\sigma'}\langle\sigma|\partial_k H(k-Et)|\sigma'\rangle \hat{c}^\dagger_{k\sigma}(t)\hat{c}_{k\sigma'}(t) \quad (66)$$

$$= \begin{pmatrix}\hat{\psi}_{+,k}(t)\\ \hat{\psi}_{-,k}(t)\end{pmatrix}^\dagger v(k-Et)\begin{pmatrix}\hat{\psi}_{+,k}(t)\\ \hat{\psi}_{-,k}(t)\end{pmatrix} \quad (67)$$

$$:= \begin{pmatrix}\hat{\psi}_{+,k}(t)\\ \hat{\psi}_{-,k}(t)\end{pmatrix}^\dagger \begin{pmatrix}\partial_k\varepsilon_+ & i\Delta W/E\\ -i\Delta W^*/E & \partial_k\varepsilon_-\end{pmatrix}\begin{pmatrix}\hat{\psi}_{+,k}(t)\\ \hat{\psi}_{-,k}(t)\end{pmatrix}, \quad (68)$$

where $\Delta = \varepsilon_+ - \varepsilon_-$. Note that this expression is exact for an arbitrary E (i.e., it contains all the nonlinear terms with respect to the vector potential). We also note that $\arg W(t)$ depends on $\arg A_{+-}(k=0)$, which has been fixed such that the asymptotic form of $a_+(t)$ becomes real [see Eq. (C25)]. As we have mentioned in the end of Sec. II B, physical observables are given as a momentum average of the single-electron expectation value calculated with the nonequilibrium Green's function (and are thus time independent). In the adiabatic limit, the electric current is given as

$$J_{\rm ad} = -i\int\frac{dk}{2\pi}{\rm Tr}[-vG^<_{\rm ad}] \quad (69)$$

$$= -\frac{E}{2\Gamma}\int\frac{dk}{2\pi}\sum_{\alpha=\pm}(\partial_k\varepsilon_\alpha)^2 f_D'(\varepsilon_\alpha) - E\int\frac{dk}{2\pi}\frac{2\Gamma\Delta^2|A_{+-}|^2}{\Delta^2+4\Gamma^2}\sum_{\alpha=\pm}f_D'(\varepsilon_\alpha), \quad (70)$$

which vanishes in the insulating system at the low temperature, as f_D' becomes zero. On the other hand, the nonperturbative correction has a temperature dependence as

$$J = \big(J^{(1)}_{\rm LZ} + J^{(2)}_{\rm LZ}\big)[f_D(\varepsilon_-(0)) - f_D(\varepsilon_+(0))]. \quad (71)$$

Here, the zero-temperature expressions $J^{(1)}_{\rm LZ}, J^{(2)}_{\rm LZ}$ are the intraband and interband currents given as

$$J^{(1)}_{\rm LZ} = \mp P_0\int_{\mp\Lambda}^0\frac{dk}{2\pi}\partial_k\Delta e^{2\Gamma k/E}, \quad (72)$$

$$J^{(2)}_{\rm LZ} = 2\sqrt{P_0}{\rm Re}\int_{\mp\Lambda}^0\frac{dk}{2\pi}|A_{+-}|\Delta e^{-i{\rm Re}\int_{k_c}^k dk'(\Delta/E+R)+2\Gamma k/E}, \quad (73)$$

where $\pm = {\rm sgn}(E)$.[2] Here, Λ is a cutoff momentum, which should be replaced by 2π divided by the lattice constant in the case of lattice systems (see Sec. IV C). $J^{(1)}_{\rm LZ}$ is asymptotically evaluated as

$$J^{(1)}_{\rm LZ} \sim \pm\frac{P_0}{2\pi}\left[-\frac{E}{2\Gamma}\frac{\partial\Delta}{\partial k} + \frac{E^2}{4\Gamma^2}\frac{\partial^2\Delta}{\partial k^2} - \cdots\right]_{k=0} \quad (74)$$

which survives since $f_D(\varepsilon_-(0)) - f_D(\varepsilon_+(0)) \sim 1$. When the first derivative of Δ vanishes as in the Landau-Zener model, the intraband tunneling current turns out to be proportional to E^2P_0. One can evaluate the interband current $J^{(2)}_{\rm LZ}$ by the similar asymptotic series expansion. The leading-order term reads as

$$J^{(2)}_{\rm LZ} \sim \frac{\sqrt{P_0}}{\pi}\left[\frac{E|A_{+-}|2\Gamma\Delta}{\Delta^2+4\Gamma^2}\right]_{k=0}, \quad (75)$$

where we have assumed ${\rm Re}\int_0^{k_c}dk'(\Delta/E+R) = 0$ for simplicity. While $J^{(2)}_{\rm LZ}$ has a smaller power $E\sqrt{P_0}$ compared with $J^{(1)}_{\rm LZ}$, the Lorentz factor makes the value small when $\Gamma \ll \Delta$. Thus, whether the intraband or interband effect is dominant depends on the strength of the dissipation.

We plot $J^{(1)}_{\rm LZ}/J^{(2)}_{\rm LZ}$ and $J^{(1)}_{\rm LZ} + J^{(2)}_{\rm LZ}$ for the Landau-Zener model in Figs. 6(a) and 6(b), respectively, as functions of E and Γ. Here, we have numerically integrated Eqs. (72)

[2]While the present formula is justified only if the decay time $1/2\Gamma$ is shorter than the adiabatic timescale, its $\Gamma \to 0$ limit partially reproduces the result in the ballistic limit as follows. The $\Gamma \to 0$ expression for the intraband current is given as $J^{(1)}_{\rm LZ} \to P_0[\Delta(\Lambda) - \Delta(0)]/2\pi$. Here $\Delta(\Lambda)$ can be regarded as the applied voltage in the Landauer picture, when two leads are sandwiching the system and the cutoff momentum is determined by the chemical potential of the leads. In this picture, we obtain the electric conductance as $P_0\,(e^2/h)$, if we drop the small contribution from $\Delta(0)$. Also, when $\Gamma \to 0$, the integral in the interband current (73) has no perturbative expression with respect to E. One can show by the saddle-point method that $J^{(2)}_{\rm LZ}$ is higher order than $J^{(1)}_{\rm LZ}$ in this limit.

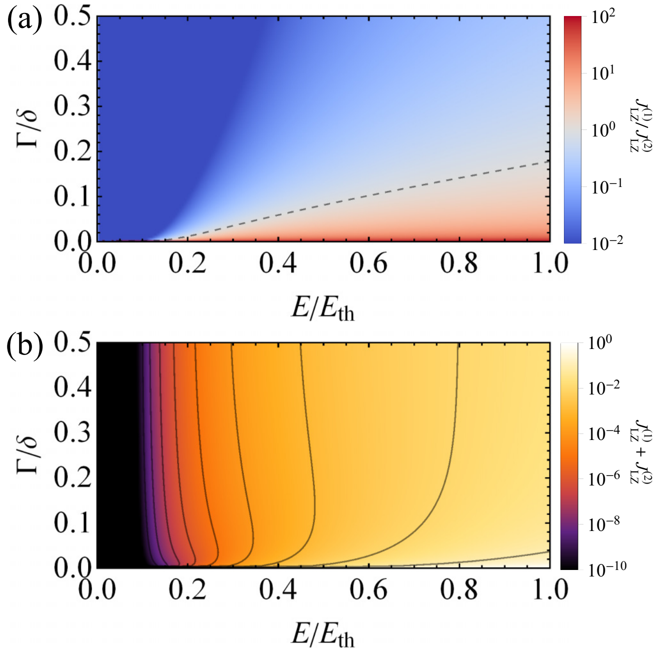

FIG. 6. Electric current response of the nonequilibrium steady state for the Landau-Zener model attached to a fermionic reservoir. (a) Ratio of the intraband and interband currents $J_{\mathrm{LZ}}^{(1)}/J_{\mathrm{LZ}}^{(2)}$ as a function of the electric field E and the dissipation Γ. Dashed line indicates $J_{\mathrm{LZ}}^{(1)} = J_{\mathrm{LZ}}^{(2)}$. (b) $J_{\mathrm{LZ}}^{(1)} + J_{\mathrm{LZ}}^{(2)}$ as a function of the electric field E and the dissipation Γ.

and (73). We find that the interband current is dominant in a wide region of the parameter space. The intraband current is dominant only when $\Gamma \lesssim 0.1\delta$, where one has a crossover from the interband-dominant to intraband-dominant regime as increasing the field strength.

Such dominance of interband contribution to the current response cannot be captured by conventional analyses of tunneling processes that only focus on tunneling probability. Namely, the intraband contribution to the current can be deduced from the tunneling probability and group velocity. In contrast, the interband contribution, which turns out to be dominant in a wide parameter range, requires analysis of phase coherence of tunneling electrons, and cannot be captured only by looking at the tunneling probability. Thus, our Green's function approach has an advantage in describing tunneling current response with an ability to incorporate the intraband and interband contributions on an equal footing.

B. Nonreciprocal transport

1. Nonreciprocal charge transport

As we have revealed in the previous study [18], the tunneling probability P_0 has a geometric factor that involves the shift vector R. In particular, for noncentrosymmetric systems, this factor exhibits nonreciprocity (depends on the sign of E):

$$\gamma_P := \frac{P_0(+|E|)}{P_0(-|E|)} = \frac{e^{2\,\mathrm{Im}\int_0^{k_c} dk(\Delta/|E|+R)}}{e^{2\,\mathrm{Im}\int_0^{k_c} dk(\Delta/|E|-R)}} = \exp\left[2\,\mathrm{Im}\int_{k_c^*}^{k_c} dk\, R\right]. \tag{76}$$

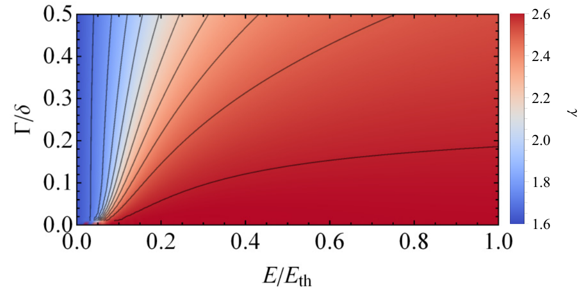

FIG. 7. Nonreciprocity ratio $\gamma = J(+E)/J(-E)$ in the steady state for a two-band model of noncentrosymmetric insulator with a nonzero shift vector, Eq. (77). Nonreciprocity is enhanced for larger electric field E and is suppressed for stronger dissipation Γ.

The shift vector R is an odd function of k when the system is inversion symmetric, and does not lead to nonreciprocity. In contrast, noncentrosymmetric systems can host nonreciprocity arising from the geometric factor.

When the tunneling process is the main mechanism to generate carriers, the nonreciprocity ratio $\gamma = J(+E)/J(-E)$ for the electric current should also be characterized by that for tunneling probability γ_P. However, since the intraband and interband currents ($J_{\mathrm{LZ}}^{(1)}$ and $J_{\mathrm{LZ}}^{(2)}$ in the previous section) are respectively proportional to P_0 and $\sqrt{P_0}$, the nonreciprocity ratio γ for the electric current should undergo a crossover from $\sqrt{\gamma_P}$ to γ_P when the dominant contribution is switched from the interband to intraband current, e.g., by sweeping the strength of the field.[3]

To demonstrate the crossover, we introduce a model for a noncentrosymmetric insulator

$$H(k) = \delta\sigma_x + m\sqrt{1+ck^2}\sigma_y + vk\sigma_z, \tag{77}$$

where the parameter m controls the strength of inversion breaking [$\sigma_x H(k)\sigma_x \neq H(-k)$] which yields a nonzero shift vector. Note that this model is time-reversal symmetric, $\sigma_x H^*(k)\sigma_x = H(-k)$, which prohibits nonreciprocal response that arises from asymmetric band structures such as magnetochiral anisotropy [6]. We show the nonreciprocity ratio γ in Fig. 7 as a function of the electric field E and the dissipation strength Γ. We choose $m = 0.5\delta$ and $c = 0.5v^2/\delta^2$, which leads to $\gamma_P = 2.62$, $\sqrt{\gamma_P} = 1.62$. We note that γ_P has no dependence on E and Γ. We can see that the nonreciprocity ratio changes from $\sim\sqrt{\gamma_P}$ to $\sim\gamma_P$ as the field strength is increased, which clearly captures the change of the dominant mechanism for the electric current from the interband to intraband effect. Namely, for the weak electric field regime, the interband effect is dominant since the phase coherence between the two bands is important for the current response with a small number

[3]In a paper by two of the present authors [56], the section on "Absence of dc nonreciprocal current in noninteracting systems" contains an incorrect argument around Eq. (14). Namely, the nonreciprocal current proportional to E^2 may exist in time-reversal symmetric noninteracting systems in general. Such nonreciprocal current $\propto E^2$ can be studied based on the Keldysh Green's function method developed in this paper, which would be an interesting future problem.

of excited electrons. For the strong electric field regime, in contrast, the intraband effect becomes dominant which means that there appear many tunnel electrons which carry current according to their group velocity. In addition, Fig. 7 shows that strong dissipation Γ suppresses nonreciprocity. In particular, we find that nonreciprocity in the crossover regime is quickly suppressed by the dissipation.

2. *Nonreciprocal spin transport*

It is interesting to investigate a different type of nonreciprocal transport that is not characterized by the nonreciprocity of the tunneling probability. The momentum distribution of the excited electrons due to the tunneling process is highly asymmetric around the gap minimum (only left or right is occupied according to the sign of the electric field), which is a peculiar property absent in metallic systems.

We can exploit this feature to obtain a nonreciprocal *spin* transport when the band dispersion has a skew around the gap minimum. Under the time-reversal symmetry, however, the gap minimum with an opposite skew exists at $-k$, so that the asymmetry in the electric current should vanish if contributions from this pair of gap minima is added up. The nonreciprocal transport due to this asymmetry may survive when we consider the spin current. We here consider an insulating model with a Rashba spin-orbit coupling

$$H(k) = (vk + \lambda s_z)\sigma_x + (\delta - \gamma k^2)\sigma_z, \tag{78}$$

where s_z is the (real) spin of the electron. This model is time-reversal symmetric since $\sigma_z s_y H^*(k) s_y \sigma_z = H(-k)$, while it lacks the inversion symmetry as $\sigma_z H(k)\sigma_z \neq H(-k)$. We plot the energy dispersion of this Hamiltonian in Fig. 8(a). Due to the Rashba spin splitting, the time-reversal partner at $-k$ has the opposite spin polarization. Thus, the tunneling current for the spin up and down differs due to the skewed dispersion, as shown in Fig. 8(b). The spin current due to this difference, shown in Fig. 8(c), does not change when the electric field is inverted, i.e., the spin current exhibits nonreciprocity. This is a different type of nonreciprocal transport which is absent in the metallic transport with the shift of the Fermi surface. Note that there are two pairs of saddle points for each spin sector of this model, and we have neglected the pair with larger threshold field, for simplicity. We also have neglected a (E-dependent) slight deviation of the crossing point $z_1 = k - Et_g$ from the gap minimum.

Recently, spin-dependent transport has been found in DNA molecules [51], and spin transport in chiral materials [chiral-induced spin selectivity (CISS)] is attracting growing interests [52]. In CISS, photoexcited electrons propagate through insulating DNA molecules and show spin accumulation due to spin-dependent decay rates. Similarly, the above-mentioned spin transport in the tunneling process indicates a spin rectification effect, and can induce spin accumulation in noncentrosymmetric and chiral semiconductors with application of electric fields. While the present mechanism of spin accumulation applies for tunneling electrons and not for photoexcited electrons in CISS, these two effects could be related with each other in that both induce spin accumulation via electron propagation through an insulator. In particular, the spin current in tunneling problem implies that application of strong DC electric fields to chiral molecules including DNAs can induce spin current generation and spin accumulation.

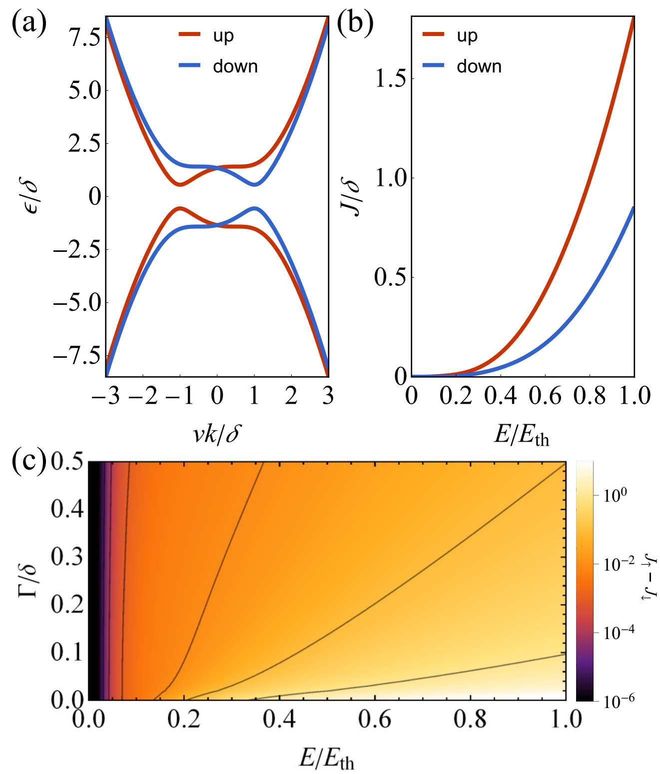

FIG. 8. Nonreciprocal spin current in the nonequilibrium steady state of a Rashba-splitted insulator, Eq. (78). $\lambda = 0.4\delta$, $\gamma = 1.25v^2/\delta$. (a) Energy dispersion. (b) Spin-resolved current as a function of electric field E for $\Gamma = 0.1\delta$. (c) Nonreciprocal spin current $J_\uparrow - J_\downarrow$ against electric field E and dissipation Γ. $J_\uparrow(-E) = -J_\downarrow(E)$ leads to directionality $J_\uparrow(E) - J_\downarrow(E) = J_\uparrow(-E) - J_\downarrow(-E)$.

C. Extension to lattice systems

So far, we have considered models in a continuous limit, such as the Landau-Zener model. Here, we briefly introduce an extension of the formalism to lattice systems with a Brillouin zone. In isolated lattice systems, the electron passes through the gap minimum periodically, with the period of the Bloch oscillation $T_B = 2\pi/|E|a_0$ (a_0 is the lattice constant). Thus, the asymptotic form of the tunneling amplitude $a_+(t)$ is modified from Eq. (52) to

$$a_+(t) \sim \sqrt{P_0} \sum_{n=-N}^{\infty} e^{in\int_0^{T_B} dt(\Delta+ER)}\Theta(t - nT_B). \tag{79}$$

Here, $N \to \infty$ should be taken after the calculation of Green's functions for the open system, to avoid the divergence of the sum. The n summation appears due to the contribution from the multiple saddle points, which has a phase difference originating from the dynamical phase factor $[W(t+T_B) = W(t)e^{i\int_0^{T_B} dt(\Delta+ER)}]$.

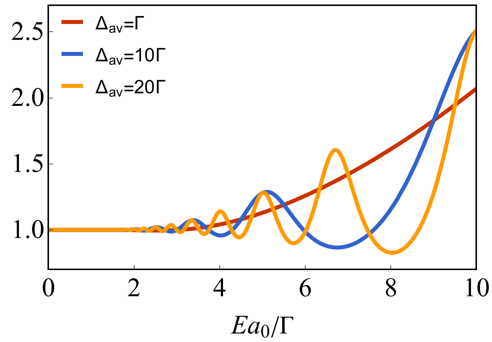

FIG. 9. The interference factor $(1+e^{-2\Gamma T_B})/|1-e^{-2\Gamma T_B - i\int_0^{T_B} dt\,\Delta}|^2$ for various values of the momentum average of the energy gap $\Delta_{av} := a_0 \int_0^{2\pi/a_0} dk/(2\pi) \times (\varepsilon_+ - \varepsilon_-)$, where $T_B = 2\pi/|E|a_0$.

By repeating the derivation in the previous sections with Eq. (79) instead of Eq. (52), one can show that the correction to the nonequilibrium Green's function is modified as

$$[G^<_{\rm LZ}(t,t)]_{\pm\pm} \to \frac{(1+e^{-2\Gamma T_B})[G^<_{\rm LZ}(t,t)]_{\pm\pm}}{|1-e^{-2\Gamma T_B - i\int_0^{T_B} dt(\Delta+ER)}|^2}, \tag{80}$$

$$[G^<_{\rm LZ}(t,t)]_{+-} \to \frac{[G^<_{\rm LZ}(t,t)]_{+-}}{1-e^{-2\Gamma T_B - i\int_0^{T_B} dt(\Delta+ER)}}, \tag{81}$$

for $t \in [0, T_B)$. The expression for an arbitrary time can be obtained by employing the periodicity $[G^<_{\rm LZ}(t+T_B, t+T_B)]_{\pm\pm} = [G^<_{\rm LZ}(t,t)]_{\pm\pm}$ and $[G^<_{\rm LZ}(t+T_B, t+T_B)]_{+-} = [G^<_{\rm LZ}(t,t)]_{+-} e^{i\int_0^{T_B} dt(\Delta+ER)}$.

The additional factor characterized by the dynamical phase and $\Gamma T_B = 2\pi\Gamma/Ea_0$ describes the interference between tunneling processes with different times. The electron excited at $t = nT_B$ acquires the dynamical phase $i\int_0^{T_B} dt(\Delta+ER)$ relative to the electron excited at $t=(n+1)T_B$. The interference becomes significant when the electric field is so large that the relaxation time $1/\Gamma$ leading to the decay of the amplitude is comparable to the period of the tunneling processes T_B. We plot the interference factor $(1+e^{-2\Gamma T_B})/|1-e^{-2\Gamma T_B - i\int_0^{T_B} dt\Delta}|^2$ in Fig. 9.

V. CONCLUSION

In this paper, we studied the nonequilibrium steady state of the insulating systems with the nonperturbative correction derived from the quantum tunneling. We established a framework for the nonequilibrium Green's function in the tunneling problem, where the Green's function in the snapshot basis is represented by the solution to the time evolution of the isolated system that the conventional approaches are based on. We perform an asymptotic evaluation of the nonequilibrium Green's function in the snapshot basis, which reproduces the result of the Boltzmann equation with the relaxation-time approximation in the adiabatic limit. By combining the Lefschetz thimble method, we also obtain the nonperturbative correction to the nonequilibrium Green's function, and discuss the electric current in the nonequilibrium steady state. We also discuss the nonreciprocal transport associated with the tunneling current, and propose the crossover of the nonreciprocity ratio in the nonmagnetic noncentrosymmetric insulators, and a nonreciprocal spin current derived from the asymmetric band dispersion in spin-splitted insulators.

The application of the present formalism in the strong-field regime turned out to be unexpectedly successful for the Landau-Zener model. This should be attributed to the fact that the asymptotic evaluation of the tunneling probability coincides with the exact solution. Such feature is absent in generic models (in particular for lattice models with an energy cutoff), and we have to substantially improve the asymptotic method adopted in this study, e.g., by a more sophisticated treatment of the Lefshetz thimble. Extension of the present formalism to many-body systems [24,26] is also an important open problem.

ACKNOWLEDGMENTS

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APPENDIX A: DERIVATION OF THE NONEQUILIBRIUM GREEN'S FUNCTIONS IN THE SNAPSHOT BASIS

Here, we derive the expressions for the nonequilibrium Green's function in the snapshot basis. Let us begin with the Heisenberg equation of the annihilation operators,

$$i\dot{\hat{c}}_{k\sigma}(t) = \sum_{\sigma'} \langle\sigma|H(k-Et)|\sigma'\rangle \hat{c}_{k\sigma'}(t) + \sum_p V_p^* \hat{b}_{k\sigma p}(t), \tag{A1}$$

$$i\dot{\hat{b}}_{k\sigma p}(t) = \omega_p \hat{b}_{k\sigma p}(t) + V_p \hat{c}_{k\sigma}(t). \tag{A2}$$

The latter one can be solved with respect to $\hat{b}$ as

$$\hat{b}_{k\sigma p}(t) = \hat{b}_{k\sigma p}(t_i) e^{-i\omega_p(t-t_i)} - iV_p \int_{t_i}^t dt' \hat{c}_{k\sigma}(t') e^{-i\omega_p(t-t')}, \tag{A3}$$

where $t_i = -\infty$ is the initial time where the system is in equilibrium. By substituting this into the former equation of motion, we obtain

$$i\dot{\hat{c}}_{k\sigma}(t) = \sum_{\sigma'} \langle\sigma|H(k-Et)|\sigma'\rangle \hat{c}_{k\sigma'}(t) + \sum_p V_p^* \hat{b}_{k\sigma p}(t_i) \times e^{-i\omega_p(t-t_i)} - i\sum_p |V_p|^2 \int_{t_i}^t dt' \hat{c}_{k\sigma}(t') e^{-i\omega_p(t-t')}. \tag{A4}$$

The memory effect described by the last term vanishes (i.e., dynamics becomes Markovian) when the fermionic reservoir satisfies the broadband condition (13): The last term is shown to be instantaneous as

$$\sum_p |V_p|^2 \int_{t_i}^t dt' \hat{c}_{k\sigma}(t') e^{-i\omega_p(t-t')}$$

$$= \int d\omega \sum_p |V_p|^2 \delta(\omega-\omega_p) \int_{t_i}^t dt' \hat{c}_{k\sigma}(t') e^{-i\omega(t-t')} \quad \text{(A5)}$$

$$= \int \frac{d\omega}{2\pi} 2\Gamma \int_{t_i}^t dt' \hat{c}_{k\sigma}(t') e^{-i\omega(t-t')} = \Gamma \hat{c}_{k\sigma}(t). \quad \text{(A6)}$$

Namely, we obtain

$$i\dot{\hat{c}}_{k\sigma}(t) = \sum_{\sigma'} \langle \sigma | H(k-Et) | \sigma' \rangle \hat{c}_{k\sigma'}(t) - i\Gamma \hat{c}_{k\sigma}(t) + \sum_p V_p^* \hat{b}_{k\sigma p}(t_i) e^{-i\omega_p(t-t_i)}. \quad \text{(A7)}$$

Then, by performing the unitary transformation (14), we obtain

$$i\frac{d}{dt}\begin{pmatrix} \hat{\psi}_{+,k}(t) \\ \hat{\psi}_{-,k}(t) \end{pmatrix} = \begin{pmatrix} -i\Gamma & W(t) \\ W^*(t) & -i\Gamma \end{pmatrix} \begin{pmatrix} \hat{\psi}_{+,k}(t) \\ \hat{\psi}_{-,k}(t) \end{pmatrix} + \sum_{p\sigma} V_p^* \begin{pmatrix} \langle \psi_{+,k}(t)|\sigma\rangle \\ \langle \psi_{-,k}(t)|\sigma\rangle \end{pmatrix} \hat{b}_{k\sigma p}(t_i) e^{-i\omega_p(t-t_i)}. \quad \text{(A8)}$$

In order to solve this differential equation, we introduce the unitary matrix $U(t)$ defined as Eq. (22). By replacing the off-diagonal matrix in the right-hand side as

$$\begin{pmatrix} 0 & W(t) \\ W^*(t) & 0 \end{pmatrix} = i\dot{U}(t)U^\dagger(t), \quad \text{(A9)}$$

we can deform Eq. (A8) into

$$i\frac{d}{dt}\left[U^\dagger(t) \begin{pmatrix} \hat{\psi}_{+,k}(t) \\ \hat{\psi}_{-,k}(t) \end{pmatrix} e^{\Gamma t} \right]$$

$$= \sum_{p\sigma} V_p^* U^\dagger(t) \begin{pmatrix} \langle \psi_{+,k}(t)|\sigma\rangle \\ \langle \psi_{-,k}(t)|\sigma\rangle \end{pmatrix} \hat{b}_{k\sigma p}(t_i) e^{-i\omega_p(t-t_i)+\Gamma t}, \quad \text{(A10)}$$

which we can solve just by integrating on $[t_i, t]$. Especially, when $\Gamma = V_p = 0$ (i.e., the case of the isolated system), we obtain

$$\begin{pmatrix} \hat{\psi}_{+,k}(t) \\ \hat{\psi}_{-,k}(t) \end{pmatrix} = U(t)U^\dagger(t_i) \begin{pmatrix} \hat{\psi}_{+,k}(t_i) \\ \hat{\psi}_{-,k}(t_i) \end{pmatrix}, \quad \text{(A11)}$$

by which the expression for $[G_0^R(t,t')]_{\alpha\beta} = -i\langle\{\hat{\psi}_{\alpha,k}(t), \psi^\dagger_{\beta,k}(t')\}\rangle_0 \Theta(t-t')$, Eq. (24), immediately follows. When $\Gamma \neq 0, V_p \neq 0$, we arrive at

$$\begin{pmatrix} \hat{\psi}_{+,k}(t) \\ \hat{\psi}_{-,k}(t) \end{pmatrix} = iG_0^R(t,t_i) \begin{pmatrix} \hat{\psi}_{+,k}(t_i) \\ \hat{\psi}_{-,k}(t_i) \end{pmatrix} e^{-\Gamma(t-t_i)} + \int_{-\infty}^{\infty} d\tau \sum_{p\sigma} V_p^* G_0^R(t,\tau) \begin{pmatrix} \langle \psi_{+,k}(\tau)|\sigma\rangle \\ \langle \psi_{-,k}(\tau)|\sigma\rangle \end{pmatrix} \times \hat{b}_{k\sigma p}(t_i) e^{-i\omega_p(\tau-t_i)-\Gamma(t-\tau)}, \quad \text{(A12)}$$

where the first term vanishes in $t_i \to -\infty$. Now, the field operator $\hat{\psi}$ is expressed by the bath operator $\hat{b}$ at the infinite past. As the bath fermions are in equilibrium at the infinite past, we can evaluate the Green's functions of $\hat{\psi}$ by using

$$\{\hat{b}^\dagger_{k\sigma p}(t_i), \hat{b}_{k\sigma' q}(t_i)\} = \delta_{\sigma\sigma'}\delta_{pq}, \quad \text{(A13)}$$

$$\langle \hat{b}^\dagger_{k\sigma p}(t_i) \hat{b}_{k\sigma' q}(t_i)\rangle = \delta_{\sigma\sigma'}\delta_{pq} f_D(\omega_p). \quad \text{(A14)}$$

For the retarded Green's function, one can derive Eq. (17) as

$$G^R(t,t') = 2\Gamma \int_{-\infty}^{t'} d\tau\, G_0^R(t,t') e^{-\Gamma(t+t'-2\tau)} \quad \text{(A15)}$$

$$= G_0^R(t,t') e^{-\Gamma(t-t')} \quad \text{(A16)}$$

by using $\sum_p |V_p|^2 e^{-i\omega_p(\tau-\tau')} = 2\Gamma\delta(\tau-\tau')$ [see Eq. (A6)], $\sum_\sigma \langle \psi_{\alpha,k}(\tau)|\sigma\rangle\langle\sigma|\psi_{\beta,k}(\tau)\rangle = \delta_{\alpha\beta}$, and $G_0^R(t,\tau)[G_0^R(t',\tau)]^\dagger = iG_0^R(t,t')\Theta(t'-\tau)$ for $t > t'$. The expression for the lesser component, Eqs. (20) and (21), can also be derived using

$$\sum_p |V_p|^2 \langle \hat{b}^\dagger_{k\sigma p}(t_i) \hat{b}_{k\sigma p}(t_i)\rangle e^{-i\omega_p(\tau-\tau')} = 2\Gamma \int \frac{d\omega}{2\pi} f_D(\omega) e^{-i\omega(\tau-\tau')}. \quad \text{(A17)}$$

APPENDIX B: NONPERTURBATIVE CONTRIBUTION TO THE DRIFT EFFECT

As can be seen in Fig. 4(b), the drift effect described by the relaxation-time approximation (49) overestimates the height of the peak. This is due to the nonperturbative effect non-negligible around the band top.

The failure of the approximation is derived from the order-by-order evaluation of the gradient expansion, formally expressed by the exponential operator $\exp(-\partial_\Gamma\partial_\tau/2)$ in Eq. (46). The exact result is recovered by replacement of the expression

$$e^{-\partial_\Gamma\partial_\tau/2} \left. \frac{\varepsilon(t-\tau)-\varepsilon(t)}{2\Gamma} \right|_{\tau=0} \to \int_0^\infty d\tau\, e^{-2\Gamma\tau}[\varepsilon(t-\tau)-\varepsilon(t)]. \quad \text{(B1)}$$

Let us consider to apply the saddle-point (thimble) method to the τ integral. The saddle point must satisfy

$$-2\Gamma + \frac{\partial_t \varepsilon(t-\tau)}{\varepsilon(t)-\varepsilon(t-\tau)} = 0. \quad \text{(B2)}$$

When τ is so small that we can approximate the denominator by $\tau\partial_t\varepsilon(t-\tau)$, we obtain $\tau = 1/2\Gamma$, which recovers the result of the gradient expansion at the first order.

On the other hand, when $\varepsilon(t) = \varepsilon(-t)$ holds, $\tau = 2t + 1/2\Gamma$ is also an approximate solution:

$$\frac{\partial_t\varepsilon(t-(2t+1/2\Gamma))}{\varepsilon(t)-\varepsilon(t-(2t+1/2\Gamma))} = \frac{-\partial_t\varepsilon(t+1/2\Gamma)}{\varepsilon(t)-\varepsilon(t+1/2\Gamma)} \simeq 2\Gamma. \quad \text{(B3)}$$

While the contribution from this saddle point is negligible for large t due to the factor of $e^{-4\Gamma t}$, it can be relevant when t is small, i.e., when the tunneling process occurs.

Let us see this contribution from the additional saddle point using a specific example. For the Landau-Zener model, $\varepsilon(t) =$

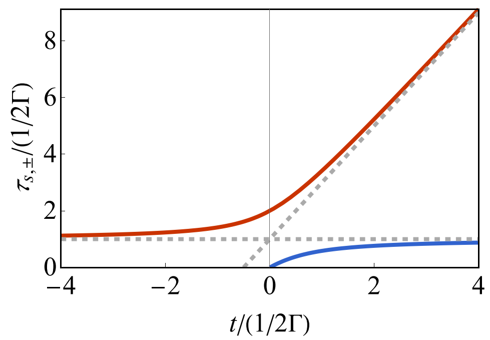

FIG. 10. The position of the saddle point $\tau_{s,\pm}$ (red for + and blue for −) as a function of t. Dashed lines are $\tau = 1/2\Gamma, 2t + 1/2\Gamma$.

$\sqrt{(vEt)^2+\delta^2}$, Eq. (B2) reads as

$$(t-\tau)^2 + \frac{t-\tau}{\Gamma} - t^2 + \frac{1}{4\Gamma^2}\frac{(t-\tau)^2}{(t-\tau)^2+(\delta/vE)^2} = 0. \tag{B4}$$

While this is a quartic equation, the last term can be neglected regardless of the value of $t-\tau$, if the adiabatic condition $1/\Gamma \ll \delta/vE$ is satisfied. We obtain

$$\tau_{s,\pm} \simeq t + \frac{1}{2\Gamma} \pm \sqrt{t^2 + \frac{1}{4\Gamma^2}} \tag{B5}$$

for the approximate position of the saddle point. As we show in Fig. 10, $\tau_{s,\pm}$ is significantly deviated from $\tau = 1/2\Gamma, 2t + 1/2\Gamma$ around the gap minimum $t = 0$, in addition to the fact that both of the two saddle points are relevant here. By applying the saddle-point method, we obtain

$$2\Gamma\int_0^\infty d\tau\, e^{-2\Gamma\tau}[\varepsilon(t-\tau)-\varepsilon(t)] \simeq \frac{E}{2\Gamma}[v_+(t)+v_-(t)\Theta(t)], \tag{B6}$$

where

$$v_\pm(t) = \frac{\sqrt{2\pi}}{e}\frac{\partial\varepsilon}{\partial k}\left(\sqrt{\frac{(\sqrt{4\Gamma^2t^2+1}\pm 1)^3}{(2\Gamma)^2\sqrt{4\Gamma^2t^2+1}}}\right)e^{-(2\Gamma t\pm\sqrt{4\Gamma^2t^2+1})}. \tag{B7}$$

We plot this result by a green line in Fig. 4, which accurately follows the numerical result.

APPENDIX C: TUNNELING AMPLITUDE EVALUATED BY THE LEFSCHETZ THIMBLE METHOD

In this Appendix, we explain how to calculate the asymptotic form of the tunneling amplitude $a_+(t)$, Eq. (8), using the Lefschetz thimble method [54].

1. Analytic continuation

First, we perform the analytic continuation of the integrand to rewrite Eq. (8) as a contour integral in the complex plane. We here introduce a complexified momentum $k - Et_1 \to z_1 \in \mathbb{C}$ (and $k - Et' \to z' \in \mathbb{C}$ in the phase factor) as the variable of integration.

We note that, in analytic continuation, we have to be careful on the treatment of the Berry connection difference $A_{++} - A_{--}$ in the phase factor of Eq. (7), which is not gauge invariant and not necessarily analytic. It is convenient to employ the alternative expression (10) for the integrand $W(t)$ with the shift vector $R = A_{++} - A_{--} - \partial_k \arg A_{+-}$ to circumvent this problem. This expression is analytic with respect to $k - Et_1$ in generic cases.

To avoid confusion, let us introduce $\tilde{A}_{+-}(z_1)$ and $\tilde{R}(z_1)$ as an analytic continuation of $|A_{+-}(k-Et_1)|$ and $R(k-Et_1)$, respectively. Then, Eq. (8) reads as

$$a_+(t) = ie^{i\arg A_{+-}(0)}\int_{C_0} dz_1 \tilde{A}_{+-}(z_1)e^{-i\int_0^{z_1}dz'(\Delta/E+\tilde{R})}, \tag{C1}$$

where $\Delta := \varepsilon_+ - \varepsilon_-$. C_0 denotes the half-line on the real axis $z_1 = x \in \mathbb{R},\ x : \mathrm{sgn}(E)\times\infty \to k - Et$.

There are exceptional cases where $|A_{+-}(k-Et_1)|$ and $R(k-Et_1)$ cannot be analytically continued. Such a situation happens when there exists a gauge choice such that $A_{++}(k) = A_{--}(k)$ and $A_{+-}(k) \in \mathbb{R}$ with $A_{+-}(^\exists k_a) = 0$ hold because the shift vector becomes $R(k) = \pi\sum_{k_a}\delta(k-k_a)$ (mod 2π). Still, in such cases, the combined quantity $|A_{+-}(k-Et_1)|e^{-i\int_0^{k-Et_1}dk'R} = \pm A_{+-}(k-Et_1)$ is analytic and does not depend on a gauge choice (up to the phase factor $e^{i\arg A_{+-}(0)}$). Thus, as an exceptional treatment, we introduce $\tilde{A}_{+-}(z_1)$ as an analytic continuation of $A_{+-}(k-Et_1)$ in the above-mentioned gauge instead, and set $\tilde{R}(z_1) = 0$.

2. Analytic property of 2 × 2 Hamiltonian

When the system is described by a 2 × 2 Hamiltonian, one can express the Hamiltonian using a pseudospin $\boldsymbol{\sigma}$ as

$$H(k) = d_0(k)I_{2\times2} + \boldsymbol{d}(k)\cdot\boldsymbol{\sigma}, \tag{C2}$$

with $\boldsymbol{\sigma}$ being the Pauli matrices. We assume that $\boldsymbol{d}$ is an analytic function of k. Then, the analytically continued variables are expressed as [18]

$$\Delta(z_1) = 2\sqrt{\boldsymbol{d}^2}, \tag{C3}$$

$$\tilde{A}_{+-}(z_1) = \frac{\sqrt{(\boldsymbol{d}\times\partial_k\boldsymbol{d})^2}}{2\boldsymbol{d}^2}, \tag{C4}$$

$$\tilde{R}(z_1) = \frac{(\boldsymbol{d}\times\partial_k\boldsymbol{d})\cdot\partial_k^2\boldsymbol{d}}{(\boldsymbol{d}\times\partial_k\boldsymbol{d})^2}\sqrt{\boldsymbol{d}^2}. \tag{C5}$$

Note that this expression includes the exceptional cases mentioned in the previous subsection, which correspond to the situation where $(\boldsymbol{d}\times\partial_k\boldsymbol{d})\cdot\partial_k^2\boldsymbol{d} \equiv 0$. Because $\tilde{R}$ is indeterminate at $k = k_a$ with $(\boldsymbol{d}\times\partial_k\boldsymbol{d})^2|_{k=k_a} = 0$, $\tilde{R}$ can be a singular function when the branch of $\sqrt{(\boldsymbol{d}\times\partial_k\boldsymbol{d})^2}$ for $\tilde{A}_{+-}$ is not appropriately chosen.

As the gap-closing point $z_1 = k_c$ with $\Delta(k_c) = 0$ plays a key role below, let us see properties of the above variables in the vicinity of $z_1 = k_c$. The gap-closing points appear in a pairwise manner [i.e., $\Delta(k_c) = \Delta(k_c^*) = 0$] because $\boldsymbol{d}(z_1^*) = [\boldsymbol{d}(z_1)]^*$ holds for Hermitian Hamiltonian $\boldsymbol{d}(k\in\mathbb{R}) \in \mathbb{R}^3$. For future convenience, we label the gap-closing points as $k_c^{(\pm1)}, k_c^{(\pm2)}, \ldots$ with $k_c^{(-n)} := (k_c^{(n)})^*$.

Since $\boldsymbol{d}^2$ is analytic, $\boldsymbol{d}^2$ should be expanded as $\boldsymbol{d}^2 = \alpha_1^{(n)}(z_1 - k_c^{(n)}) + \alpha_2^{(n)}(z_1 - k_c^{(n)})^2 + \cdots$, with $\alpha_1^{(n)} \neq 0$ for generic cases. Namely, the gap-closing point behaves as a square-root branch point

$$\Delta(z_1) \sim 2\sqrt{\alpha_1^{(n)}(z_1 - k_c^{(n)})}. \tag{C6}$$

In a similar way, we assume that $(\partial_k \boldsymbol{d})^2 = \beta_0^{(n)} + \beta_1^{(n)}(z_1 - k_c^{(n)}) + \cdots$ and $(\boldsymbol{d} \times \partial_k \boldsymbol{d}) \cdot \partial_k^2 \boldsymbol{d} = \eta_0^{(n)} + \eta_1^{(n)}(z_1 - k_c^{(n)}) + \cdots$ with $\eta_0^{(n)} \neq 0$. Then, we obtain

$$(\boldsymbol{d} \times \partial_k \boldsymbol{d})^2 = \boldsymbol{d}^2(\partial_k \boldsymbol{d})^2 - \frac{1}{4}(\partial_k \boldsymbol{d}^2)^2 \tag{C7}$$

$$= -\frac{1}{4}\alpha_1^{(n)2} + \alpha_1^{(n)}\big(\beta_0^{(n)} - \alpha_2^{(n)}\big)\big(z_1 - k_c^{(n)}\big) + \cdots, \tag{C8}$$

which leads to

$$\tilde{A}_{+-}(z_1) \sim \frac{\zeta_n \mathrm{sgn}(\mathrm{Im} k_c^{(n)})}{4i(z_1 - k_c^{(n)})}, \tag{C9}$$

$$\tilde{R}(z_1) \sim -\frac{4\eta_0^{(n)}}{\alpha_1^{(n)3/2}}\sqrt{z_1 - k_c^{(n)}} \tag{C10}$$

as leading-order expressions. $\zeta_n = \zeta_{-n} = \pm 1$ arises from the multivaluedness of $\sqrt{(\boldsymbol{d} \times \partial_k \boldsymbol{d})^2}$.

3. Saddle points

In order to apply the Lefschetz thimble method to the evaluation of Eq. (C1), we need to identify the position of the saddle point of $f(z_1)$ with $a_+(t) = ie^{i \arg A_{+-}(0)} \int_{C_0} dz_1 e^{f(z_1)}$. The saddle point is given as the solution of $\partial_{z_1} f(z_1) = 0$, i.e., it satisfies [see Eq. (C1)]

$$\frac{\partial}{\partial z_1} \ln \tilde{A}_{+-}(z_1) - i\frac{\Delta(z_1)}{E} - i\tilde{R}(z_1) = 0. \tag{C11}$$

For simplicity, we focus on $\tilde{R} = 0$ cases here. Results for $\tilde{R} \neq 0$ can be recovered by replacing Δ by $\Delta + E\tilde{R}$ in the final expression (see Ref. [18] for details).

For now, we consider $E > 0$. Since the second term diverges in $E \to 0$, the saddle-point approach the gap-closing point k_c. However, the first term also diverges in this limit since

$$\frac{\partial}{\partial z_1} \ln \tilde{A}_{+-}(z_1) \sim -\frac{\partial}{\partial z_1} \ln(z_1 - k_c) = -\frac{1}{z_1 - k_c} \tag{C12}$$

follows from Eq. (C9). Combined with Eq. (C6), the solutions of Eq. (C11), $z_1 = k_s$, at the leading order of E are given as

$$k_s^{(n,m)} - k_c^{(n)} \sim \left(\frac{E^2}{4\alpha_1^{(n)}}\right)^{1/3} e^{-\pi i + 4\pi i m/3} \tag{C13}$$

with $m = 0, 1, 2$. Due to the branch point, $\arg(k_s^{(n,m)} - k_c^{(n)})$ is mod 4π here. We note that, in contrast to the gap-closing point, $z_1 = (k_s^{(n,m)})^*$ is not the saddle point.

Let us evaluate the integral along the thimble (steepest descent) $\mathcal{J}_{n,m}$ associated with the saddle point $z_1 = k_s^{(n,m)}$. Since $f(z_1) - f(k_s^{(n,m)}) \in \mathbb{R}$ ($z_1 \in \mathcal{J}_{n,m}$) takes the maximal value at $z_1 = k_s^{(n,m)}$, the integral can be approximated as

$$\int_{\mathcal{J}_{n,m}} dz_1 e^{f(z_1)} \sim \int_{\mathcal{J}_{n,m}} dz_1 e^{f(k_s^{(n,m)}) + f''(k_s^{(n,m)})(z_1 - k_s^{(n,m)})^2/2} \tag{C14}$$

known as Laplace's method. Using

$$f''(k_s^{(n,m)}) \sim 3\left(\frac{2\alpha_1^{(n)2}}{E^4}\right)^{1/3} e^{-2\pi i m/3}, \tag{C15}$$

we can parametrize the steepest descent around $z_1 = k_s^{(n,m)}$ as $z_1 - k_s^{(n,m)} = (\alpha_1^{(n)})^{-1/3} x e^{-i\pi/2 + 4\pi i m/3}$ with $x \in \mathbb{R}$. Here, the direction of the contour around the saddle point $k_s^{(n,m)}$ is counterclockwise seen from the gap-closing point $k_c^{(n)}$. Combined with

$$e^{f(k_s^{(n,m)})} \sim i\zeta_n \mathrm{sgn}(\mathrm{Im} k_c^{(n)})\left(\frac{e^2\alpha_1^{(n)}}{16E^2}\right)^{1/3} e^{-4\pi i m/3} e^{-i\int_0^{k_c^{(n)}} dz' \Delta/E}, \tag{C16}$$

we obtain the asymptotic form of the integral as

$$\int_{\mathcal{J}_{n,m}} dz_1 e^{f(z_1)} \sim \zeta_n \mathrm{sgn}(\mathrm{Im} k_c^{(n)})\sqrt{\frac{\pi}{3}}\frac{e^{2/3}}{2} e^{-i\int_0^{k_c^{(n)}} dz' \Delta/E}. \tag{C17}$$

According to the exact result obtained by the DDP method [30], the prefactor $\sqrt{\pi/3}e^{2/3}/2 = 0.9965\ldots$ should be replaced by unity when the higher-order terms of the adiabatic perturbation theory are taken into account. Hereafter, we drop this prefactor.

When $E < 0$, the position of the saddle point around $k_c^{(n)}$ reads as

$$k_s^{(n,m)} - k_c^{(n)} \sim \left(\frac{|E|^2}{4\alpha_1^{(n)}}\right)^{1/3} e^{\pi i - 4\pi i m/3}, \tag{C18}$$

which corresponds to $(k_s^{(-n,m)})^*$ in the $E > 0$ case. The expression for the integral coincides with Eq. (C17) (note that E in the exponent becomes negative).

4. Tunneling amplitude

Let us apply the Lefschetz thimble method. Using Cauchy's integral theorem, we can deform the contour of the integral C_0 to a set of steepest descents [54,55]

$$C = \sum_{n,m} N_{n,m} \mathcal{J}_{n,m} - \Gamma(t), \tag{C19}$$

where the sum of the contour is defined as $\int_{\Gamma_1 \pm \Gamma_2} := \int_{\Gamma_1} \pm \int_{\Gamma_2}$. Here, $\Gamma(t)$ represents the steepest descent extending from the end point of the original contour C_0, i.e., $z_1 = k - Et$. The Morse index $N_{n,m} = \langle C_0, \mathcal{K}_{n,m}\rangle \in \{-1, 0, 1\}$ counts the (oriented) number of intersection between the original contour C_0 and the steepest ascent $\mathcal{K}_{n,m}$ associated with $k_s^{(n,m)}$. The orientation is defined as $\langle \mathcal{J}_{n,m}, \mathcal{K}_{n',m'}\rangle = \delta_{n,n'}\delta_{m,m'}$. Namely, if we neglect the contribution from $\Gamma(t)$, we can rewrite Eq. (C1) as a sum of Eq. (C17):

$$a_+(t) \sim i\sum_{n,m} N_{n,m}\zeta_n \mathrm{sgn}(\mathrm{Im} k_c^{(n)}) e^{-i\int_0^{k_c^{(n)}} dz' \Delta/E + i \arg A_{+-}(k)}. \tag{C20}$$

The remaining task is to identify the Morse index $N_{n,m}$. As the extension to the case of the multiple pairs of gap-closing points is straightforward, here let us assume that $N_{n,m} = \delta_{n,1}\delta_{m,0}N_{1,0}$ holds for $E > 0$, and the thimble $\mathcal{J}_{1,0}$ passes through $z_1 = k - Et_g^{(1)}$, i.e., the momentum at $t_1 = t_g^{(1)}$. Without calculating the steepest descent directly, whether the latter assumption is consistent can be verified by $\mathrm{Re}f(k_s^{(1,0)}) < \mathrm{Re}f(k - Et_g^{(1)})$, which must hold since they are on the same steepest ascent $\mathcal{K}_{1,0}$. The position of $z_1 = k - Et_g^{(1)}$ can also be identified by comparing $\mathrm{Im}f$. Note that, while $z_1 = k - Et_g^{(1)}$ coincides with the gap minimum for the Landau-Zener model, it is not necessarily the case for generic models [e.g., Eq. (78)]. In particular, t_g can be a function of E.

As the steepest ascent $\mathcal{K}_{1,0}$ has an intersection with C_0 when $t > t_g^{(1)}$ (as $z_1 = x \in [k - Et, +\infty)$ for $z_1 \in C_0$), the Morse index is given as

$$N_{1,0} = -\mathrm{sgn}\big(\mathrm{Im}k_c^{(1)}\big)\Theta\big(t - t_g^{(1)}\big). \tag{C21}$$

Here, the sign factor arises because C_0 is clockwise (counterclockwise) seen from the gap-closing point $k_c^{(1)}$ in the upper (lower) half-plane.

When $E < 0$, $N_{n,m} = \delta_{n,-1}\delta_{m,0}N_{-1,0}$ should hold since $-i\int_0^{k_c^{(-n)}} dz'\Delta/E = [-i\int_0^{k_c^{(n)}} dz'\Delta/|E|]^*$. Now, the original contour is $C_0 = (-\infty, k - Et]$, and is counterclockwise (clockwise) seen from $k_c^{(-1)}$ on the upper (lower) half-plane. Namely,

$$N_{-1,0} = \mathrm{sgn}\big(\mathrm{Im}k_c^{(-1)}\big)\Theta\big(t - t_g^{(1)}\big). \tag{C22}$$

We can summarize the above results as

$$a_+(t) \sim -i\zeta_1 \mathrm{sgn}(E)\sqrt{P_0}\Theta\big(t - t_g^{(1)}\big) \times e^{-i\mathrm{Re}\int_0^{k_c^{(1)}} dz'(\Delta/E+\tilde{R}) + i\arg A_{+-}(0)}, \tag{C23}$$

where

$$P_0 = e^{2\mathrm{Im}\int_0^{k_c^{(1)}} dz'[\Delta/|E| + \mathrm{sgn}(E)\tilde{R}]} \tag{C24}$$

is the tunneling probability.

When there is only one pair of the gap-closing points ($z = k_c^{(\pm 1)}$), we can set $t_g^{(1)} = 0$ by choosing k and $A_{+-}(0)$ such that the asymptotic form of the tunneling amplitude is real: $a_+(t) \sim \sqrt{P_0}\Theta(t)$. This expression is used in the main text for simplicity. We note that in such a case the interband matrix element $W(t)$ reads as

$$W(t) = i\zeta_1|E||A_{+-}(k - Et)|e^{-i\mathrm{Re}\int_{k_c^{(1)}}^{k-Et} dz'(\Delta/E+\tilde{R})}, \tag{C25}$$

which is used for the evaluation of the electric current in Sec. IV A ($\zeta_1 = 1$ is assumed in the main text).

APPENDIX D: EVALUATION OF THE TIME-DIFFERENCE FACTOR IN THE GRADIENT EXPANSION

In the evaluation of $e^{-\partial_s\partial_\tau - \partial_{s'}\partial_{\tau'}} I(s, s')$ with $t > t'$, we have to deal with $\langle T(t, t')| := e^{-\partial_s\partial_\tau} e^{-s(t-t')}\langle\overline{\psi}_{\alpha,k}(t,\tau)|F(s)$ with $s = \Gamma + i\varepsilon_\alpha(t)$, $\tau = 0$, and an arbitrary function $F(s)$. As we have mentioned in the main text, $e^{-s(t-t')}$ acts as a time-translation operator as

$$\langle T(t, t')| = e^{-s(t-t')}e^{-\partial_s\partial_\tau}e^{(t-t')\partial_\tau}\langle\overline{\psi}_{\alpha,k}(t,\tau)|F(s) \tag{D1}$$

$$= e^{-s(t-t')}e^{-\partial_s\partial_\tau}\langle\overline{\psi}_{\alpha,k}(t,\tau + t - t')|F(s). \tag{D2}$$

As $\tau + t - t'$ is no longer small, we need to shift the origin time of the slow component. Using the definition of the slow component (34), we obtain

$$\langle T(t, t')| = e^{-s(t-t')}e^{-\partial_s\partial_\tau}e^{i\varepsilon_\alpha(t)(\tau+t-t') - i\varepsilon_\alpha(t')\tau}\langle\overline{\psi}_{\alpha,k}(t',\tau)|F(s) \tag{D3}$$

$$= e^{-\Gamma(t-t')}e^{-\partial_s\partial_\tau}e^{-i[\varepsilon_\alpha(t) - \varepsilon_\alpha(t')]\partial_s}\langle\overline{\psi}_{\alpha,k}(t',\tau)|F(s), \tag{D4}$$

which can be rewritten as $\langle T(t, t')| = e^{-\partial_s\partial_\tau} e^{-\Gamma(t-t')}\langle\overline{\psi}_{\alpha,k}(t',\tau)|F(s)$ with $s = \Gamma + i\varepsilon_\alpha(t')$, $\tau = 0$. Using this expression, we obtain $[G^<_{\mathrm{ad}}(t, t')]_{\alpha\beta}$ as

$$[G^<_{\mathrm{ad}}(t, t')]_{\alpha\beta} = i2\Gamma e^{-\Gamma(t-t')}e^{-\partial_s\partial_\tau - \partial_{s'}\partial_{\tau'}} \times \frac{f_D(-is)}{s + s'}\langle\overline{\psi}_{\alpha,k}(t',\tau)|\overline{\psi}_{\beta,k}(t',\tau')\rangle, \tag{D5}$$

evaluated at $s = \Gamma + i\varepsilon_\alpha(t')$, $s' = \Gamma - i\varepsilon_\beta(t')$, $\tau = \tau' = 0$.

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