Non-adiabatic extension of the Zak phase and charge pumping in the Rice-Mele model

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(Dated: September 18, 2018)

In this study, the Landau-Zener transition method was applied to analytically investigate the Rice-Mele model and its non-adiabatic effect on the Zak phase and topological charge pumping. The effective lower band wave function picks up the St"ockelberg phase as well as the usual dynamical phase at avoided crossings. However, the St"ockelberg phase is averaged out by integrating over momentum space. Therefore, the probability of transitioning to the upper band is crucial. A non-adiabatic extension of the Zak phase is formulated, corresponding to the particle’s center of mass. From this extension, we further formulate the deviation from the quantization of topological charge pumping, and the breakdown of the quantization of topological charge pumping is quantitatively estimated for the broad parameter regime.

**Introduction.**— The theory of topological physics has been realized and is being investigated in detail in real experimental systems. In particular, systems of cold atoms in optical lattices have great possibility to simulate the physics since the systems have high parameter controllability, isolation from environment, and no impurity [1, 2]. Very recently, as a typical verification experiment in one-dimensional topological physics, topological charge pumping phenomena [3] have been realized in cold atoms in an one dimensional optical lattice [4, 5]. Therefore, again it is important to theoretically consider the topological physics and obtain new knowledge that has not been obtained so far.

Motivated by the experimental successes of topological charge pumping, various studies of 1D topological physics have been conducted in recent years. For example, the interaction effect for topological charge pumping under adiabatic conditions has been extensively studied [7–11]. The breakdown of the quantization of topological charge pumping has also been discussed [12, 13]. However, there are still some areas in this field that have not yet been investigated in detail.

In the past three decades, a large number of papers on theoretical topological physics have been submitted. The fundamental framework of topological physics has been theoretically developed [14, 15]. In general, the topological properties are based on the following assumptions: the bulk band gap exists, and the system is close to equilibrium, i.e., the model is under adiabatic conditions. This naturally brings up the question, “How does non-adiabaticity affect topological properties?” It is an important task to answer the question.

However, there is a lack of studies on the theoretical formulation and quantitative evaluation of non-adiabatic effects. Therefore, this paper discusses the effects of non-adiabaticity on topological properties using a typical model, focusing on the properties of the lower band ground state, especially the lower band topological properties of the system. The target model is the Rice-Mele (RM) model [16]. The RM model is a standard theoretical model of topological physics. It exhibits essential topological properties such as quantization of the Zak phase [17] and topological charge pumping [15, 16]. The RM model is much close to some experimental cold atom systems in an optical superlattice [5, 6, 18]. In this study, we primarily deal with the weakly non-adiabatic effect, where the probability of transition to the upper band is small. The non-adiabatic effect on non-interacting topological charge pumping is formulated by applying the Landau–Zener (LZ) transition well [19, 21]. A similar prescription is in Refs. [22, 24]. After formulating the non-adiabatic effect, the breakdown of the quantization of charge pumping is estimated using the obtained formula.

The aim of this work is different from that of previous works such as [23, 24], which focused on the St"ockelberg interferometer.

**Rice-Mele model.**— We start to consider the bulk momentum representation of the RM model. The Bloch vector representation is written by the following form

$$\hat{h}_{RM}(k,t) = d_x(k,t)\sigma_x + d_y(k,t)\sigma_y + d_z(k,t)\sigma_z,$$

where $\sigma_i$ ($i = x, y, z$) is the Pauli matrix; $d_x(k,t) = J_1(t) + J_2(t)\cos k$; $d_y(k,t) = J_2(t)\sin k$; and $d_z(k,t) = -\Delta_0 \cos \Omega t$, $J_1(t) = J_0 + \delta_0 \sin (\Omega t)$; $J_2(t) = J_0 - \delta_0 \sin (\Omega t)$; and $\Omega = 2\pi/T$. $T$ is the interval time of one cycle in the RM model. $J_0 > 0$, $\delta_0 > 0$ and $\Delta_0 > 0$. The energy spectrum is two band, given by $E_{\pm}(k,t) = \pm |d|$. When we focus on a certain wave number $k$, the $t$ dependent spectrum at $k$ can be regarded as a two-level system.
including some avoided crossings in a certain parameter regime (see Fig. 1 (b)). Assuming that the two bands never touch each other along one cycle $T$ and a specific case $\Delta_0 > 2\delta_0$ and $\delta_0 > \delta_0$, an avoided crossing appears around $t = T/4 \equiv t_1$ and $3T/4 \equiv t_2$ for any fixed $k$. At avoided crossings, a non-adiabatic transition may occur depending on the sweep speed $\Omega$. The energy landscape is shown in Fig. 1 (a). In what follows, the focus is placed on the energy landscape. Here, the LZ transition around the avoided crossing point for a certain fixed $k$ is considered. Around the avoided crossing points $t = t_1$ and $t_2$, the $\hat{h}_{\text{RM}}$ can be linearized in terms of $t$ as $t = t_1 \pm \delta t$ and $t = t_2 \pm \delta t$. The linearized Hamiltonian for $\hat{h}_{\text{RM}}$ is generally given in the following form:

$$\hat{h}_{\text{RM}}(k, \delta t) = A(k)\hat{\sigma}_x + B(k)\hat{\sigma}_y + \Delta_0 \delta t \hat{\sigma}_z. \quad (2)$$

Here, $A(k)$ and $B(k)$ are $k$-dependent functions (independent of $t$), and the $O(\delta t^2)$ order terms are dropped. By introducing the rotational transformation of the Pauli matrix, $\hat{h}_{\text{RM}}(k, t)$ can be transformed into the following form:

$$\hat{h}_{\text{RM}}(k, \delta t) = -\sqrt{A^2(k) + B^2(k)}\hat{\sigma}_x - \Delta_0 \delta t \hat{\sigma}_z, \quad (3)$$

where $\hat{\sigma}_{x(z)}$ is a rotated $x(z)$-component Pauli matrix. $\hat{h}_{\text{RM}}(k, \delta t)$ is the canonical form for applying the LZ transition formula. The above linearized form is justified around the avoided crossing points $t = t_1$ and $t_2$.

Now, the general LZ application form is defined as $\hat{h}_{\text{RM}}(k, \delta t) \equiv -\Delta(k)\hat{\sigma}_x - \frac{\Delta_0}{2}\hat{\sigma}_z$, then $\Delta(k) \equiv 2\sqrt{A^2(k) + B^2(k)}$, $v = 2\Delta_0\Omega$. Here, the adiabaticity parameter is introduced by $\hat{\delta}(k) = \Delta^2(k)/(4v)$. The details of the transformation for Eq. (3) are given in Appendix A.

Landau-Zener transition.— The LZ transition is the transition between the lower and upper band at avoided crossings. The linearized RM model $\hat{h}_{\text{RM}}(k, \delta t)$ of Eq. (3) has two avoided crossings: at $t = t_1$ and $t = t_2$. Here, the LZ transition matrix $\Gamma(k)$ can be introduced around the avoided crossing points. The matrix is known by the following form $^{[21,22,26]}$

$$\Gamma(k) = \left[ \begin{array}{c} \sqrt{1 - p_{\text{LZ}}(k)}e^{-i\gamma_{\text{nb}}(k)} \\ p_{\text{LZ}}(k) \end{array} \right],$$

$$\Gamma_{\text{LZ}}(k) = \left[ \begin{array}{c} \sqrt{1 - p_{\text{LZ}}(k)}e^{-i\gamma_{\text{nb}}(k)} \\ p_{\text{LZ}}(k) \end{array} \right],$$

where $\gamma_{\text{nb}}(k)$ is the St"uckelberg phase (a non-adiabatic berry phase), and $p_{\text{LZ}}(k) = e^{2\pi\hat{\delta}(k)}$ is the probability of transition from the lower to the upper band. In the matrix $\Gamma(k)$, the diagonal terms are lower-to-lower and upper-to-upper state transitions, and the off-diagonal terms are lower-to-upper state transition and vice versa. The detailed derivation of $\Gamma(k)$ is given in Appendix B. The origin of the St"uckelberg phase is purely mathematical. To solve the Schr"odinger equation for $\hat{h}_{\text{RM}}(k, \delta t)$, the special function needs to be introduced (Weber function) $^{[26]}$. At this time, the St"uckelberg phase appears. Then the coefficients of the wave function obtain the non-trivial phase factor through avoided crossings. The explicit form of the St"uckelberg phase is given by the following form: $^{[25,26]}

$$\gamma_{\text{nb}}(k) = \pi + \hat{\delta}(k)\ln \hat{\delta}(k) - 1 + \arg(\Gamma(1 - i\hat{\delta}(k))). \quad (5)$$

where $\Gamma(z)$ is the imaginary gamma function. As explained in detail below, the adiabatic-impulse approximation is employed. Therefore, the matrix $\Gamma(k)$ acts on very narrow time intervals, $t_1 - 0 \leq t \leq t_1 + 0$ and $t_2 - 0 \leq t \leq t_2 + 0$. Accordingly, the dynamical phase is not accumulated in such a narrow time regime.

**Time evolution in adiabatic-impulse approximation.**— The adiabatic-impulse approximation is applied to the band structure. Here, we assume a very narrow avoided crossing regime is assumed for the target parameter regime in the RM model. In other time regimes, the system is under adiabatic conditions, i.e., only the non-adiabatic effect around the avoided crossings is considered. The schematic figure of the adiabatic-impulse approximation is shown in Fig. 2. Under these conditions, the time evolution of the wave function expanded by the instantaneous eigenstates of the two bands is considered, with a focus on the change in the lower band occupation. First, we prepare the wave function constituted by the linear combination of the instantaneous lower and upper band periodic function,

$$|\Psi(k, t)\rangle = c_1(k, t)|u_1(k, t)\rangle + c_2(k, t)|u_2(k, t)\rangle,$$

where $c_{1(2)}(k, t) \in \mathbb{C}$ is the coefficient of the lower (upper) band instantaneous eigenstate, and $|u_1(2)(k, t)\rangle$ is determined by the Bloch theorem at time $t$. Then, the time evolution of $c_{1(2)}(k, t)$ can be calculated from the adiabatic-impulse approximation. The temporal gauge for $|\Psi(k, t)\rangle$ is taken here $^{[27]}$. In the adiabatic regime, the time evolution is obtained by considering the follow-
ing unitary operator:
\[
U(k, t, t') = \begin{bmatrix}
e^{-i \int_{t'}^{t} E_{+}(k, t'')dt''} & 0 \\
0 & e^{-i \int_{t'}^{t} E_{-}(k, t'')dt''}
\end{bmatrix}.
\] (7)

The operator \(U\) acts on the coefficient vector \((c_2, c_1)^t\) and gives the adiabatic time evolution from \(t'\) to \(t''\). On the other hand, around the avoided crossing corresponding to the impulse regime, the time evolution of \(c(2)_{t}(k, t)\) can be obtained by acting upon the LZ transition matrix \(\Gamma(k)\). The coefficient \(c(2)_{t}(k, t)\) is connected to \(c(1)_{t}(k, 0)\) by acting the unitary operator \(U\) and the LZ transition matrix \(\Gamma(k)\). Accordingly, by introducing the coefficient vector defined by \(c(k, t) = (c_2(k, t), c_1(k, t))^t\), the one cycle time evolution can be written down in the following form:
\[
c(k, T) = U(k, T, t_2 + 0)\Gamma(k)U(k, t_2 - 0, t_1 + 0) \times (\Gamma(k)U(k, t_1 - 0, 0)c(k, 0)).
\] (8)

From this relation, the time evolution of the wave function \(\Psi(k, t)\) can be obtained. The time evolution includes the interband transition effect. This is undeniably a non-adiabatic effect. In this study, we put \(c_1(k, 0) = 1\) as an initial state. For the time evolution described by Eq. (8), only the dynamics of the lower band, i.e., the dynamics of \(c_1(k, t)\), is of interest. Thus, the leakage from the lower-to-upper bands may be regarded as dissipation from the lower band state \(22\), and the dynamics of \(c_2(k, t)\) can be ignored. Then, the lower band component \(c_1(k, T)\) is effectively given by
\[
c_1(k, T) = [1 - \mathbb{P}_{LZ}]e^{2\gamma_{nb}(k)}e^{i \int_{0}^{T} E_{-}(k, t'')dt''} \times c_1(k, 0) + \mathcal{O}(\mathbb{P}_{LZ}(k)^2).
\] (9)

Here, since the focus is placed on the weak transition to the upper band, i.e., \(\mathbb{P}_{LZ}(k)\) is small, we take into account first order of \(\mathbb{P}_{LZ}(k)\). It is noted that in Eq. (9) the coefficient \(c_1(k, t)\) picks up the St"uckelberg phase \(\gamma_{nb}(k)\) twice since the LZ transition matrix \(\Gamma(k)\) acts twice along the time evolution.

*Non-adiabatic extension of the Zak phase.*— By using the representation of Eq. (9), a non-adiabatic extension of the Zak phase can be formulated. The Zak phase is known to correspond to the charge polarization in a strong correlated electron system \(28, 29\). To formulate the extended form, first by using the lower band sector of \(\Psi(k, t)\), the lower band Wannier function \(W(t)\) \(15\) is introduced:
\[
W(t) = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{imk} |m\rangle \otimes c_1(k, t)|u_1(k, t)\rangle = \int_{-\pi}^{\pi} \frac{dk_{\parallel} p_{LZ}(k)}{2\pi} \otimes c_1(k, t)|u_1(k, t)\rangle.
\] (10)

Here, \(m\) is a lattice site; \(|m\rangle\) is the state where a particle is localized at site \(m\), and \(N\) is the total number of lattice sites in one spatial period. From \(W(t)\), the center of mass (CM) is given as \(\langle W(t)|\dot{x}|W(t)\rangle\), where \(\dot{x}\) is the position operator of the particle as viewed from the continuous space. In general, the CM is known to correspond to the Zak phase \(4, 13\). Hereafter, the CM is denoted by \(P(t)\). If \(c_1(k, t) = 1\), i.e., the initial state at \(t = 0\) is in the lower band insulating state, the CM at \(t = T\), \(P(T)\) can be given as follows (a detailed calculation is given in Appendix C):
\[
P(T) = P_0(T) - \delta P(T)
\]
\[
+ \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \mathbb{P}_{LZ}(k) \partial_k \mathbb{P}_{LZ}(k)
\]
\[
- \frac{1}{2\pi} \int_{-\pi}^{\pi} dk [1 - \mathbb{P}_{LZ}]^2 \partial_k \gamma_{nb}(k),
\] (11)

\[
P_0(T) = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \langle u_1(k, T)|\partial_k u_1(k, T)\rangle,
\] (12)

\[
\delta P(T) = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \gamma_{d}(k)\langle u_1(k, T)|\partial_k u_1(k, T)\rangle,
\] (13)

where \(\gamma_{d}(k) = 2\mathbb{P}_{LZ}(k) - \mathbb{P}_{LZ}^2(k)\), \(P_0(T)\) is the adiabatic Zak phase, and \(\delta P(T)\) is regarded to be the non-adiabatic effect inducing the deviation from the adiabatic Zak phase. Furthermore, the third and fourth terms of the right-hand side of Eq. (11) get to zero because the integrants are periodic for \(k\) and odd about \(k = 0\). As a result, the effect of the St"uckelberg phase is averaged out for the \(k\) integral. Therefore, \(P(T) = P_0(T) - \delta P(T)\). The \(P(T)\) can be regarded as a non-adiabatic extension of the Zak phase.

Here, it should be noted that, as seen from the expression of Eq. (11), the St"uckelberg phase only deforms the integrant in the above integral compared to the adiabatic case, i.e., it only deforms the Berry curvature locally, and if for Eq. (11) the adiabatic limit is taken from \(\mathbb{P}_{LZ}(k) \to 0\), the \(P(T)\) smoothly connects to \(P_0(t)\).

From Eq. (11), the total deviation \(P(T) - P(0)\) is further considered, which is the total shift of the CM during one pumping cycle. The total deviation \(P(T) - P(0)\) is just the total pumped charge current \(15\) denoted by \(Q\). The \(Q\) is given in the following form:
\[
Q = P(T) - P(0) = C_N - \delta Q,
\] (14)

\[
C_N = \frac{i}{2\pi} \int_{0}^{T} dt \int_{-\pi}^{\pi} dk \partial_k \langle u_1(k, t)|\partial_k u_1(k, t)\rangle,
\] (15)

\[
\delta Q = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \gamma_{d}(k)\langle u_1(k, T)|\partial_k u_1(k, T)\rangle,
\] (16)

where \(C_N\) is the lower band Chern number in the temporal gauge \(15\) and known to take an integer value \(3, 31\). \(\delta Q\) represents the non-adiabatic effect. The case \(\delta Q \neq 0\) indicates the breakdown of the quantization of \(Q\).

*Breakdown of the quantization of \(Q\).*— Now, the extent of breakdown in the quantization of \(Q\) is quantitatively evaluated. Here, it should be noted that the formulation of Eq. (11) does not cover all non-adiabatic regimes \(0 \leq \Omega \leq \infty\), and the driving regime considered is weakly non-adiabatic, where \(\mathbb{P}_{LZ}(k)\) is small, i.e., Eq. (9) is valid. For such a situation, the form of Eq. (10) is justifies.
In the base of the assumption, we plot the values of $Q$ on the $J_0 - \Omega$ and $\Delta_0 - \Omega$ planes in Figs. 3(a) and (b). Also, figure 3(c) shows the behavior of $Q$ with increasing driving frequency $\Omega$. The vertical dashed lines represent the qualitative signature of the breakdown point of the quantization of $Q$, defined as $\Omega = 4\delta_0$. For all cases, the minimum of $\Omega$ is 0.01.

In the base of the assumption, we plot the values of $Q$ in the $J_0 - \Omega$ plane with $\delta_0 = 0.2$ and $\Delta_0 = 1$. (b) The values of $Q$ in the $\Delta_0 - \Omega$ plane with $J_0 = 0.25\pi d_0\delta_0 = 0.2$. (c) The detailed behavior of $Q$ with increasing driving frequency $\Omega$. The vertical dashed lines represent the qualitative signature of the breakdown point of the quantization of $Q$, defined as $\Omega = 4\delta_0$. For all cases, the minimum of $\Omega$ is 0.01.

FIG. 3. Deviation from the quantization of charge pumping. (a) The values of $Q$ in the $J_0 - \Omega$ plane with $\delta_0 = 0.2$ and $\Delta_0 = 1$. (b) The values of $Q$ in the $\Delta_0 - \Omega$ plane with $J_0 = 0.25\pi d_0\delta_0 = 0.2$. (c) The detailed behavior of $Q$ with increasing driving frequency $\Omega$. The vertical dashed lines represent the qualitative signature of the breakdown point of the quantization of $Q$, defined as $\Omega = 4\delta_0$. For all cases, the minimum of $\Omega$ is 0.01.

In the base of the assumption, we plot the values of $Q$ on the $J_0 - \Omega$ and $\Delta_0 - \Omega$ planes in Figs. 3(a) and (b). Also, figure 3(c) shows the behavior of $Q$ in typical parameter sets. The parameter spaces satisfy the conditions $\Delta_0 > 2\delta_0$ and $J_0 > \delta_0$. In calculating the $Q$ at each point shown in Figs. 3(a) and (b), most values of $p_{\text{LZ}}(k)$ on the BZ are less than 0.5. The dependence upon $\Omega$ can be clearly observed from the results displayed in Figs. 3(a), (b), and (c): as $\Omega$ increases, $\delta Q$ increases, and $Q$ deviates from unity. Here, it is interesting and important to estimate the breakdown by comparing the minimum band gap $\Delta E$ of the instantaneous spectrum with $\Omega$. In general, the adiabatic condition is expected to break down under the condition $\Delta E < \Omega$. This expectation is qualitative. Let us consider how accurate this qualitative expectation is. In the system under study, the energy gap depends on $k$. Thus, we pick up the minimum energy gap $\Delta E_{\text{km}}$ in the BZ at the avoided crossing, and $\Delta E_{\text{km}}$ is used for comparison. For the target parameter regime, the minimum energy gap, obtained from the energy spectrum at $k = \pm \pi$, is $\Delta E_{\text{km}} = 4\delta_0$. From this value of $\Delta E_{\text{km}}$, the qualitative breakdown of the quantization of $Q$ is expected to start at $\Omega = 4\delta_0$. We plot the qualitative breakdown in Fig. 3(c). Here, interestingly the result in Fig. 3(c) shows that the breakdown of the quantization of $Q$ obtained by Eq. (14) starts earlier than the qualitative breakdown point $\Omega = 4\delta_0$. This fact seems to be established in a wide parameter area as seen from the result in Fig. 3(a) and (b). Here, the black dotted lines in Figs. 3(a) and (b) represent the qualitative breakdown line.

About experimental verification.—We mention the verification of our result for real experimental cold atom systems. Measuring the CM is not so difficult because there is an established experimental method, e.g., the band mapping method in a real experimental system [9, 10]. The RM model has already been implemented in an optical super lattice system [11] and there also exists a continuous RM model [12]. Their experimental systems can reach our considering parameter regime in terms of $J_0$, $\delta_0$ and $\Delta_0$ in the RM model in this study. However, there are still some experimental limitations. For example, perfect full occupation of the lower band state has not been realized [13] due to the finite temperature effect. Harmonic trapping also breaks the translational symmetry of the system. These obstacles must be overcome before a high-accuracy observation of the CM shift is carried out, since the deviation from the quantization value in our estimation is at most 1 to 2 percent in weakly non-adiabatic regime.

Conclusion.—A weakly non-adiabatic effect for the Zak phase and topological charge pumping in the RM model has been discussed. The dynamics of the lower band state has been formulated by applying the adiabatic impulse approximation and using the LZ transition method. Using the wave function obtained from the dynamics after one cycle $T$, a simple formula describing a non-adiabatic extension of the Zak phase and total pumped current has been derived. This formula of the total pumped current $Q$ indicates the breakdown of the quantization of topological charge pumping. Furthermore, the breakdown of the quantization of charge pumping has been quantitatively evaluated for some broad parameter regimes and compared the starting point of the breakdown with the qualitative expectation value obtained from the minimum band gap. We found that the breakdown starts earlier than the qualitative starting point in a wide parameter area in the RM model. The breakdown can be measured in future experiments in a cold atoms in an optical lattice.

The general idea and prescription used to derive Eq. (14) are an effective way to investigate the non-adiabatic effect of wider topological models.

ACKNOWLEDGMENTS

Y. K. acknowledges the support of a Grant-in-Aid for JSPS Fellows (No.17J00486).

APPENDIX A: HAMILTONIAN TRANSFORMATION FOR THE LZ TRANSITION

We show a transformation for the RM Hamiltonian around an avoided crossing. The RM model needs to be transformed into the suitable form for the LZ transition.
Thus, the rotational transformation of the Pauli matrix is considered. In general, the rotated Pauli matrix $\tilde{\sigma}_j$ along the $i$-component spin ($i = 1(x), 2(y), 3(z)$) axis is given by the following formula:

$$\tilde{\sigma}_j(\theta) = e^{-i\theta \bar{\sigma}_j} \sigma_j e^{i\theta \bar{\sigma}_j} = \tilde{\sigma}_j \cos \theta + \epsilon_{ijk} \tilde{\sigma}_k \sin \theta. \quad (A1)$$

Here, $\theta$ is the rotational angle along the $i$-axis.

Consider a Hamiltonian described by $H(k) = A(k)\tilde{\sigma}_x + B(k)\tilde{\sigma}_y$, where $A(k)$ and $B(k)$ are functions of $k$. $H(k)$ can be reduced to a form including only one component of the Pauli matrix by acting the rotational transformation of the Pauli matrix along the $z$-component spin axis, with the angle $\theta_z = \arctan[A(k)/B(k)] + \pi$:

$$H(k) = A(k)\tilde{\sigma}_x + B(k)\tilde{\sigma}_y \rightarrow -\sqrt{A(k)^2 + B(k)^2}\tilde{\sigma}_x. \quad (A2)$$

Through this transformation, Eq. (4) is obtained from Eq. (2).

**APPENDIX B: DERIVATION OF THE LZ TRANSITION MATRIX**

In this appendix, we show how to derive the LZ transition matrix of Eq. (1). To this end we follow and summarize ref. [21]. We start with the following two level Hamiltonian:

$$h_{LZ}(t) = -\frac{\Delta}{2}\tilde{\sigma}_x - \frac{V t}{2}\tilde{\sigma}_z, \quad (A3)$$

where $\Delta$, $V$, and $t$ are the off-set energy, sweeping velocity, and time, respectively. To match the Hamiltonian of Eq. (3) with Eq. (A3), $\Delta \leftrightarrow \Delta(k)$ and $v \leftrightarrow V$ need to be considered. Since the two-level system Hamiltonian $h_{LZ}(t)$ is considered, the time-dependent wave function can be written as $|\psi(t)\rangle = b_+(t)|\rho_+(t)\rangle + b_-|\rho_-(t)\rangle$, where $\sum_{a=\pm} |b_a(t)|^2 = 1$, and $|\rho_+(t)\rangle$ is an upper (lower) instantaneous eigenstate at $t$.

The goal is to find the approximated time evolution of the wave function of the two-level system. To obtain the dynamics of the two-level system described by $h_{LZ}(t)$, the basis $|\phi_{\uparrow}(t)\rangle$ for $\tilde{\sigma}_z$ is further introduced. The bases are defined as $\tilde{\sigma}_z|\phi_{\downarrow}(t)\rangle = \pm|\phi_{\uparrow}(t)\rangle$. To solve the Schrödinger equation, it is more effective to use the bases $|\phi_{\downarrow}(t)\rangle$ than the instantaneous eigenstate $|\rho_{\uparrow}(t)\rangle$. By using the bases $|\phi_{\downarrow}(t)\rangle$, the time dependent wave function can be set as $|\psi(t)\rangle = a_1(t)|\phi_{\uparrow}\rangle + a_2(t)|\phi_{\downarrow}\rangle$. Then, from the Hamiltonian $h_{LZ}(t)$, the Schrödinger equation for $a_1(t)$ is given as follows ($\hbar = 1$):

$$i\frac{d}{dt} \begin{bmatrix} a_1(t) \\ a_2(t) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -V t & -\Delta \\ \Delta & V t \end{bmatrix} \begin{bmatrix} a_1(t) \\ a_2(t) \end{bmatrix}. \quad (A4)$$

This equation can be solved approximately. Through the following variable transformation from $t \rightarrow Z$, the equation of Eq. (A4) is transformed into the Weber equations [21]:

$$\frac{d^2a_1(Z)}{dZ^2} + (2\delta + i + Z^2)a_1(Z) = 0, \quad (A5)$$

$$Z = \sqrt{\frac{V}{2} t}, \quad \delta = \frac{\Delta^2}{4V}. \quad (A6)$$

Here, $Z$ is the redefined time, and $\delta$ is the adiabaticity parameter. It is known that an asymptotic solution of Eq. (A5) can be constructed using the parabolic cylinder functions [33]. In particular, an asymptotic form of the solution for $|Z| \gg 1$ (it is assumed that $V$ is large $V \gg 1$) is clearly given as follows [21]:

For $Z \ll -1$,

$$\begin{bmatrix} a_1(Z) \\ a_2(Z) \end{bmatrix} \approx \begin{bmatrix} A_+ \Xi_1 e^{i\Phi(-Z)} \\ (-e^{-\frac{\delta}{2}} A_+ + e^{\frac{\delta}{2}} A_-) \Xi_2 e^{-i\Phi(-Z)} \end{bmatrix}. \quad (A7)$$

For $Z \gg 1$,

$$\begin{bmatrix} a_1(Z) \\ a_2(Z) \end{bmatrix} \approx \begin{bmatrix} A_- \Xi_1 e^{i\Phi(Z)} \\ (-e^{-\frac{\delta}{2}} A_+ + e^{\frac{\delta}{2}} A_-) \Xi_2 e^{-i\Phi(Z)} \end{bmatrix}. \quad (A8)$$

Here, $A_\pm$ is an arbitrary constant factor, and $\Phi(Z)$, $\Xi_1$, and $\Xi_2$ are given as [21]:

$$\Phi(Z) = \frac{Z^2}{2} + \delta \ln(\sqrt{Z}). \quad (A9)$$
\[ \Xi_1 = \sqrt{2\pi} \left[ \Gamma(1 + i\delta) \right]^{-1} e^{-\frac{i\eta}{2}}, \]  
\[ \Xi_2 = \frac{1}{\sqrt{\delta}} e^{i\frac{\eta}{2} - \Phi}, \]  

where \( \Phi(Z) \) is a dynamical phase, which will later be obtained by integrating the linearized spectrum of \( h_{LZ}(Z) \), and \( \Gamma(z) \) is the complex gamma function.

The LZ transition matrix is constructed using Eqs. (A7) and (A8). First, the LZ transition matrix \( T_{LZ} \) is introduced, including the following four components:

\[ T_{LZ} = \begin{bmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{bmatrix}. \]  

The components are complex numbers. Now, the components \( N_{11}, N_{12}, N_{21}, \) and \( N_{22} \) of \( T_{LZ} \) must be determined.

To determine these components, the bases are switched to instantaneous eigenstate bases \( | \phi_+^{(t)} \rangle \), and the time evolution of the coefficient \( b(t) = (b_+(t), b_-(t))^t \) from \( t = -t_0 \) to \( t = t_0 \) is considered. The \( b(t_0) \) can be connected from the \( b(-t_0) \) by acting the operators as follows:

\[ b(t_0) = U(t_0, +0) T_{LZ} U(-0, -0) b(-t_0), \]  

where \( U(t_a, t_b) \) is the unitary operator introduced by Eq. (7). It is assumed that the LZ transition occurs in very narrow time interval. This operation is the adiabatic-impulse approximation. Here, as shown in Eq. (A4), the time evolution of the Hamiltonian \( h_{LZ}(t) \) is solved in terms of the basis \( | \phi_+^{(t)} \rangle \).

Therefore, the relation can be immediately expected at \( V|t| \gg \Delta \). At \( V|t| \gg \Delta \), the off-diagonal terms of Eq. (A3) can be dropped. Then, \( b(t) \) can be related with \( a(t) \). For \( t = -t_0 \), the instantaneous eigenstate can be reduced to \( | \rho_+ \rangle = | \phi_+ \rangle \) and \( | \rho_- \rangle = | \phi_- \rangle \). On the other hand, for \( t = t_0 \), \( | \rho_+ \rangle = -| \phi_+ \rangle \) and \( | \rho_- \rangle = | \phi_- \rangle \). As a result, 

\[ (b_+, b_-)^t = (a_1, a_2)^t \]  

is obtained for \( t = -t_0 \), and 

\[ (b_+, b_-)^t = (-a_2, a_1)^t \]  

is obtained for \( t = t_0 \). By substituting the relations into Eq. (A13) under the assumption \( |Z| \gg 1 \), the following relation about \( a(Z_0) \) is obtained:

\[ a(Z_0) = \left[ \begin{array}{c} -a_2(Z_0) \\ a_1(Z_0) \end{array} \right] = \left[ \begin{array}{cc} e^{-i\eta(0,t_0)} & 0 \\ 0 & e^{i\eta(0,t_0)} \end{array} \right] \left[ \begin{array}{cc} N_{11} & N_{12} \\ N_{21} & N_{22} \end{array} \right] \left[ \begin{array}{c} e^{-i\eta(0,t_0)} \\ e^{i\eta(0,t_0)} \end{array} \right] \left[ \begin{array}{c} a_1(-Z_0) \\ a_2(-Z_0) \end{array} \right]. \]  

Here, \( \eta(t_0, 0) = \int_{0}^{t_0} \frac{\Delta^2}{2} + (Vt)^2 \)dt. The \( \eta(t_0, 0) \) can be calculated by using the spectrum of \( h_{LZ}(Z) \) and an integration formula, \( \int \sqrt{x + a^2} \)dx = \( x\sqrt{x^2 + a^2} + a^2 \ln \left[ x + \sqrt{x^2 + a^2} \right] \). After some calculations,

\[ \eta(t_0, 0) = \left[ \frac{Z_0^2}{2} + \delta \ln \sqrt{Z_0} \right] + \frac{1}{2} \left[ \delta - \delta \ln \delta \right]. \]  

The first bracket term in the right-hand side is a dynamical phase, and the remaining bracket term in the right-hand side is known to be part of the St"uckelberg phase \( \Delta Z \).

Now, the components \( N_{11}, N_{12}, N_{21}, \) and \( N_{22} \) of matrix \( T_{LZ} \) are determined. By substituting Eqs. (A7) and (A8) into Eq. (A14), the following equation is obtained:

\[ \left[ \begin{array}{c} e^{i\Phi(Z_0)} A_+ - e^{-i\Phi(Z_0)} A_- \\ \Xi_2 e^{-i\Phi(Z_0)} A_+ \end{array} \right] = \left[ \begin{array}{c} e^{-2i\eta(0,t_0)} N_{11} e^{i\Phi(Z_0)} - N_{12} e^{-2i\eta(0,t_0)} e^{-i\Phi(Z_0)} A_+ + N_{21} e^{i\Phi(Z_0)} - e^{2i\eta(0,t_0)} N_{22} e^{-2i\eta(0,t_0)} e^{-i\Phi(Z_0)} A_- \\ N_{21} e^{i\Phi(Z_0)} - e^{2i\eta(0,t_0)} N_{22} e^{-2i\eta(0,t_0)} e^{-i\Phi(Z_0)} \end{array} \right]. \]  

Here, the above equation is an identity for \( A_+ \) and \( A_- \). Therefore, the four conditions and then all of the components of \( T_{LZ} \) are obtained. \( N_{22} \) is calculated as a concrete example. From Eq. (A16),

\[ N_{22} = \Xi_2 e^{-\eta(0,t_0)} e^{-2i\eta(0,t_0)}. \]
The following part of the right-hand side in the above equation is calculated by using some properties of the gamma function:

\[
\Xi_1 \Xi_2^{-1} e^{-\pi/2\delta} = \frac{\sqrt{2\pi\delta}}{\Gamma(1+i\delta)} e^{-(\pi/2)\delta} e^{i\pi/4} = \frac{\sqrt{2\pi\delta} \Gamma(1-i\delta)}{\Gamma(1+i\delta) \Gamma(1-i\delta)} e^{-(\pi/2)\delta} e^{i\pi/4}
\]

\[
= \frac{\sqrt{2\pi\delta} |\Gamma(1-i\delta)|}{\sinh(\pi\delta)} e^{-(\pi/2)\delta + i\pi/4 + i\arg(\Gamma(1-i\delta))}
\]

\[
= (1 - e^{-i2\pi\delta}) \left[ \frac{|\Gamma(1-i\delta)| e^{i(\pi/2)\delta}}{\sqrt{2\pi\delta}} \right] e^{i\pi/4 + i\arg(\Gamma(1-i\delta))}
\]

\[
= (1 - e^{-i2\pi\delta})^{1/2} e^{i\pi/4 + i\arg(\Gamma(1-i\delta))}.
\] (A18)

Here,

\[
\frac{|\Gamma(1-i\delta)| e^{i(\pi/2)\delta}}{\sqrt{2\pi\delta}} = \frac{\delta |\Gamma(-i\delta)| e^{i(\pi/2)\delta}}{\sqrt{2\pi\delta}}
\]

\[
= \sqrt{\frac{\delta}{2\pi}} \left[ \frac{\pi}{(-\delta) \sinh(-\pi\delta)} \right]^{1/2} e^{i\pi/2}\delta = (1 - e^{-i2\pi\delta})^{-1/2}.
\] (A19)

As a result,

\[
N_{22} = \sqrt{1 - p_{LZ}} \exp \left[ i \left( \frac{\pi}{4} + \delta |\ln \delta - 1| + \arg(\Gamma(1-i\delta)) \right) \right].
\] (A20)

\(N_{11}, N_{12},\) and \(N_{21}\) can be obtained by the same procedure.

**APPENDIX C: CALCULATION OF THE CENTER OF MASS**

The center of mass at \(t = T\) is calculated using Eq. (11). To begin with, \(\hat{x}|W(T)\rangle\) is

\[
\hat{x}|W(T)\rangle = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \sum_{m} e^{-km} |m\rangle \otimes \partial_{k} \left[ c_{1}(k,T) |u_{1}(k,T)\rangle \right]
\]

\[
= \frac{i}{2\pi} \int_{-\pi}^{\pi} \sum_{m} e^{-km} |m\rangle \otimes \left[ \partial_{k}c_{1}(k,T) |u_{1}(k,T)\rangle + c_{1}(k,T) |\partial_{k}u_{1}(k,T)\rangle \right].
\] (A21)

This equation is multiplied by \(\langle W(T)\rangle\), and the following equation is obtained:

\[
\langle W(T)\rangle |\hat{x}|W(T)\rangle = \frac{i}{2\pi} \int_{-\pi}^{\pi} dkc_{1}^{*}(k,T) \partial_{k}c_{1}(k,T) + \frac{i}{2\pi} \int_{-\pi}^{\pi} dk |c_{1}(k,T)|^{2} \langle u_{1}(k,T) | \partial_{k}u_{1}(k,T) \rangle).
\] (A22)

Here, \(c_{1}(k,T)\) of Eq. (11) is substituted with Eq. (A22), and the periodic condition \(E_{-}(\pi, T) = E_{-}(\pi, T)\) is used. The center of mass is given as follows:

\[
\langle W(T)\rangle |\hat{x}|W(T)\rangle = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \left[ (1 - p_{LZ}(k))(-\partial_{k}p_{LZ}(k)) + 2(1 - p_{LZ}(k))^{2} (i\partial_{k}\gamma_{nd}(k)) \right]
\]

\[
+ \frac{i}{2\pi} \int_{-\pi}^{\pi} dk (1 - p_{LZ}(k))^{2} \langle u_{1}(k,T) | \partial_{k}u_{1}(k,T) \rangle).
\] (A23)

The above equation corresponds to Eq. (11).

In general, considering two functions for \(k, f(k), g(k)\), which satisfy \(f(k) = f(-k)\) and \(g(k) = g(-k)\),

\[
\int_{-\pi}^{\pi} dk f(k) \partial_{k}g(k) = \int_{0}^{\pi} dk f(k) \partial_{k}g(k) + \int_{-\pi}^{0} dk f(k) \partial_{k}g(k)
\]

\[
= \int_{0}^{\pi} dk f(k) \partial_{k}g(k) - \int_{0}^{\pi} dk f(k') \partial_{k}g(k') = 0.
\] (A24)

From this and the periodicity of \(p_{LZ}(k)\) and \(\gamma_{nd}(k)\) for \(k\), the first term in the right-hand side of Eq. (A23) vanishes.
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