Nonadiabatic Control of Geometric Pumping

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We study nonadiabatic effects of geometric pumping. With arbitrary choices of periodic control parameters, we go beyond the adiabatic approximation to obtain the exact pumping current. We find that a geometrical interpretation for the nontrivial part of the current is possible even in the nonadiabatic regime. The exact result allows us to find a smooth connection between the adiabatic Berry phase theory at low frequencies and the Floquet theory at high frequencies. We also study how to control the geometric current. Using the method of shortcuts to adiabaticity with the aid of an assisting field, we illustrate that it enhances the current.

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Introduction.—In 1983, Thouless discovered a phenomenon called geometric pumping. In electron systems, a slow periodic variation of control parameters gives a nontrivial current without bias [1,2]. The mechanism is described by the geometric Berry phase [3], which shows that it is a topological phenomenon. While the original study was applied to a one-dimensional system with a lattice potential, we can find various processes driven by Berry phase in mesoscopic quantum dot systems [4], and in stochastic systems described by the classical master equation [5–13] or the quantum master equation [14–20]. The experimental verification can be seen in many works [21–28]. The pumped system is also interesting from a viewpoint of stochastic thermodynamics. In small systems with appreciable fluctuations, by using the method of full counting statistics [29–31], we can examine the fluctuation theorem [32–35].

Although the phenomenon is a purely dynamical one, the theoretical description relies on the static picture. The use of the adiabatic approximation is crucial not only for theoretical analysis but also for establishing the geometrical picture. Since the adiabatic approximation is justified only at the case when the parameter change is sufficiently slow, it is important to ask how much the adiabatic description makes sense for nonideal fast manipulations. It is known that the geometric phase for nonadiabatic systems is still useful [36–38], but we have not fully understood the corresponding phenomenon for the geometric pumping. A breakdown of the fluctuation theorem in the adiabatic regime was reported in [39–41] and it is an interesting problem to study how the nonadiabatic effect changes the result. While nonadiabatic effects in the geometric pumping have been studied in many works [42–48], we need a nonperturbative analytical method to obtain a clear picture of the nonadiabatic pumping. Establishing the nonadiabatic description is important not only for finding the fundamental properties but also for realizing efficient control of systems in applications.

In this Letter, we treat the stochastic master equation to study the nonadiabatic effect. We propose a method incorporating the effect to the solution of the equation. We find that a geometrical interpretation is still possible for the pumping current under modulation with arbitrary speed, which allows us to discuss controlling the nontrivial contributions to the current.

Master equation.—The system we treat in this Letter is coupled to several reservoirs to provide particle transfer. The process is stochastic and the time evolution of the system is described by the master equation

$$\frac{d}{dt}|p(t)\rangle = W(t)|p(t)\rangle. \qquad (1)$$

$|p(t)\rangle$ is represented as $|p(t)\rangle = [p_1(t), p_2(t), \ldots]^T$ where the ith component represents the probability of the ith microscopic state of the system being occupied. $W(t)$ is a transition-rate matrix with each component $W_{ij}(t)$ representing the transition rate from state j to state i at t. The system is coupled to reservoirs and $W(t)$ is decomposed as $W(t) = \sum_\nu W^{(\nu)}(t)$ where ν labels the reservoirs. $W_{ij}^{(\nu)}(t)$ is defined in a similar way. The off diagonal components of

$W^{(\nu)}(t)$ are nonnegative and the diagonal components must satisfy the condition $\sum_i W_{ij}^{(\nu)}(t) = 0$. To find a nontrivial contribution to the current, we modulate the system periodically without the average bias between the left ($\nu = L$) and right ($\nu = R$) couplings.

Assuming that the transition-rate matrix is diagonalizable, we represent the solution of the master equation by an orthonormal set of the instantaneous left and right eigenstates of $W(t)$, denoted as $\{\langle\phi_n(t)|, |\phi_n(t)\rangle\}$ with the eigenvalues $\{\epsilon_n(t)\}$ where n is the index specifying the corresponding eigenvalue. Since the transition-rate matrix is non-Hermitian, the left eigenstate is not equal to the conjugate of the right eigenstate. See the Supplemental Material [49] for details. We write

$$|p(t)\rangle = \sum_n C_n(t) e^{\int_0^t dt' \epsilon_n(t')} |\tilde{\phi}_n(t)\rangle, \tag{2}$$

$$|\tilde{\phi}_n(t)\rangle = e^{-\int_0^t dt' \langle\phi_n(t')|\dot{\phi}_n(t')\rangle} |\phi_n(t)\rangle, \tag{3}$$

where the dot denotes the time derivative. $|\tilde{\phi}_n(t)\rangle$ represents the eigenstate with a geometric "phase" which is an analog of the Berry phase, or the Aharonov-Anandan phase, in quantum mechanics [3,36–38]. This state vector has the property of the gauge invariance, that is the invariance under the transformation $[\langle\phi_n(t)|, |\phi_n(t)\rangle] \to [\langle\phi_n(t)|R_n^{-1}(t), R_n(t)|\phi_n(t)\rangle]$ where $R_n(t) \in \mathbb{R}$ with $R_n(0) = 1$. To find the geometric current, we use the adiabatic approximation, namely, the time dependence of the coefficients $C_n(t)$ is neglected. The physical meaning of this approximation is that the system follows an instantaneous eigenstate of the system when the time variation of $W(t)$ is small. To examine effects of fast driving, we need to treat mixing between different eigenstates.

The master equation has, at least, one stationary state with zero eigenvalue. For simplicity, we assume that this stationary state, denoted with the label $n = 1$, is unique. Then, $C_1(t) = 1$ and the other states with $n \neq 1$ have negative eigenvalues $\epsilon_n(t) < 0$. The equation for $C_n(t)$ with $n \neq 1$ is given by

$$\frac{dC_n(t)}{dt} e^{\int_0^t dt' \epsilon_n(t')} + \sum_{m(\neq n)} C_m(t) e^{\int_0^t dt' \epsilon_m(t')} \langle\tilde{\phi}_n(t)|\dot{\tilde{\phi}}_m(t)\rangle = 0. \tag{4}$$

When we consider a slow modulation, we expect that the time evolution does not make transitions to different eigenstates. This means that the overlap in the second term on the left hand side of Eq. (4), $\langle\tilde{\phi}_n(t)|\dot{\tilde{\phi}}_m(t)\rangle = \langle\tilde{\phi}_n(t)|\dot{W}(t)|\tilde{\phi}_m(t)\rangle/[\epsilon_m(t) - \epsilon_n(t)]$ with $m \neq n$, is negligible. In addition, in systems described by the master equation, we have an exponentially decaying factor $e^{\int_0^t dt' \epsilon_m(t')}$ for $m \neq 1$, which further justifies the approximation. The factor is absent for $m = 1$ with $\epsilon_1(t) = 0$ and it is reasonable to keep this term. Then, neglecting the contributions with $m \neq 1$, we obtain a nonadiabatic approximate solution

$$|p(t)\rangle \simeq |\tilde{\phi}_1(t)\rangle + \sum_{n\neq 1} (\delta_n(t) + C_n e^{\int_0^t dt' \epsilon_n(t')}) |\tilde{\phi}_n(t)\rangle, \tag{5}$$

where C_n is a constant determined from the initial condition, and

$$\delta_n(t) = -\int_0^t dt' \langle\tilde{\phi}_n(t')|\dot{\tilde{\phi}}_1(t')\rangle e^{\int_{t'}^t dt'' \epsilon_n(t'')}. \tag{6}$$

See the Supplemental Material [49] for details of the derivation. The adiabatic approximation for $|p(t)\rangle$ is obtained by setting $\delta_n(t) = 0$. $\delta_n(t)$ depends on the whole history of the time evolution and represents nonadiabatic effects. This function is not periodic in t even when $W(t)$ is periodic. However, it rapidly falls into a periodic behavior at large t. $\delta_n(t)$ falls into the same trajectory after transient evolutions at first several periods [49]. A similar function appears in quantum systems to treat a nonreciprocal effect for Landau-Zener tunneling [50], where the function was evaluated by using a contour integral in a complex plane.

Pumping current.—Using the solution of the master equation (1), Eq. (5), we can evaluate the current through the system. Formally, it can be defined by introducing a counting field [9]. To make the discussion concrete, we treat the two-state case where the number of the components of $|p(t)\rangle$ is two and Eq. (5) becomes the exact solution. When we set that the first (second) component of $|p(t)\rangle$ represents the probability that the system is empty (filled), the average current through the system from the left to right reservoirs is given by $J = \lim_{T\to\infty}(1/T) \int_0^T dt(W_{12}^{(R)}(t)p_2(t) - W_{21}^{(R)}(t)p_1(t))$ [49]. In this expression, the long-time averaged current is independent of the initial condition and of the last term in the brackets of Eq. (5). This implies that we can calculate the exact current by using the approximated state in Eq. (5) even if we go beyond the two-state case. The neglected term in Eq. (4) incorporates an exponentially decaying factor and does not contribute to the current after the second modulation cycle.

In the adiabatic approximation for the current, J is given by the sum of the dynamical part J_d and the geometric part J_g. The former is given by the dynamical "phase" term and the latter by the geometric term [9]. In the present treatment, the dynamical part is the same and the geometric part is separated into the adiabatic part and the nonadiabatic part $J_g = J_{\mathrm{ad}} + J_{\mathrm{nad}}$. The explicit form of each part is respectively given by

$$J_d = \frac{1}{T_0}\int_0^{T_0} dt \frac{k_{\rm in}^{(L)}(t)k_{\rm out}^{(R)}(t) - k_{\rm out}^{(L)}(t)k_{\rm in}^{(R)}(t)}{k_{\rm in}(t)+k_{\rm out}(t)}, \quad (7)$$

$$J_{\rm ad} = \frac{1}{T_0}\int_0^{T_0} dt p^{(R)}(t)\frac{d}{dt}p_{\rm out}(t), \quad (8)$$

$$J_{\rm nad} = \lim_{T\to\infty}\frac{1}{T_0}\int_T^{T+T_0} dt p^{(R)}(t)\frac{d}{dt}\delta_2(t), \quad (9)$$

where we put $W_{12}(t)=k_{\rm out}(t)=k_{\rm out}^{(L)}(t)+k_{\rm out}^{(R)}(t)$, $W_{21}(t)=k_{\rm in}(t)=k_{\rm in}^{(L)}(t)+k_{\rm in}^{(R)}(t)$, and $p^{(R)}(t)=[k_{\rm in}^{(R)}(t)+k_{\rm out}^{(R)}(t)]/[k_{\rm in}(t)+k_{\rm out}(t)]$, $p_{\rm out}(t)=k_{\rm out}(t)/[k_{\rm in}(t)+k_{\rm out}(t)]$. Here, $k_{\rm in}(t)$ represents the incoming rate and $k_{\rm out}(t)$ the outgoing rate, and the superscript denotes the coupling to the left or right reservoir. We consider the case where each parameter is represented as a function of ωt with the period $T_0=2\pi/\omega$. The dynamical part is independent of ω and is negligible for no-biased pumping. $J_{\rm ad}$ is represented by using the geometric term and is proportional to ω. Therefore, within the adiabatic approximation, the current is enhanced by increasing ω, though the expression is only valid in the limit $\omega\to 0$. This behavior is interfered by the presence of $J_{\rm nad}$. We stress that the above form of the current is exact. By knowing the explicit form of the nonadiabatic part, we can optimize the current as we discuss below. It is a straightforward task to find a similar expression of the current in general multilevel systems.

Geometrical picture.—The nonadiabatic part, Eq. (9), has a similar form to the adiabatic part, Eq. (8), which leads to a geometrical interpretation. Suppose that we control the system by using two time-dependent periodic parameters $\boldsymbol{k}(t)=[k_1(t),k_2(t)]$. The adiabatic current $J_{\rm ad}$ arises only when the orbit of $\boldsymbol{k}$ encloses a finite area. The adiabatic current is represented by a flux penetrating the surface. This geometrical picture is also applied to the nonadiabatic part. We extend the parameter space and introduce a third axis $k_3=\delta_2$. Although δ_2 is a function of k_1 and k_2, we leave it independent for the moment and use the relation after the calculation. In the extended space $\tilde{\boldsymbol{k}}=(\boldsymbol{k},k_3)$, J_g is written as

$$J_g = \oint_{\tilde{C}} d\tilde{\boldsymbol{k}}\cdot\boldsymbol{A}(\boldsymbol{k}) = \int_{\tilde{S}} d\tilde{\boldsymbol{S}}(\tilde{\boldsymbol{k}})\cdot\boldsymbol{B}(\boldsymbol{k}), \quad (10)$$

where $\tilde{C}$ represents the closed contour in the $\tilde{\boldsymbol{k}}$ space and $\boldsymbol{A}(\boldsymbol{k})$ is the "gauge field":

$$\boldsymbol{A}(\boldsymbol{k}) = \frac{\omega}{2\pi}\begin{pmatrix} p^{(R)}\partial_1 p_{\rm out} \\ p^{(R)}\partial_2 p_{\rm out} \\ p^{(R)} \end{pmatrix}. \quad (11)$$

This vector function is independent of k_3. The adiabatic part is represented by the first and second components of $\boldsymbol{A}$ and the nonadiabatic part is by the third component. We can

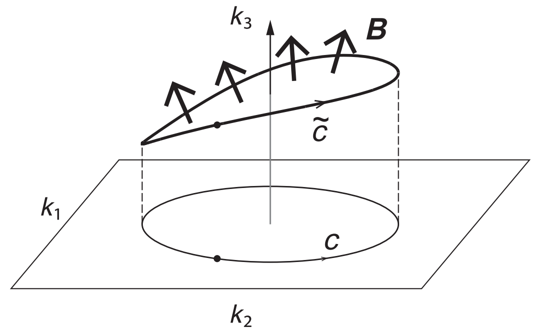

FIG. 1. Trajectories in the parameter space. When we consider a periodic trajectory C in the (k_1,k_2) plane, k_3 is changed accordingly and we have a closed contour $\tilde{C}$. The current is determined by the magnetic field penetrating a surface $\tilde{S}$ specified by $\tilde{C}=\partial\tilde{S}$.

introduce the corresponding "magnetic field" $\boldsymbol{B}(\boldsymbol{k})=\nabla\times\boldsymbol{A}(\boldsymbol{k})$. The third (first and second) component of $\boldsymbol{B}(\boldsymbol{k})$ corresponds to the adiabatic (nonadiabatic) part. Using the Stokes theorem, we obtain the last expression in Eq. (10). The integral represents a surface integral where the surface $\tilde{S}$ is defined by using the closed contour $\tilde{C}$. This is pictorially represented as in Fig. 1. This surface is not unique and we can consider a convenient choice. This geometrical representation does not mean that the result is independent of the control speed. $\boldsymbol{B}$ is written in terms of purely geometric variables k_1 and k_2, but the third axis is determined by the dynamics.

Structure of the transition-rate matrix.—Since the current is linear in W, the decomposition of the current can also be applied to the transition-rate matrix as $W(t)=W_d(t)+W_g(t)$. The explicit form of $W_g(t)$ is given by

$$W_g(t) = (\dot{p}_{\rm out}(t)+\dot{\delta}_2(t))\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}. \quad (12)$$

The solution of the master equation $|p(t)\rangle$ is given by the adiabatic state of $W_d(t)$. $W_g(t)$ is interpreted as a counterdiabatic term known in shortcuts to adiabaticity [49,51–56]. It has a geometrical meaning [57], which is consistent with the geometrical interpretation for J_g.

Using the decomposition of $W(t)$, we can also find a relation to the Floquet theory. The time-evolution operator $U(t)=T\exp\left(\int_0^t dt' W(t')\right)$, where T is the time-ordering operator, is written at $t=T_0=2\pi/\omega$ as $U(T_0)=e^{T_0W_F}$ to define the effective transition-rate matrix W_F. Since the solution of the master equation is characterized as a stationary state of W_F, W_F must be related to $W_d(t)$. In fact, we can write

$$W_F = \frac{\bar{k}}{k_{\rm in}(0)+k_{\rm out}(0)}\frac{W_d(T_0)-e^{-2\pi\bar{k}/\omega}W_d(0)}{1-e^{-2\pi\bar{k}/\omega}}, \quad (13)$$

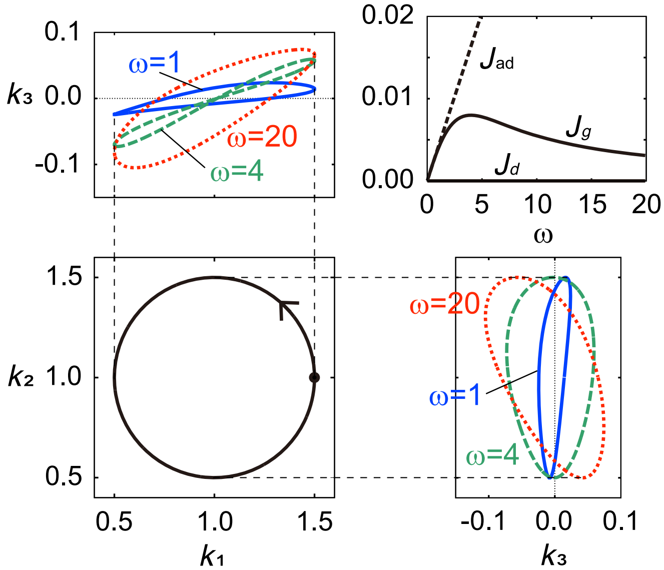

FIG. 2. The frequency dependence of the current (top right) and trajectories in the parameter space at several values of ω. We set $k_1 = k_{\rm in}^{(L)}(t) = k_0(1+\frac{1}{2}\cos\omega t)$, $k_2 = k_{\rm in}^{(R)}(t) = k_0(1+\frac{1}{2}\sin\omega t)$, $k_{\rm out}^{(L)} = k_0$, and $k_{\rm out}^{(R)} = k_0$. All the quantities are plotted in unit of k_0.

where $\bar{k} = (1/T_0)\int_0^{T_0} dt[k_{\rm in}(t) + k_{\rm out}(t)]$. See the Supplemental Material [49] for details. In the adiabatic limit $\omega \to 0$, we find $W_F \sim W_d(T_0)$, which is consistent with the above consideration. In the opposite limit, the function can be expanded in powers of $1/\omega$, which is equivalent to the Floquet-Magnus expansion [58,59]. This relation is useful since we can find the decomposition of $W(t)$ by using the expansion at high frequencies.

Nonadiabatic effects on geometric current.—A typical behavior of the current is shown in Fig. 2. We use a similar protocol as used in Ref. [9]. Since we use a protocol with no net bias, the dynamical current is negligibly small. At low ω, the adiabatic current is dominant, which is proportional to ω. It is considerably disturbed by the nonadiabatic effects at high ω. The total current approaches zero as $1/\omega$, as is found from the Floquet-Magnus expansion. Thus, the nonadiabatic effect inhibits the linearity of the geometric current with respect to ω.

The behavior of the current is understood from the geometrical picture. Since the third component of the flux $B_3(\boldsymbol{k}) = \partial_1 A_2(\boldsymbol{k}) - \partial_2 A_1(\boldsymbol{k})$ determines the adiabatic current, the geometric current coincides with the adiabatic current if the trajectory $\tilde{C}$ is parallel to the (k_1, k_2) plane. In Fig. 2, we see that, as the frequency increases, the trajectory is distorted from a flat plane to cancel out the adiabatic part.

In Fig. 3, we plot the current when the trajectory C is slightly deformed while keeping the dynamical current invariant (see the Supplemental Material [49] for details). We still observe nonadiabatic effects affecting linear growth. To keep the adiabatic current, we need to design

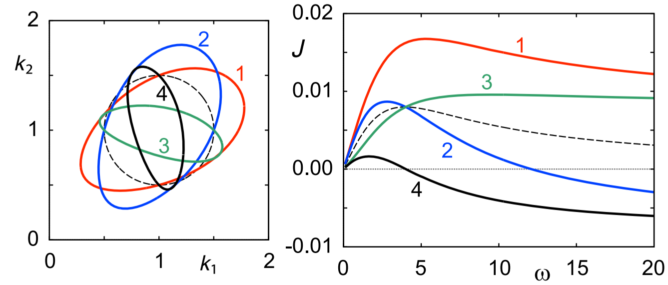

FIG. 3. Left: Elliptic trajectories (1–4) keeping the dynamical current invariant. The dashed line represents the original protocol used in Fig. 2. Right: The corresponding total current. The dynamical part is zero in each protocol. See the Supplemental Material [49] for details.

the protocol such that the plane is kept parallel to the (k_1, k_2) plane. Since we cannot choose the trajectory $\tilde{C}$ arbitrary, this is a difficult problem in general.

Assisted adiabatic pumping.—To obtain a desirable enhancement of the geometric current, we use a method of counterdiabatic driving. We introduce the counterdiabatic term into the original transition matrix so that the adiabatic state of the original matrix becomes the exact solution. Although the idea is implemented for the Schrödinger equation for isolated quantum systems, the generalization to other equations such as the master equation and the Fokker-Planck equation is a straightforward task. We can find several applications in previous studies [60–63].

In the master equation, the transition-rate matrix is diagonalized as $W(t) = \sum_n \epsilon_n(t)|\phi_n(t)\rangle\langle\phi_n(t)|$ and the adiabatic state is defined by Eq. (2) with time-independent coefficients $\{C_n\}$. We modify the transition-rate matrix $W(t) \to W(t) + W_{\rm CD}(t)$ so that the solution of the modified master equation is given by the adiabatic state. The counterdiabatic term $W_{\rm CD}(t)$ is given by

$$W_{\rm CD}(t) = \sum_{m,n(m\neq n)} |\phi_m(t)\rangle\langle\phi_m(t)|\dot{\phi}_n(t)\rangle\langle\phi_n(t)|. \quad (14)$$

For the two-state case, $W_{\rm CD}(t)$ can be explicitly written as

$$W_{\rm CD}(t) = \dot{p}_{\rm out}(t)\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}. \quad (15)$$

This form is slightly different from $W_g(t)$ in Eq. (12). We see that the addition of the counterdiabatic term is obtained by replacements $k_{\rm in}(t) \to k_{\rm in}(t) - \dot{p}_{\rm out}(t)$ and $k_{\rm out}(t) \to k_{\rm out}(t) + \dot{p}_{\rm out}(t)$. Since these variables represent the transition rates, $|\dot{p}_{\rm out}(t)|$ cannot be large and the method fails for rapid changes of parameters.

The inclusion of the counterdiabatic term ensures that the exact solution of the master equation is given by the adiabatic state of the original transition-rate matrix. $k_{\rm in}(t)$ and $k_{\rm out}(t)$ are, respectively, represented by the sum of the left and right parts and we still have degrees of freedom to

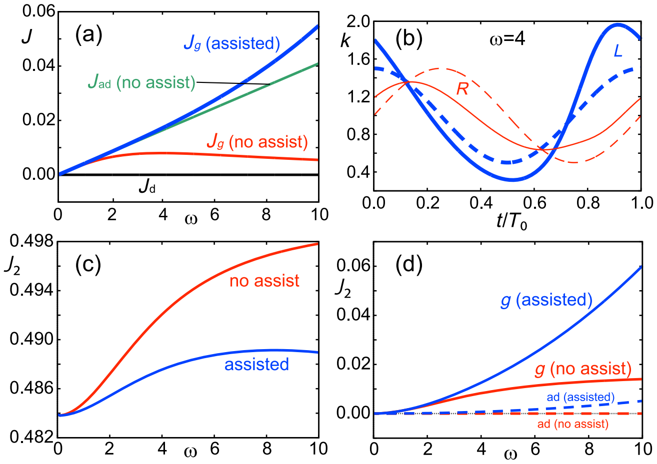

FIG. 4. Assisted adiabatic pumping. We use the same protocol as used in Fig. 2 for the original system before assist. (a) The geometric current with an assisting field is represented by the blue line. The other lines are the same as in the top right panel of Fig. 2. (b) Dashed lines representing protocols before assist are changed to solid lines by the assisting field. Bold blue lines represent the left amplitude $k_{\rm in}^{(L)}$ and thin red lines do the right amplitude $k_{\rm in}^{(R)}$. We take $\omega = 4.0$. (c) The current fluctuations before or after assist [49]. (d) The geometric part (solid lines) and the adiabatic part (dashed lines) of the current fluctuations.

implement the counterdiabatic term. We can use them to keep the dynamical part of the current invariant and to set that the geometric part of the current is given by the adiabatic part of the original current without assist [49].

Although the above procedure works in principle, we have no clear picture on how the assisting field enhances the current. In addition, the manipulation is restricted in realistic situations and we cannot control each element in the transition-rate matrix independently. In our choice in the above examples, we set that $k_{\rm out}$ is time independent. The introduction of the counterdiabatic term inevitably breaks this condition. To keep the time independence of $k_{\rm out}$, we can consider scaling. After the introduction of the counterdiabatic term, we write the transition-rate matrix as

$$W(t) + W_{\rm CD}(t) = \left(1 + \frac{\dot{p}_{\rm out}(t)}{k_{\rm out}}\right) \begin{pmatrix} -\frac{1-\frac{\dot{p}_{\rm out}(t)}{k_{\rm in}(t)}}{1+\frac{\dot{p}_{\rm out}(t)}{k_{\rm out}}} k_{\rm in}(t) & k_{\rm out} \\ \frac{1-\frac{\dot{p}_{\rm out}(t)}{k_{\rm in}(t)}}{1+\frac{\dot{p}_{\rm out}(t)}{k_{\rm out}}} k_{\rm in}(t) & -k_{\rm out} \end{pmatrix}. \tag{16}$$

The prefactor of the right-hand side is positive and is scaled out by the redefinition of the timescale as $d\tilde{t} = dt[1 + \dot{p}_{\rm out}(t)/k_{\rm out}]$. We still have a degree of freedom to decompose the new component $k_{\rm in}(t)$ into the left and right parts and use it to keep the dynamical current invariant. In this case, the geometric current is not equal to the adiabatic current in the original system and is not proportional to the frequency. However, we confirm that the deviation is not so large and the geometric current can be kept growing as a function of the frequency. The result is shown in Fig. 4 (see the Supplemental Material [49] for details). The obtained protocol indicates that we need to shift the oscillation of the assisting field to the left compared to the original one to prevent the deviation. The required field becomes larger when we consider faster driving and the control fails at some frequency where $|\dot{p}_{\rm out}(t)|$ exceeds the threshold.

In Fig. 4, we also plot the current fluctuation that is decreasing by the introduction of the assisting field. Generally, the counterdiabatic term leads to an increase in the energy cost characterized by the fluctuation and a broadening of the work distribution [64,65]. This expectation, i.e., the increment of the fluctuation for the geometric part under the assisting field, is verified as can be seen on the bottom right panel of Fig. 4. Although we cannot control the dynamical part of the fluctuation as we did for the average, we find a decrease of the total fluctuation as a result of the decrease of the dynamical fluctuation. The suppression of the fluctuations implies the stability of the assisted driving. A variational formulation of the counterdiabatic driving for quantum systems also indicates a stable driving [66]. In the Supplemental Material [49], we examine several examples to confirm the stability by slightly modifying the amplitudes in several ways.

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Note added in the proof.—After the completion of this work, we learned about Ref. [67] where a similar method is used for adiabatic pumping.

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