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Adiabatically steered open quantum systems: Master equation and optimal phase

J. Salmilehto,^{1,*} P. Solinas,¹ J. Ankerhold,² and M. Möttönen^{1,3}

¹Department of Applied Physics/COMP, Aalto University, P.O. Box 14100, FI-00076 Aalto, Finland

²Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, DL-89069 Ulm, Germany

³Low Temperature Laboratory, Aalto University, P.O. Box 13500, FI-00076 Aalto, Finland

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We introduce an alternative way to derive the generalized form of the master equation recently presented by J. P. Pekola *et al.* [Phys. Rev. Lett. **105**, 030401 (2010)] for an adiabatically steered two-level quantum system interacting with a Markovian environment. The original derivation employed the effective Hamiltonian in the adiabatic basis with the standard interaction picture approach but without the usual secular approximation. Our approach is based on utilizing a master equation for a nonsteered system in the first superadiabatic basis. It is potentially efficient in obtaining higher-order equations. Furthermore, we show how to select the phases of the adiabatic eigenstates to minimize the local adiabatic parameter and how this selection leads to states which are invariant under a local gauge change. We also discuss the effects of the adiabatic noncyclic geometric phase on the master equation.

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I. INTRODUCTION

The adiabatic theorem [1,2] has been one of the workhorses of quantum physics for decades. It states that if the external control parameters of the system Hamiltonian vary slowly enough, the system remains very accurately in one of its initial instantaneous eigenspaces. As slowly varying quantum systems appear in many fields of physics, a multitude of applications for the theorem exists. In recent years, adiabatically steered quantum systems have attracted a lot of interest due to their connection to geometric phases in cyclic evolution [3–5]. These phases provide a potential alternative to quantum information processing [6–8] in which the quantum gates are implemented by purely geometric means [9-18]. This geometric quantum computation has been shown to offer inherent robustness against control errors [19-22] due to the fact that geometric phases depend only on some global geometric properties. Different ways to describe geometric phases in open systems have been introduced [23-28] and methods to account for the effect of the environment on the system evolution have been studied [19,29-36] along with techniques to reduce the unwanted noise. However, a consistent description of the combined effect of adiabatic steering and noise was missing until recently, when a master equation was introduced in Refs. [37] and [38].

In the approach of Ref. [37], it was shown that the typically applied secular approximation [32,39] is not suitable in describing adiabatic evolution. Taking into account all the relevant contributions leads to a master equation which ensures relaxation to a proper basis and shows that the ground-state dynamics are not influenced by zero-temperature Markovian noise in the adiabatic limit. Thus the system exhibits inherent robustness. The master equation derived in Ref. [37] was generalized to hold for a generic system-environment coupling operator in Ref. [38]. Furthermore, the master equation was applied to describe Cooper pair pumping [40–42] in Refs. [37] and [38].

In this paper, we introduce an alternative derivation of the master equation for adiabatically steered quantum systems coupled to a Markovian environment. Our derivation is based on utilizing a nonsteered master equation in the first superadiabatic basis. We show that the master equation we obtain is the same as in Ref. [38]. Our method is potentially more efficient in obtaining higher order expansions in the adiabatic parameter. In addition, we introduce a way to select the complex phases of the adiabatic basis states such that the local adiabatic parameter is minimized, leading to vanishing diagonal elements for the operator describing the steering. We show that this selection results in locally phase-invariant basis states. Finally, we discuss how to account for the time-local accumulation speed of the geometric phase in the environment-induced transitions.

The structure of this paper is as follows. In the next section, we introduce our model describing the open quantum system. In Sec. III, we derive the master equation for a nonsteered system subject to decoherence. In Sec. IV, we use the nonsteered master equation to obtain the full master equation for adiabatic steering. In Sec. V, we introduce the optimal phase selection for the adiabatic eigenstates and demonstrate the main implications of such a selection. We conclude the paper in Sec. VI.

II. MODEL

We consider a quantum system with a Hamiltonian \hat{H}_S which depends on a set of real control parameters $\{q_k\}$ that vary in time. The system is assumed to be interacting with the environment so that the total Hamiltonian is

$$\hat{H}(t) = \hat{H}_S(t) + \hat{V}(t) + \hat{H}_E,$$
 (1)

where $\hat{V}(t)$ is the coupling between the system and its environment and \hat{H}_E is the Hamiltonian of the environment. We assume that the coupling is of the generic form $\hat{V} = \hat{A} \otimes \hat{X}(t)$, where \hat{A} is the system part of the coupling operator and $\hat{X}(t)$ acts in the Hilbert space of the environment. Let $|m; \vec{q}(t)\rangle$ be the instantaneous eigenstate of $\hat{H}_S(t)$, and $E_m(t)$ the corresponding eigenenergy defined

^{*}juha.salmilehto@tkk.fi

by $\hat{H}_S[\vec{q}(t)] | m; \vec{q}(t) \rangle = E_m[\vec{q}(t)] | m; \vec{q}(t) \rangle$. In the context of adiabatic evolution, $\{|m; \vec{q}(t)\rangle\}$ is referred to as the *adiabatic basis*. We assume that the adiabatic states are normalized and nondegenerate.

Let the Hamiltonian $\hat{H}_S(t)$ be diagonalized in a fixed basis $\{|m_f\rangle\}$ using the eigendecomposition as $\hat{H}_S(t) = \hat{D}^{\dagger}(t)\hat{H}_S(t)\hat{D}(t)$, implying that $\langle n_f|\hat{H}_S(t)|m_f\rangle = E_m(t)\delta_{nm}$. We define a similar transformation for the total density operator $\hat{\rho}(t)$ in the Schrödinger picture as $\hat{\rho}(t) = \hat{D}^{\dagger}(t)\hat{\rho}(t)\hat{D}(t)$. It follows from the Schrödinger equation that the evolution of $\hat{\rho}(t)$ is governed by the effective Hamiltonian for the adiabatic basis

$$\hat{H}^{(1)}(t) = \hat{H}_S(t) + \hbar \hat{w}(t) + \hat{V}(t) + \hat{H}_E, \tag{2}$$

where $\hat{\hat{V}}(t) = \hat{D}^{\dagger}(t)\hat{V}(t)\hat{D}(t) = \hat{D}^{\dagger}(t)\hat{A}\hat{D}(t) \otimes \hat{X}(t)$ and $\hat{w}(t) = -i\hat{D}^{\dagger}(t)\hat{D}(t)$. Omitting the environment and assuming adiabatic evolution, a more accurate approximation for the exact evolving state is achieved if the adiabatic states are corrected by

$$|\delta m; \vec{q}(t)\rangle = -i\hbar \sum_{k \neq m} |k; \vec{q}(t)\rangle \frac{\langle k; \vec{q}(t)| \frac{\partial}{\partial t} |m; \vec{q}(t)\rangle}{E_m - E_k}, \quad (3)$$

in the first order in the perturbation theory. The basis formed by the corrected states $\{|m\rangle + |\delta m\rangle\}$ is usually referred to as the *first superadiabatic basis* [3].

We introduce the local adiabatic parameter as $\alpha(t) = \hbar ||\hat{w}(t)||/\Delta(t)$, where we compare the Hilbert-Schmidt norm of the operator arising from the adiabatic evolution $||\hat{w}(t)|| = \sqrt{\text{Tr}_S\{\hat{w}(t)^{\dagger}\hat{w}(t)\}}$ to an instantaneous minimum energy gap in the spectrum $\Delta(t)$. Here Tr_S denotes the trace over the system degrees of freedom, and in the following we use Tr_E to denote the trace over the environment degrees of freedom. The parameter $\alpha(t)$ typically yields a good estimate for the degree of adiabaticity of the evolution [25,38]. In cyclic evolution with the period T, the parameter scales as 1/T, and thus, in adiabatic evolution we should have $\alpha(t) \ll 1$.

III. MASTER EQUATION FOR A NONSTEERED SYSTEM

Let us study the dynamics of a generic nonsteered two-level quantum system coupled to its environment. Denote the ground and excited states of \hat{H}_S in the Schrödinger picture as $|g\rangle$ and $|e\rangle$, respectively, with corresponding eigenenergies E_g and E_e . We apply the standard method [37–39] to obtain the master equation for a nonsteered system as

$$\frac{d\rho_{gg}}{dt} = -(\Gamma_{ge} + \Gamma_{eg})\rho_{gg} + \text{Re}\{\tilde{\Gamma}_0\rho_{ge}\} + \Gamma_{eg}, \tag{4}$$

and

$$\begin{split} \frac{d\rho_{ge}}{dt} &= i\omega_{01}\rho_{ge} - (\tilde{\Gamma}_{+} + \tilde{\Gamma}_{-})\rho_{gg} \\ &- \left(\frac{\Gamma_{eg}}{2} + \frac{\Gamma_{ge}}{2} + \Gamma_{\varphi}\right)\rho_{ge} + (\Gamma_{\alpha} + \Gamma_{\beta})\rho_{eg} + \tilde{\Gamma}_{+}, \quad (5) \end{split}$$

where $\rho_{rs} = \langle r | \hat{\rho}_S | s \rangle$ with $r,s \in \{g,e\}$, and $\omega_{01} = (E_e - E_g)/\hbar$. The transition rates are defined as

$$\begin{split} \Gamma_{ge} &= \frac{|\langle e|\hat{A}|g\rangle|^2}{\hbar^2} S_X(-\omega_{01}), \\ \Gamma_{eg} &= \frac{|\langle e|\hat{A}|g\rangle|^2}{\hbar^2} S_X(+\omega_{01}), \\ \tilde{\Gamma}_0 &= \frac{\langle e|\hat{A}|g\rangle(\langle g|\hat{A}|g\rangle - \langle e|\hat{A}|e\rangle)}{\hbar^2} S_X(0), \\ \tilde{\Gamma}_{\pm} &= \frac{\langle g|\hat{A}|e\rangle(\langle e|\hat{A}|e\rangle - \langle g|\hat{A}|g\rangle)}{2\hbar^2} S_X(\pm\omega_{01}), \\ \Gamma_{\varphi} &= \left(\frac{|\langle e|\hat{A}|e\rangle|^2}{2\hbar^2} + \frac{|\langle g|\hat{A}|g\rangle|^2}{2\hbar^2} - \frac{\langle g|\hat{A}|g\rangle\langle e|\hat{A}|e\rangle}{\hbar^2}\right) S_X(0), \\ \Gamma_{\alpha} &= \frac{\langle g|\hat{A}|e\rangle^2}{2\hbar^2} S_X(\omega_{01}), \\ \Gamma_{\beta} &= \frac{\langle g|\hat{A}|e\rangle^2}{2\hbar^2} S_X(-\omega_{01}). \end{split}$$

The spectral density is denoted $S_X(\omega) = \int_{-\infty}^{\infty} d\tau \operatorname{Tr}_E \{\hat{\rho}_E \hat{X}(\tau) \hat{X}(0)\} e^{i\omega\tau}$. Note that we neglect the drive, that is, omit all terms proportional to \hat{w} . Furthermore, Eqs. (4) and (5) include all the nonsecular terms neglected in the usual application of the approach in Ref. [39].

For details concerning the derivation of Eqs. (4) and (5), see the Appendix. Especially, we neglect the possible imaginary parts of the transition rates, that is, the Lamb shift, by assuming that the system time scales are longer than the environment autocorrelation time.

IV. MASTER EQUATION FOR ADIABATIC STEERING

We aim to derive the full master equation for the system coupled to its environment in adiabatic steering using the master equation for a nonsteered system. Define a unitary transformation $\hat{D}_1(t)$ making $\hat{H}_S(t) + \hbar \hat{w}(t)$ diagonal in the fixed basis $\{|0\rangle, |1\rangle\}$. Thus the evolution of the density matrix $\hat{\rho}^{(2)} = \hat{D}_1^{\dagger} \hat{\rho} \hat{D}_1 = \hat{D}_1^{\dagger} \hat{D}^{\dagger} \hat{\rho} \hat{D}_1$ is governed by the effective Hamiltonian for the first superadiabatic basis.

$$\hat{\tilde{H}}^{(2)}(t) = \hat{\tilde{H}}_{S}^{(2)}(t) + \hbar \hat{w}_{1}(t) + \hat{\tilde{V}}^{(2)}(t) + \hat{H}_{E}, \tag{6}$$

where $\hat{\tilde{H}}_{S}^{(2)}(t) = \hat{D}_{1}^{\dagger}(t)[\hat{H}_{S}(t) + \hbar \hat{w}(t)]\hat{D}_{1}(t), \quad \hat{\tilde{V}}^{(2)}(t) = \hat{D}_{1}^{\dagger}(t)\hat{\tilde{V}}(t)\hat{D}_{1}(t), \text{ and } \hat{w}_{1} = -i\hat{D}_{1}^{\dagger}(t)\hat{D}_{1}(t).$

Assume that the superadiabatic correction, \hat{w}_1 , is negligible with respect to the adiabatic one so that we can write Eq. (6) as $\hat{H}^{(2)}(t) \approx \hat{H}_S^{(2)}(t) + \hat{V}^{(2)}(t) + \hat{H}_E$. Since this Hamiltonian describes effectively a nonsteered system, we can employ the approach of Sec. III to write a master equation similar to Eqs. (4) and (5) as

$$\frac{d\rho_{gg}^{(2)}}{dt} = -\left(\Gamma_{ge}^{(2)} + \Gamma_{eg}^{(2)}\right)\rho_{gg}^{(2)} + \text{Re}\left\{\tilde{\Gamma}_{0}^{(2)}\rho_{ge}^{(2)}\right\} + \Gamma_{eg}^{(2)}, \quad (7)$$

and

$$\begin{split} \frac{d\rho_{ge}^{(2)}}{dt} &= i\omega_{01}^{(2)}\rho_{ge}^{(2)} - (\tilde{\Gamma}_{+}^{(2)} + \tilde{\Gamma}_{-}^{(2)})\rho_{gg}^{(2)} \\ &- \left(\frac{\Gamma_{eg}^{(2)}}{2} + \frac{\Gamma_{ge}^{(2)}}{2} + \Gamma_{\varphi}^{(2)}\right)\rho_{ge}^{(2)} + \left(\Gamma_{\alpha}^{(2)} + \Gamma_{\beta}^{(2)}\right)\rho_{eg}^{(2)} \\ &+ \tilde{\Gamma}_{-}^{(2)}, \end{split} \tag{8}$$

where we have marked the relevant terms in the superadiabatic basis with the superscript (2) to avoid confusing them with the adiabatic ones. The transformation $\hat{D}_1(t)$ can be approximated using the perturbation theory for the adiabatic correction. This results in the superadiabatic eigenstates which we can obtain from Eq. (3) up to the linear order in $\alpha(t)$ in the two-state model as

$$|g^{(2)}\rangle = |g\rangle - |e\rangle \frac{w_{ge}^*}{w_{01}},\tag{9}$$

and

$$|e^{(2)}\rangle = |e\rangle + |g\rangle \frac{w_{ge}}{\omega_{01}},$$
 (10)

with the eigenenergies $E_g^{(2)}=E_g+\hbar w_{gg}$ and $E_e^{(2)}=E_e+\hbar w_{ee}$, respectively. Here, we denote matrix elements of the adiabatic correction $w_{sr}=-i\ \langle s|\dot{r}\rangle$, where $r,s\in\{g,e\}$. Thus, the superadiabatic angular frequency up to this order becomes $\omega_{01}^{(2)}=\omega_{01}+(w_{ee}-w_{gg})$.

The matrix elements in Eqs. (7) and (8) can be written using the superadiabatic eigenstates to obtain the master equation for adiabatic steering up to the linear order in $\alpha(t)$. We restrict our derivation to the linear order since, in the adiabatic limit, $\alpha(t) \to 0$, making the contributions beyond the linear one negligible. If we assume that the system is driven adiabatically but does not necessarily remain in the ground state at all times, we cannot assume that density matrix elements ρ_{ge} become small enough to be neglected due to their order in this limit. Hence, we are only considering $\alpha(t)$ as a small parameter and neglect all terms with α^2 or higher order. If we rewrite $\rho_{gg}^{(2)}$ and $\rho_{ge}^{(2)}$ using Eqs. (9) and (10), the master equation becomes

$$\begin{split} \dot{\rho}_{gg} &- 2 \frac{\text{Re}(w_{ge}^* \dot{\rho}_{ge})}{\omega_{01}} \\ &= - \left(\Gamma_{ge}^{(2)} + \Gamma_{eg}^{(2)} \right) \left(\rho_{gg} - 2 \frac{\text{Re}(w_{ge}^* \rho_{ge})}{\omega_{01}} \right) \\ &+ \text{Re} \left\{ \tilde{\Gamma}_{0}^{(2)} \left(\rho_{ge} + 2 \frac{w_{ge}}{\omega_{01}} \rho_{gg} - \frac{w_{ge}}{\omega_{01}} \right) \right\} + \Gamma_{eg}^{(2)}, \end{split} \tag{11}$$

and

$$\begin{split} \dot{\rho}_{ge} + 2 \frac{w_{ge}}{\omega_{01}} \dot{\rho}_{gg} \\ &= i [\omega_{01} + (w_{ee} - w_{gg})] \left(\rho_{ge} + 2 \frac{w_{ge}}{\omega_{01}} \rho_{gg} - \frac{w_{ge}}{\omega_{01}} \right) \\ &- (\tilde{\Gamma}_{-}^{(2)} + \tilde{\Gamma}_{-}^{(2)}) \left(\dot{\rho}_{gg} - 2 \frac{\text{Re}(w_{ge}^* \dot{\rho}_{ge})}{\omega_{01}} \right) \\ &- \left(\frac{\Gamma_{eg}^{(2)}}{2} + \frac{\Gamma_{ge}^{(2)}}{2} + \Gamma_{\varphi}^{(2)} \right) \left(\rho_{ge} + 2 \frac{w_{ge}}{\omega_{01}} \rho_{gg} - \frac{w_{ge}}{\omega_{01}} \right) \\ &+ \left(\Gamma_{\alpha}^{(2)} + \Gamma_{\beta}^{(2)} \right) \left(\rho_{eg} + 2 \frac{w_{ge}^*}{\omega_{01}} \rho_{gg} - \frac{w_{ge}^*}{\omega_{01}} \right) + \tilde{\Gamma}_{+}^{(2)}, \end{split}$$
(12)

where we have neglected all terms of order α^2 or higher, except in the $\Gamma^{(2)}$ terms, which we treat later. We can solve $\dot{\rho}_{gg}$ and $\dot{\rho}_{gg}$ from these equations to obtain the full master equation. In addition, we employ Eqs. (9) and (10) to rewrite the rates in the superadiabatic approximation. To present the full master equation, we adopt a notation which will not reduce the generality of the equations but simplify them. In the nested commutator expression for the master equation for a nonsteered system [see Eq. (A1) in the Appendix], the coupling operator is only found in places where it is commuting with other operators, and hence, provided that the Lamb shift is neglected, we can add any operator comparable to the identity operator to it without affecting the nested expression. Thus, the system part of the coupling operator can be chosen traceless in the two-state basis. We adopt this convention by introducing $m_1 = \langle g | \hat{A} | g \rangle = -\langle e | \hat{A} | e \rangle$ and $m_2 = \langle g | \hat{A} | e \rangle$. Note that $m_1 \in \mathbb{R}$, whereas $m_2 \in \mathbb{C}$ in the case of a general coupling operator. The master equation up to the linear order in $\alpha(t)$ and the quadratic order in the system-environment coupling becomes

$$\begin{split} \dot{\rho}_{gg} &= -2 \text{Im}(w_{ge}^* \rho_{ge}) + S(\omega_{01}) |m_2|^2 - [S(-\omega_{01}) + S(\omega_{01})] \\ &\times |m_2|^2 \rho_{gg} + 2 [\text{Im}(m_2) \text{Im}(\rho_{ge}) + \text{Re}(m_2) \text{Re}(\rho_{ge})] \\ &\times S(0) m_1 - 2 \frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}} \\ &\times \{ [\text{Im}(m_2) \text{Im}(w_{ge}) + \text{Re}(m_2) \text{Re}(w_{ge})] \\ &\times [\text{Im}(m_2) \text{Im}(\rho_{ge}) + \text{Re}(m_2) \text{Re}(\rho_{ge})] \} \\ &+ 2 \frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}} \{ \text{Im}(m_2) \text{Im}(w_{ge}) \\ &+ \text{Re}(m_2) \text{Re}(w_{ge}) \} m_1 \rho_{gg} - 2 \frac{S(0) - S(\omega_{01})}{\omega_{01}} m_1 \\ &\times \{ \text{Im}(m_2) \text{Im}(w_{ge}) + \text{Re}(m_2) \text{Re}(w_{ge}) \} \end{split}$$

and

$$\begin{split} \dot{\rho}_{ge} &= i w_{ge} (2 \rho_{gg} - 1) + i (w_{ee} - w_{gg}) \rho_{ge} + i \omega_{01} \rho_{ge} - S(\omega_{01}) \\ &\times m_1 m_2 + [S(-\omega_{01}) + S(\omega_{01})] m_1 m_2 \rho_{gg} - 2S(0) m_1^2 \rho_{ge} \\ &- i [S(-\omega_{01}) + S(\omega_{01})] m_2 [\text{Im}(\rho_{ge}) \text{Re}(m_2) - \text{Im}(m_2) \\ &\times \text{Re}(\rho_{ge})] - 2 \frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}} m_1^2 w_{ge} \rho_{gg} \\ &+ 2 \frac{S(0) - S(\omega_{01})}{\omega_{01}} m_1^2 w_{ge} - i m_2 \frac{S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}} \\ &\times \{\text{Im}(m_2) \text{Re}(w_{ge}) - \text{Im}(w_{ge}) \text{Re}(m_2)\} \\ &- 2 \frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}} m_1 \{i m_2 [\text{Im}(w_{ge}) \\ &\times \text{Re}(\rho_{ge}) - \text{Im}(\rho_{ge}) \text{Re}(w_{ge})] - [\text{Im}(m_2) \text{Im}(w_{ge}) \\ &+ \text{Re}(m_2) \text{Re}(w_{ge})] \rho_{ge} \}. \end{split}$$

Here, we applied a shortened notation for the spectral densities $S(\omega) = S_X(\omega)/\hbar^2$. We would like to emphasize that in this section, we assume that the system is externally steered; that is, the system Hamiltonian is time dependent. Even though we do not explicitly make the approximation of adiabatic rates [39], that is, assume that the evolution time is much longer than the environment autocorrelation time so that ω_{01} , m_1 , m_2 , and the matrix elements of \hat{w} vary slowly in time, the approximation is implicitly assumed. This assumption

stems from the fact that we use the master equation for a nonsteered system in the linear order in $\alpha(t)$. Furthermore, we have neglected corrections proportional to $\partial_{\omega}S(\omega)|_{\omega=\pm\omega_{01}}$ when estimating the preceding power spectra, since they correspond to driving-induced Lamb shift contributions which are neglected also in the derivation in Refs. [37] and [38]. In Sec. V, we show that w_{gg} and w_{ee} vanish from Eq. (14) for a specific choice of the phases of the adiabatic basis states.

Let us explicitly reformulate and assess the range of validity of the master equation [see Eqs. (13) and (14)]. The approximation of adiabatic rates requires that the external drive does not change the Hamiltonian governing the system on the time scale of the memory time of the bath; that is, we assume that $\tau_{\rm corr} \ll 1/||\hat{w}||$, where $\tau_{\rm corr}$ is the environment correlation time. Furthermore, we require that the dynamics of the density operator occur on time scales longer than the environment autocorrelation time, so that $\tau_{\rm corr} \ll 1/\omega_0$, where $1/\omega_0$ is a typical system transition time relating to the offdiagonal elements of the density matrix. As mentioned in the Appendix, we apply the Markov approximation by assuming that $\tau_{\rm corr} \ll 1/\gamma$, where $1/\gamma$ is a typical relaxation time of the system. Moreover, the assumptions we employ demand that $1/\omega_0 \ll 1/\gamma, 1/||\hat{w}||$. Combining the used approximations leads to a requirement of time scale separation $\tau_{\rm corr} \ll 1/\omega_0 \ll$ $1/\gamma, 1/||\hat{w}||$.

Remarkably, our master equation is identical to that derived in Ref. [38], however, the manner in which the master equation was derived is different. In Ref. [38], one starts from the effective Hamiltonian for the adiabatic basis presented in Eq. (2) and formulates a nested commutator expression for the derivative of the reduced system density operator in the adiabatic basis, applying $\hbar \hat{w}(t) + \hat{V}(t)$ as the perturbation,

$$\begin{split} & \frac{d\hat{\sigma}_{I}(t)}{dt} = i[\hat{\sigma}_{I}(t), \hat{w}_{I}(t)] \\ & - \frac{1}{\hbar^{2}} \mathrm{Tr}_{E} \bigg\{ \int_{0}^{t} dt' \bigg[[\hat{\rho}_{I}(t), \hat{\bar{V}}_{I}(t')], \hat{\bar{V}}_{I}(t) \bigg] \bigg\} \\ & + \frac{i}{\hbar^{2}} \mathrm{Tr}_{E} \bigg\{ \int_{0}^{t} dt' \int_{0}^{t'} dt'' [[\hat{\rho}_{I}(t), [\hat{w}_{I}(t'), \hat{\bar{V}}_{I}(t'')]], \hat{\bar{V}}_{I}(t)] \bigg\}, \end{split}$$

$$(15)$$

in the interaction picture. Using this operator directly results in the same master equation that we obtained. Thus, we find that with respect to adiabatic temporal evolution, it makes no difference whether one uses the effective Hamiltonian for the adiabatic basis and takes $\hbar \hat{w}(t) + \tilde{V}(t)$ as the perturbation, as done in Refs. [37] and [38], or whether one uses our approach to express the effective Hamiltonian for the superadiabatic basis assuming that the superadiabatic correction is small, thus taking $\hat{\hat{V}}^{(2)}(t)$ as the perturbation and writing the superadiabatic basis states up to the linear order in $\alpha(t)$. Our discovery reaffirms that the superadiabatic basis approximates the exact evolving state in the next order in α , so using only the bath coupling as the perturbation will result in describing the dynamics in the same order as the effective Hamiltonian for the adiabatic basis does. This result is an important consistency check for the master equation derived in Refs. [37] and [38]; see Eqs. (13) and (14).

The original way [37,38] of deriving the full master equation can be extended to obtain master equations in higher orders in α by applying the nesting procedure iteratively [see Eq. (15)]. Our method can also be used to obtain higher order master equations by using higher order perturbation theory to write the matrix elements required to utilize the master equation for nonsteered systems. Since our technique is based on applying algebraic operations, it is potentially simpler to obtain higher order equations with it than with the nesting procedure, which results in complicated integral expressions.

As an example, let us illustrate how to obtain the master equation up to the second order in $\alpha(t)$ using our method for a two-level system. We begin by defining a unitary transformation $\hat{D}_2(t)$ making $\hat{H}_S^{(2)}(t) + \hbar \hat{w}_1(t)$ diagonal in the fixed basis $\{|0\rangle, |1\rangle\}$. Thus the relevant density matrix becomes $\hat{\rho}^{(3)} = \hat{D}_2^{\dagger} \hat{\rho}^{(2)} \hat{D}_2$ and its evolution is governed by the effective Hamiltonian for the second superadiabatic basis,

$$\hat{\tilde{H}}^{(3)}(t) = \hat{\tilde{H}}_{S}^{(3)}(t) + \hbar \hat{w}_{2}(t) + \hat{\tilde{V}}^{(3)}(t) + \hat{H}_{E},$$
 (16)

where $\hat{H}_S^{(3)}(t) = \hat{D}_2^{\dagger}(t)[\hat{H}_S^{(2)}(t) + \hbar \hat{w}_1(t)]\hat{D}_2(t), \hat{V}^{(3)}(t) = \hat{D}_2^{\dagger}(t)$ $\hat{V}^{(2)}(t)\hat{D}_2(t)$, and $\hat{w}_2 = -i\hat{D}_2^{\dagger}(t)\hat{D}_2(t)$. Assuming that \hat{w}_2 is negligible with respect to \hat{w}_1 , we can again resort to the approach in Sec. III and write a master equation similar to Eqs. (4) and (5). Finding the relevant matrix elements is slightly more complicated than in the case of the master equation up to the linear order in $\alpha(t)$. We essentially wish to describe $\hat{D}(t)\hat{D}_1(t)\hat{D}_2(t)|m\rangle$, where $|m\rangle$ is a fixed state, up to the second order in $\alpha(t)$. We first write the first superadiabatic eigenstates up to the second order in $\alpha(t)$ as

$$|g^{(3)}\rangle = |g\rangle - |e\rangle \frac{w_{ge}^*}{\omega_{01}} + |e\rangle \frac{w_{ee}w_{ge}^*}{\omega_{01}^2}, \qquad (17)$$

and

$$|e^{(3)}\rangle = |e\rangle + |g\rangle \frac{w_{ge}}{\omega_{01}} + |g\rangle \frac{w_{gg}w_{ge}}{\omega_{01}^2}, \tag{18}$$

with the eigenenergies $E_g^{(3)}=E_g+\hbar w_{gg}-\hbar|w_{ge}|^2/\omega_{01}$ and $E_e^{(3)}=E_e+\hbar w_{ee}+\hbar|w_{ge}|^2/\omega_{01}$, respectively. Additionally, we must account for the lowest order in $||\hat{w}_1(t)||\sim \alpha(t)^2$ to obtain the states of interest up to the second order in $\alpha(t)$ as

$$\hat{D}(t)\hat{D}_1(t)\hat{D}_2(t)|0\rangle \approx |g^{(3)}\rangle - |e\rangle \frac{w_{1,ge}^*}{\omega_{01}},$$
 (19)

and

$$\hat{D}(t)\hat{D}_1(t)\hat{D}_2(t)|1\rangle \approx |e^{(3)}\rangle + |g\rangle \frac{w_{1,ge}}{\omega_{01}},$$
 (20)

and the angular frequency as $\omega_{01}^{(3)} = \omega_{01}^{(2)} + 2|w_{ge}|^2/\omega_{01} + (w_{1,ee} - w_{1,gg})$. Here we denote $w_{1,gg} = -i \langle 0|\hat{D}_1^{\dagger}(t)\hat{D}_1(t)|0\rangle$, $w_{1,ee} = -i \langle 1|\hat{D}_1^{\dagger}(t)\hat{D}_1(t)|1\rangle$, and $w_{1,ge} = -i \langle 0|\hat{D}_1^{\dagger}(t)\hat{D}_1(t)|1\rangle$. Using these definitions, one could write the matrix elements in the relevant master equation for a nonsteered system to obtain the master equation for adiabatic steering up to the second order in $\alpha(t)$.

V. OPTIMAL PHASE SELECTION

Assume that we have nondegenerate adiabatic eigenstates $|g\rangle$ and $|e\rangle$ that are normalized and smooth during the temporal evolution, and that they can be obtained from the fixed states with a unitary transformation as $\hat{D}|0\rangle = |g\rangle$ and $\hat{D}|1\rangle =$ $|e\rangle$. Thus, the operator determining the adiabatic evolution becomes $\hat{w} = -i\hat{D}^{\dagger}\hat{D}$ [see Eq. (2)]. However, the choice for the complex phases of the states is essentially arbitrary, and hence its effect on \hat{w} should be studied. This means that we could also work with basis states that differ from $|g\rangle$ and $|e\rangle$ by phase factors which depend on the point in the control cycle. In this section, we show that this degree of freedom can be used to minimize the local adiabatic parameter, while in the corresponding master equation it leads only to renormalized matrix elements. Furthermore, we discuss how to account for the noncyclic geometric phase leading to a slightly different but generally more feasible phase selection.

Let us choose new phases for the states by multiplying them with phase factors $e^{i\lambda_g}$ and $e^{i\lambda_e}$, where $\lambda_g, \lambda_e \in \mathbb{R}$, so that a phase selection operator $\hat{\Omega}$ is defined as

$$\hat{\Omega} = e^{i\lambda_g} |0\rangle \langle 0| + e^{i\lambda_e} |1\rangle \langle 1|, \tag{21}$$

yielding the new transformation as $\hat{\hat{D}}=\hat{D}\hat{\Omega}$. Note that the new states defined by the transformation are still eigenstates of the original Hamiltonian. With this transformation, the operator for the drive becomes

$$\begin{split} \hat{\hat{w}} &= -i \hat{\hat{D}}^{\dagger} \dot{\hat{\hat{D}}} \\ &= -i \hat{\Omega}^{\dagger} \hat{D}^{\dagger} (\dot{\hat{D}} \hat{\Omega} + \hat{D} \dot{\hat{\Omega}}) \\ &= \dot{\lambda}_{g} |0\rangle \langle 0| + \dot{\lambda}_{e} |1\rangle \langle 1| - i \hat{\Omega}^{\dagger} \hat{D}^{\dagger} \dot{\hat{D}} \hat{\Omega}, \end{split}$$
(22)

where we have used the unitarity of \hat{D} . The matrix elements in the phase-shifted basis become

$$\langle 0|\hat{w}|0\rangle = \dot{\lambda}_{g} - i \langle 0|\hat{D}^{\dagger}\dot{D}|0\rangle = \dot{\lambda}_{g} + w_{gg},$$

$$\langle 1|\hat{w}|1\rangle = \dot{\lambda}_{e} - i \langle 1|\hat{D}^{\dagger}\dot{D}|1\rangle = \dot{\lambda}_{e} + w_{ee},$$

$$\langle 0|\hat{w}|1\rangle = -ie^{i(\lambda_{e} - \lambda_{g})} \langle 0|\hat{D}^{\dagger}\dot{D}|1\rangle = e^{i(\lambda_{e} - \lambda_{g})}w_{ge},$$

$$\langle 1|\hat{w}|0\rangle = -ie^{i(\lambda_{g} - \lambda_{e})} \langle 1|\hat{D}^{\dagger}\dot{D}|0\rangle = e^{i(\lambda_{g} - \lambda_{e})}w_{eg}.$$
(23)

Thus, the phase shift induces a shift in the diagonal elements and a phase shift in the off-diagonal elements.

Since the choice of the phases of the eigenstates changes the \hat{w} terms of the master equation and affects the quantum evolution, it has to be fixed by physical reasoning. One way to avoid artifact effects arising from the phase choice is to minimize the Hilbert-Schmidt norm $||\hat{w}|| = \sqrt{\text{Tr}_S\{\hat{w}^{\dagger}\hat{w}\}}$ at each time instant. For this task, it suffices to minimize

$$\operatorname{Tr}_{S}\{\hat{w}^{\dagger}\hat{w}\} = |\langle 0|\hat{w}|0\rangle|^{2} + |\langle 1|\hat{w}|1\rangle|^{2} + |\langle 1|\hat{w}|0\rangle|^{2} + |\langle 0|\hat{w}|1\rangle|^{2}. \tag{24}$$

The last two terms consist of the off-diagonal terms and the phase selection has no effect on them. Thus, the minimum is found when we select the diagonal elements in Eq. (24) to vanish, yielding

$$\lambda_g(t) = -\int_0^t dt' w_{gg}(t') + \lambda_g^0 = i \int_0^t dt' \langle g | \dot{g} \rangle + \lambda_g^0,$$

$$\lambda_e(t) = -\int_0^t dt' w_{ee}(t') + \lambda_e^0 = i \int_0^t dt' \langle e | \dot{e} \rangle + \lambda_e^0,$$
(25)

and

$$\begin{aligned} \langle 0|\hat{\bar{w}}|1\rangle &= e^{i(\lambda_{e}^{0} - \lambda_{g}^{0})} e^{i\int_{0}^{t} dt'[w_{gg}(t') - w_{ee}(t')]} w_{ge} \\ &= e^{i(\lambda_{e}^{0} - \lambda_{g}^{0})} e^{\int_{0}^{t} dt'[\langle g|\hat{g}\rangle - \langle e|\hat{e}\rangle]} w_{oe}. \end{aligned}$$
(26)

The absolute phases are not fixed since we have a degree of freedom in the selection of the constant parts λ_e^0 and λ_g^0 . Note that the primary selection of the smooth eigenstates $|g\rangle$ and $|e\rangle$ determines the accumulating phase. We denote the integrals as simply over time, but one should bear in mind that they contribute a path in the parameter space. Used in conjunction with our master equation, the preceding phase selection results in w_{gg} and w_{ee} vanishing in Eq. (14). Furthermore, it minimizes the local adiabatic parameter $\tilde{\alpha}(t) = ||\hat{w}(t)||/\omega_{01}(t)$. Thus we refer to it as *optimal phase selection*, although it may not yield the most accurate evolution, as discussed here.

Utilizing the optimal phase selection scheme with our master equation requires a careful consideration of the used approximations, in particular, the approximation of adiabatic rates. We used this approximation in the derivation of the master equation [see Eqs. (13) and (14)] to state that ω_{01} , m_1 , m_2 , and the matrix elements of \hat{w} vary slowly in time. With the optimal phase selection, the corresponding parameters are $\tilde{\omega}_{01} = \omega_{01}$, $\tilde{m}_1 = m_1$, $\tilde{m}_2 = e^{i(\lambda_e - \lambda_g)} m_2$, $\tilde{w}_{gg} = \tilde{w}_{ee} = 0$, and $\tilde{w}_{ge} = e^{i(\lambda_e - \lambda_g)} w_{ge}$. Since the approximation of adiabatic rates applies for the derivatives of the accumulating phases defined in Eq. (25), any possible shift in the power spectra induced by the optimal phase selection can be neglected since it would only lead to higher order terms in the master equation. Thus, the master equation can be used directly by replacing the original variables with the phase-shifted ones.

With the optimal selection, the phase-shifted basis states become $|\tilde{g}\rangle = e^{i\lambda_0^0} e^{-\int_0^t dt'\langle g|\hat{g}\rangle} |g\rangle$ and $|\tilde{e}\rangle = e^{i\lambda_0^0} e^{-\int_0^t dt'\langle g|\hat{e}\rangle} |e\rangle$. Thus we have $\langle \tilde{g}|\tilde{g}\rangle = \langle \tilde{e}|\tilde{e}\rangle = 0$ independent of $|g\rangle$ and $|e\rangle$ and the selection renders the phase-shifted states also to be invariant under a local gauge change; that is, $|g\rangle \to e^{i\beta(t)} |g\rangle$ has no effect on $|\tilde{g}\rangle$ and $|e\rangle \to e^{i\eta(t)} |e\rangle$ has no effect on $|\tilde{e}\rangle$, where $\beta(t)$ and $\eta(t)$ are any smooth functions. For a closed path in the parameter space γ , we have

$$\lambda_{g}(t_{b}) - \lambda_{g}(t_{a}) = i \oint_{\gamma} \langle g | \dot{g} \rangle,$$

$$\lambda_{e}(t_{b}) - \lambda_{e}(t_{a}) = i \oint_{\gamma} \langle e | \dot{e} \rangle,$$
(27)

where we have denoted t_a and t_b the virtual starting and ending time instants for the path, respectively. These are the Berry phases accumulated over the path for the phase-shifted basis states and, as such, cannot be removed by any continuous local gauge change [3]. Thus, selecting the optimal local phase for a closed loop in the parameter space implies a gauge-invariant accumulated phase at the end of the loop. However, the optimal phase selection neglects the effects of the accumulation speed

of the geometric phase on the environment-induced transitions in the master equation. Although this effect is negligible in the adiabatic limit, it is useful to provide means to take it into account consistently.

To go beyond the optimal phase selection, we need to study the adiabatic noncyclic geometric phase acquired during the evolution [43,44]. The adiabatic noncyclic geometric phase acquired by the nth eigenstate [44] can be defined as

$$\gamma_n(t) = \arg\{\langle n; \vec{q}(t_0) | n; \vec{q}(t) \rangle\}$$

$$+ i \int_0^t d\tau \, \langle n; \vec{q}(\tau) | \partial_\tau | n; \vec{q}(\tau) \rangle, \qquad (28)$$

where $|n;\vec{q}(t_0)\rangle$ is an essentially arbitrary reference eigenvector not orthogonal to $|n;\vec{q}(t)\rangle$. The phase $\gamma_n(t)$ is invariant under any local phase transformation of the basis states and independent of the speed at which we traverse the open path in the control parameter space. To allow for the accumulating phase of the basis vectors to describe the noncyclic geometric phase, one can define a phase transformation of the eigenstates $|n\rangle = e^{-i\arg\{\langle n';\vec{q}(t_0)|n';\vec{q}(t)\rangle\}}\,|n'\rangle$, where $n\in\{g,e\}$ and $|n'\rangle$ describes an eigenstate with an arbitrary continuous local phase. This transformation produces

$$w_{nn} = -\partial_t \arg\{\langle n'; \vec{q}(t_0) | n'; \vec{q}(t) \rangle\} - i \langle n' | \dot{n}' \rangle$$

= $-\dot{\gamma}_n(t)$. (29)

Thus the time-local accumulation speed of the geometric phase can be made to appear in the master equation [Eqs. (13) and (14)]. However, the accumulation speed in Eq. (29) is dependent on the reference point $|n';\vec{q}(t_0)\rangle$, and thus, redefining the reference typically changes the accumulation speed at all times. This can become a problem since the accumulation speed affects in general the resulting physical quantities, which should not depend on the choice of the reference point. A possible way to correct for this inconsistency is to use the geodesic approach [43].

VI. CONCLUSIONS

We devised a way to derive the full master equation for adiabatically steered quantum systems in the two-state approximation under the influence of decoherence starting from an interaction-picture-based derivation, in which the external drive was first omitted. The full master equation was obtained by approximating the transformation to the superadiabatic basis using the perturbation theory and exploiting the master equation for the nonsteered system. We showed that the master equation we obtain in this way is the same as the one obtained in Ref. [38] by a longer calculation. We concluded that our manner of obtaining the master equation is a consequence of the superadiabatic basis approximating the exact evolving state in the linear order in the adiabatic parameter $\alpha(t)$. Furthermore, there is no need to evaluate high-order nested commutators of integrals in our method if it is extended beyond the linear order in $\alpha(t)$, as opposed to the method in Refs. [37] and [38]. A detailed study of the efficiency of these two approaches is left for future research.

There exists a gauge degree of freedom in the choice of the phases of the basis states during the evolution. We have demonstrated a way to choose the phases in a way which minimizes the local adiabatic parameter and simplifies the derived master equation. We showed that this choice produces basis states which are invariant under a local gauge change. Furthermore, we have discussed how to account in a gauge-invariant manner for the effects of the accumulation speed of the adiabatic noncyclic geometric phase on the environment-induced transitions.

APPENDIX: NONSTEERED MASTER EQUATION IN THE TWO-STATE BASIS

The reduced system density matrix in the interaction picture $\hat{\sigma}_I(t) = \mathrm{Tr}_E\{\hat{\rho}_I(t)\}$ can be used to derive the relevant master equation assuming a stationary environment, that is, $\frac{d\hat{\rho}_E}{dt} = \frac{i}{\hbar}[\hat{\rho}_E,\hat{H}_E] = 0$. We define the operators in the interaction picture as $\hat{Z}_I(t) = e^{i\hat{H}_E t/\hbar}\hat{U}_S^\dagger(t,0)\hat{Z}(t)\hat{U}_S(t,0)e^{-i\hat{H}_E t/\hbar}$, where $\hat{Z}(t)$ is the operator in the Schrödinger picture and $\hat{U}_S(t,0)$ is the time-evolution operator. For a time-dependent system Hamiltonian, the time-evolution operator is $\hat{U}_S(t,0) = \mathcal{T}e^{-i\int_0^t \hat{H}_S(\tau)d\tau/\hbar}$ but simplifies to $\hat{U}_S(t,0) = e^{-i\hat{H}_St/\hbar}$ for nonsteered systems studied in this Appendix.

If we assume that the system interacts weakly with the environment, the master equation acquires the standard form (Redfield equation [45]),

$$\frac{d\hat{\sigma}_I(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_E \{ [[\hat{\sigma}_I(t) \otimes \hat{\rho}_E, \hat{V}_I(t')], \hat{V}_I(t)] \}, \tag{A1}$$

in the interaction picture, where we have utilized the Born-Markov approximation [45]. The transformation from the interaction picture to the Schrödinger picture unfolds when we employ

$$\hat{\rho}_S(t) = \hat{U}_S(t,0)\hat{\sigma}_I(t)\hat{U}_S^{\dagger}(t,0), \tag{A2}$$

which can be used to obtain the density matrix transformation componentwise as

$$\rho_{gg}(t) = \sigma_{I,gg}(t),
\rho_{ee}(t) = \sigma_{I,ee}(t),
\rho_{ge}(t) = e^{i\omega_{01}t}\sigma_{I,ge}(t),
\rho_{eg}(t) = e^{-i\omega_{01}t}\sigma_{I,eg}(t).$$
(A3)

Derivating Eq. (A2) yields the transformation of the derivative as

$$\frac{d\hat{\rho}_S(t)}{dt} = \frac{i}{\hbar} [\hat{\rho}_S(t), \hat{H}_S(t)] + \hat{U}_S(t, 0) \frac{d\hat{\sigma}_I(t)}{dt} \hat{U}_S^{\dagger}(t, 0). \quad (A4)$$

Using Eqs. (A1) and (A4), we define the diagonal matrix element

$$\langle g | \frac{d\hat{\rho}_{S}(t)}{dt} | g \rangle = -\frac{1}{\hbar^{2}} \int_{0}^{t} dt' \operatorname{Tr}_{E} \{ \langle g | [[\hat{\sigma}_{I}(t)]] \rangle \},$$

$$\otimes \hat{\rho}_{E}, \hat{V}_{I}(t')], \hat{V}_{I}(t)] | g \rangle \},$$
(A5)

and the off-diagonal matrix element

$$\langle g | \frac{d\hat{\rho}_{S}(t)}{dt} | e \rangle = i \omega_{01} \rho_{ge}(t) - e^{i\omega_{01}t} \frac{1}{\hbar^{2}} \int_{0}^{t} dt' \operatorname{Tr}_{E} \{ \langle g | [[\hat{\sigma}_{I}(t)] \\ \otimes \hat{\rho}_{E}, \hat{V}_{I}(t')], \hat{V}_{I}(t)] | e \rangle \}, \tag{A6}$$

for the nonsteered master equation. Note that our derivation is based on assuming that the system relaxation time is long compared to the environment correlation time $\tau_{\rm corr}$, so that the environment has no memory; that is, we are in the Markov regime [39]. This allows us to neglect any variation of $\hat{\sigma}_I(t)$ between time t and time $t + \tau_{\rm corr}$. The integral expressions in Eqs. (A5) and (A6) simplify to give Eqs. (4) and (5) when we expand the commutators, use the closure relation for the adiabatic basis, and utilize ${\rm Tr}_E\{\hat{\rho}_E\hat{X}(t')\hat{X}(t)\} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_X(\omega) e^{-i\omega(t'-t)}$ and Eq. (A3). Furthermore, we assume that the system time scales are longer than the system autocorrelation time to approximate the spectral densities in

the remaining integral expressions. This treatment leads to neglecting the Lamb shift.

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