Adiabatically steered open quantum systems: Master equation and optimal phase

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We introduce an alternative way to derive the generalized form of the master equation recently presented in Ref. [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 non-steered system in the first super-adiabatic basis. It is potentially efficient in obtaining higher-order equations. Furthermore, we show how to select the phases of the adiabatic basis states to minimize the local adiabatic parameter and how to apply this optimal phase selection scheme to our 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 [22, 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, 38].

In the approach of Ref. [37], it was shown that the typically applied secular approximation [31, 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, 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 non-steered master equation in the first super-adiabatic basis. We show that the master equation we obtain is the same as in Ref. [38] and that our method is potentially simpler to apply to 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.

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 non-steered system subject to decoherence. In Sec. IV, we use the non-steered master equation to obtain the full master equation for adiabatic steering. In Sec. V, we introduce the optimal phase selection for the adiabatic basis states 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

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

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 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 non-degenerate.

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

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

where $\hat{\tilde{V}}(t) = \hat{D}^\dagger(t)\hat{V}(t)\hat{D}(t) = \hat{D}^\dagger(t)\hat{A}\hat{D}(t)\otimes\hat{X}(t)$ and $\hat{w}(t) = -i\hat{D}^\dagger(t)\dot{\hat{D}}(t)$. 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

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

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 $||\hat{w}(t)|| = \sqrt{\mathrm{Tr}_S\{\hat{w}(t)^\dagger\hat{w}(t)\}}$ 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 will use Tr_E to denote the trace over the environment degrees of freedom. The parameter $\alpha(t)$ should give 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 NON-STEERED SYSTEM

Let us study the dynamics of a generic non-steered two-level 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. The standard method [39] for 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, i.e., $\frac{d\hat{\rho}_E}{dt} = \frac{i}{\hbar}[\hat{\rho}_E, \hat{H}_E] = 0$. 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 $\hat{U}_S(t,0) = e^{-i\int_0^t \hat{H}_S(\tau)d\tau/\hbar}$ but simplifies to $\hat{U}_S(t,0) = e^{-i\hat{H}_S t/\hbar}$ for non-steered systems studied in this Section.

If we assume that the system interacts weakly with the environment, the master equation acquires the standard form [43]

$$\frac{d\hat{\sigma}_I(t)}{dt} = -\frac{1}{\hbar^2}\int_0^t dt'\,\mathrm{Tr}_E([[\hat{\sigma}_I(t)\otimes\hat{\rho}_E, \hat{V}_I(t')], \hat{V}_I(t)]), \tag{4}$$

in the interaction picture, where we have utilized the Born-Markov approximation [44]. Equation (4) is recast into the Schrödinger picture as

$$\frac{d\rho_{gg}}{dt} = -(\Gamma_{ge} + \Gamma_{eg})\rho_{gg} + \Re e\{\tilde{\Gamma}_0\rho_{ge}\} + \Gamma_{eg}, \tag{5}$$

and

$$\begin{aligned}\frac{d\rho_{ge}}{dt} &= i\omega_{01}\rho_{ge} - (\tilde{\Gamma}_+ + \tilde{\Gamma}_-)\rho_{gg} \\ &\quad - \left(\frac{\Gamma_{eg}}{2} + \frac{\Gamma_{ge}}{2} + \Gamma_\varphi\right)\rho_{ge} + (\Gamma_\alpha + \Gamma_\beta)\rho_{eg} + \tilde{\Gamma}_+,\end{aligned} \tag{6}$$

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

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

The spectral density is denoted by $S_X(\omega) = \int_{-\infty}^{\infty} d\tau\,\mathrm{Tr}_E\{\hat{\rho}_E\hat{X}(\tau)\hat{X}(0)\}e^{i\omega\tau}$. Note that we neglect the drive, i.e., omit all terms proportional to $\hat{w}$. Furthermore, Eqs. (5) and (6) include all the nonsecular terms neglected in the usual approach [39].

For futher details concerning the derivation of Eqs. (5) and (6) see Appendix. Especially, we neglect the possible imaginary parts of the transition rates, i.e., the Lamb shift, by assuming that the system time scales are longer than the system autocorrelation time.

IV. MASTER EQUATION FOR ADIABATIC STEERING

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

$$\hat{\tilde{H}}^{(2)}(t) = \hat{\tilde{H}}_S^{(2)}(t) + \hbar\hat{w}_1(t) + \hat{\tilde{V}}^{(2)}(t) + \hat{H}_E, \tag{7}$$

where $\hat{\tilde{H}}_S^{(2)}(t) = \hat{D}_1^\dagger(t)(\hat{\tilde{H}}_S(t) + \hbar\hat{w}(t))\hat{D}_1(t)$, $\hat{\tilde{V}}^{(2)}(t) = \hat{D}_1^\dagger(t)\hat{\tilde{V}}(t)\hat{D}_1(t)$, and $\hat{w}_1 = -i\hat{D}_1^\dagger(t)\dot{\hat{D}}_1(t)$.

Assume that the super-adiabatic correction, $\hat{w}_1$, is negligible with respect to the adiabatic one so that we can write Eq. (7) as $\hat{\tilde{H}}^{(2)}(t) \approx \hat{\tilde{H}}_S^{(2)}(t) + \hat{\tilde{V}}^{(2)}(t) + \hat{H}_E$. Since this Hamiltonian describes effectively a non-steered system, we can employ the approach of Sec. III to write a master equation similar to Eqs. (5) and (6) as

$$\frac{d\rho_{gg}^{(2)}}{dt} = -(\Gamma_{ge}^{(2)} + \Gamma_{eg}^{(2)})\rho_{gg}^{(2)} + \Re e\{\tilde{\Gamma}_0^{(2)}\rho_{ge}^{(2)}\} + \Gamma_{eg}^{(2)}, \tag{8}$$

and

$$\begin{aligned}\frac{d\rho_{ge}^{(2)}}{dt} &= i\omega_{01}^{(2)}\rho_{ge}^{(2)} - (\tilde{\Gamma}_+^{(2)} + \tilde{\Gamma}_-^{(2)})\rho_{gg}^{(2)} \\ &\quad - \left(\frac{\Gamma_{eg}^{(2)}}{2} + \frac{\Gamma_{ge}^{(2)}}{2} + \Gamma_\varphi^{(2)}\right)\rho_{ge}^{(2)} + (\Gamma_\alpha^{(2)} + \Gamma_\beta^{(2)})\rho_{eg}^{(2)} \\ &\quad + \tilde{\Gamma}_+^{(2)},\end{aligned} \tag{9}$$

where we have marked the relevant terms in the super-adiabatic 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

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

and

$$|e^{(2)}\rangle = |e\rangle + |g\rangle \frac{w_{ge}}{\omega_{01}}, \tag{11}$$

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

The matrix elements in Eqs. (8) and (9) can be written using the super-adiabatic 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 $\alpha(t) \sim 1/T$ and in the adiabatic limit, $T \to \infty$ 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 the density matrix elements ρ_{ge} to 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. Using Eqs. (8) and (9), this yields

$$\begin{aligned}&\dot{\rho}_{gg} - 2\frac{\Re e(w_{ge}^*\dot{\rho}_{ge})}{\omega_{01}} \\ &= -(\Gamma_{ge}^{(2)} + \Gamma_{eg}^{(2)})\left(\rho_{gg} - 2\frac{\Re e(w_{ge}^*\rho_{ge})}{\omega_{01}}\right) \\ &+ \Re e\left\{\tilde{\Gamma}_0^{(2)}\left(\rho_{ge} + 2\frac{w_{ge}}{\omega_{01}}\rho_{gg} - \frac{w_{ge}}{\omega_{01}}\right)\right\} + \Gamma_{eg}^{(2)},\end{aligned} \tag{12}$$

and

$$\begin{aligned}&\dot{\rho}_{ge} + 2\frac{w_{ge}}{\omega_{01}}\dot{\rho}_{gg} \\ &= i[\omega_{01} + (w_{ee} - w_{gg})]\left(\rho_{ge} + 2\frac{w_{ge}}{\omega_{01}}\rho_{gg} - \frac{w_{ge}}{\omega_{01}}\right) \\ &- (\tilde{\Gamma}_+^{(2)} + \tilde{\Gamma}_-^{(2)})\left(\dot{\rho}_{gg} - 2\frac{\Re e(w_{ge}^*\dot{\rho}_{ge})}{\omega_{01}}\right) \\ &- \left(\frac{\Gamma_{eg}^{(2)}}{2} + \frac{\Gamma_{ge}^{(2)}}{2} + \Gamma_\varphi^{(2)}\right)\left(\rho_{ge} + 2\frac{w_{ge}}{\omega_{01}}\rho_{gg} - \frac{w_{ge}}{\omega_{01}}\right) \\ &+ (\Gamma_\alpha^{(2)} + \Gamma_\beta^{(2)})\left(\rho_{eg} + 2\frac{w_{ge}^*}{\omega_{01}}\rho_{gg} - \frac{w_{ge}^*}{\omega_{01}}\right) + \tilde{\Gamma}_+^{(2)}.\end{aligned} \tag{13}$$

We can solve $\dot{\rho}_{gg}$ and $\dot{\rho}_{ge}$ from these equations to obtain the full master equation. In addition, we employ Eqs. (10) and (11) to rewrite the rates in the super-adiabatic 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 of Eq. (4), 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 choosen traceless in the two-state basis. We will adopt this convention by introducing $m_1 = \langle g|\hat{A}|g\rangle = -\langle e|\hat{A}|e\rangle$ and $m_2 = \langle g|\hat{A}|e\rangle$. Notice 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 $\alpha(t)$ becomes

$$\dot{\rho}_{gg} = -2\Im m(w_{ge}^*\rho_{ge}) + S(\omega_{01})|m_2|^2 - [S(-\omega_{01}) + S(\omega_{01})]|m_2|^2\rho_{gg} + 2[\Im m(m_2)\Im m(\rho_{ge}) + \Re e(m_2)\Re e(\rho_{ge})]S(0)m_1$$
$$- 2\frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}}\{[\Im m(m_2)\Im m(w_{ge}) + \Re e(m_2)\Re e(w_{ge})][\Im m(m_2)\Im m(\rho_{ge}) + \Re e(m_2)\Re e(\rho_{ge})]\}$$
$$+ 2\frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}}\{\Im m(m_2)\Im m(w_{ge}) + \Re e(m_2)\Re e(w_{ge})\}m_1\rho_{gg}$$
$$- 2\frac{S(0) - S(\omega_{01})}{\omega_{01}}m_1\{\Im m(m_2)\Im m(w_{ge}) + \Re e(m_2)\Re e(w_{ge})\} \tag{14}$$

and

$$\dot{\rho}_{ge} = iw_{ge}(2\rho_{gg} - 1) + i(w_{ee} - w_{gg})\rho_{ge} + i\omega_{01}\rho_{ge} - S(\omega_{01})m_1m_2 + [S(-\omega_{01}) + S(\omega_{01})]m_1m_2\rho_{gg} - 2S(0)m_1^2\rho_{ge}$$
$$- i[S(-\omega_{01}) + S(\omega_{01})]m_2[\Im m(\rho_{ge})\Re e(m_2) - \Im(m_2)\Re e(\rho_{ge})]$$
$$- 2\frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}}m_1^2w_{ge}\rho_{gg} + 2\frac{S(0) - S(\omega_{01})}{\omega_{01}}m_1^2w_{ge}$$
$$- im_2\frac{S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}}\{\Im m(m_2)\Re e(w_{ge}) - \Im m(w_{ge})\Re e(m_2)\}$$
$$- 2\frac{2S(0) - S(-\omega_{01}) - S(\omega_{01})}{\omega_{01}}m_1\{im_2[\Im m(w_{ge})\Re e(\rho_{ge}) - \Im m(\rho_{ge})\Re e(w_{ge})]$$
$$- [\Im m(m_2)\Im m(w_{ge}) + \Re e(m_2)\Re e(w_{ge})]\rho_{ge}\}. \tag{15}$$

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, i.e., the system Hamiltonian is time-dependent. Even though we do not explicitly make the approximation of adiabatic rates [39], i.e., assume 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 non-steered system in the linear order in $\alpha(t)$. In Sec. V, we show that w_{gg} and w_{ee} vanish from Eq. (15) when we select the phases of the adiabatic basis states in an optimal manner.

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 $\hbar\hat{w}(t) + \hat{\tilde{V}}(t)$ as the perturbation

$$\frac{d\hat{\tilde{\sigma}}_I(t)}{dt} = i[\hat{\tilde{\sigma}}_I(t), \hat{w}_I(t)] - \frac{1}{\hbar^2}\mathrm{Tr}_E\left\{\int_0^t dt'\left[[\hat{\tilde{\rho}}_I(t), \hat{\tilde{V}}_I(t')], \hat{\tilde{V}}_I(t)\right]\right\}$$
$$+ \frac{i}{\hbar^2}\mathrm{Tr}_E\left\{\int_0^t dt'\int_0^{t'} dt''\left[\left[\hat{\tilde{\rho}}_I(t), [\hat{w}_I(t'), \hat{\tilde{V}}_I(t'')]\right], \hat{\tilde{V}}_I(t)\right]\right\}, \tag{16}$$

in the interaction picture. Using this operator directly, results in the same master equation to the one 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 $\hbar\hat{w}(t)+\hat{\tilde{V}}(t)$ as the perturbation as was done in Refs. [37, 38] or whether one uses our approach to express the effective Hamiltonian for the super-adiabatic basis assuming that the super-adiabatic correction is small, thus taking $\hat{\tilde{V}}^{(2)}(t)$ as the perturbation and writing the super-adiabatic basis states up to the linear order in $\alpha(t)$.

Our discovery reaffirms that the super-adiabatic basis approximates the exact evolving state in the next order in α so that 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, 38], see Eqs. (14) and (15). 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 iteratively the nesting procedure [see Eq. (16)]. Our procedure can be used as well to obtain higher-order master equations by using higher-order perturbation theory to approximate the evolving basis states up to higher orders in α. Since our procedure is based on applying algebraic operations, it is potentially simpler to obtain higher order equations with it than with nesting which results in complicated integral expressions.

V. OPTIMAL PHASE SELECTION

Assume that we have nondegenerate adiabatic basis states $|g\rangle$ and $|e\rangle$, that are normalized and smooth during the time 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 $\hat{w}=-i\hat{D}^\dagger\dot{\hat{D}}$ [see Eq. (2)]. However, the complex phases of the states are arbitrary, and hence their 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 time dependent phase factors. In this Section, we show that this freedom can be used to minimize the local adiabatic parameter, while in the corresponding master equation it leads to renormalized matrix elements only.

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

$$\hat{\Omega}=e^{i\lambda_g}\,|0\rangle\,\langle 0|+e^{i\lambda_e}\,|1\rangle\,\langle 1|\,, \tag{17}$$

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

$$\begin{aligned}\hat{\tilde{w}}&=-i\hat{\tilde{D}}^\dagger\dot{\hat{\tilde{D}}}\\&=-i\hat{\Omega}^\dagger\hat{D}^\dagger(\dot{\hat{D}}\hat{\Omega}+\hat{D}\dot{\hat{\Omega}})\\&=\dot{\lambda}_g\,|0\rangle\,\langle 0|+\dot{\lambda}_e\,|1\rangle\,\langle 1|-i\hat{\Omega}^\dagger\hat{D}^\dagger\dot{\hat{D}}\hat{\Omega},\end{aligned} \tag{18}$$

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

$$\begin{aligned}\langle 0|\hat{\tilde{w}}|0\rangle&=\dot{\lambda}_g-i\,\langle 0|\hat{D}^\dagger\dot{\hat{D}}|0\rangle=\dot{\lambda}_g+w_{gg},\\\langle 1|\hat{\tilde{w}}|1\rangle&=\dot{\lambda}_e-i\,\langle 1|\hat{D}^\dagger\dot{\hat{D}}|1\rangle=\dot{\lambda}_e+w_{ee},\\\langle 0|\hat{\tilde{w}}|1\rangle&=-ie^{i(\lambda_e-\lambda_g)}\,\langle 0|\hat{D}^\dagger\dot{\hat{D}}|1\rangle=e^{i(\lambda_e-\lambda_g)}w_{ge},\\\langle 1|\hat{\tilde{w}}|0\rangle&=-ie^{i(\lambda_g-\lambda_e)}\,\langle 1|\hat{D}^\dagger\dot{\hat{D}}|0\rangle=e^{i(\lambda_g-\lambda_e)}w_{eg}.\end{aligned} \tag{19}$$

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

In order to obtain the optimal selection, we minimize the Hilbert-Schmidt norm $||\hat{\tilde{w}}||=\sqrt{\mathrm{Tr}_S\{\hat{\tilde{w}}^\dagger\hat{\tilde{w}}\}}$ at each time instance since the local adiabatic parameter for evolution using a phase shifted basis is defined using it as $\alpha(t)=||\hat{\tilde{w}}(t)||/\omega_{01}(t)$, where $t\geq 0$ and we assume that the drive is engaged at time zero. For this task, it suffices to minimize

$$\begin{aligned}\mathrm{Tr}_S\{\hat{\tilde{w}}^\dagger\hat{\tilde{w}}\}=&\,|\,\langle 0|\hat{\tilde{w}}|0\rangle\,|^2+|\,\langle 1|\hat{\tilde{w}}|1\rangle\,|^2\\&+|\,\langle 1|\hat{\tilde{w}}|0\rangle\,|^2+|\,\langle 0|\hat{\tilde{w}}|1\rangle\,|^2.\end{aligned} \tag{20}$$

The last 2 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. (20) to vanish, yielding

$$\begin{aligned}\lambda_g(t)&=-\int_0^t dt'w_{gg}(t')+\lambda_g^0=i\int_0^t dt'\,\langle g|\dot{g}\rangle+\lambda_g^0,\\\lambda_e(t)&=-\int_0^t dt'w_{ee}(t')+\lambda_e^0=i\int_0^t dt'\,\langle e|\dot{e}\rangle+\lambda_e^0,\end{aligned} \tag{21}$$

and

$$\begin{aligned}\langle 0|\hat{\tilde{w}}|1\rangle&=e^{i(\lambda_e^0-\lambda_g^0)}e^{i\int_0^t dt'[w_{gg}(t')-w_{ee}(t')]}w_{ge}\\&=e^{i(\lambda_e^0-\lambda_g^0)}e^{\int_0^t dt'[\langle g|\dot{g}\rangle-\langle e|\dot{e}\rangle]}w_{ge}.\end{aligned} \tag{22}$$

The phases are not fixed since we have a degree of freedom in the selection of the constant parts. Notice 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 conjuction with our master equation, the optimal phase selection results in w_{gg} and w_{ee} vanishing in Eq. (15).

With the optimal selection, the phase shifted basis states become $|\tilde{g}\rangle=e^{i\lambda_g^0}e^{-\int_0^t dt'\langle g|\dot{g}\rangle}\,|g\rangle$ and $|\tilde{e}\rangle=$

$e^{i\lambda_e^0} e^{-\int_0^t dt' \langle e|\dot{e}\rangle} |e\rangle$. Thus we have $\langle\tilde{g}|\dot{\tilde{g}}\rangle = \langle\tilde{e}|\dot{\tilde{e}}\rangle = 0$ independent of $|g\rangle$ and $|e\rangle$ and the selection renders the phase shifted states to be also invariant under a local gauge change, i.e., $|g\rangle \to e^{i\beta(t)}|g\rangle$ 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

$$\begin{aligned} \lambda_g(t_b) - \lambda_g(t_a) &= i \oint_\gamma \langle g|\dot{g}\rangle\,, \\ \lambda_e(t_b) - \lambda_e(t_a) &= i \oint_\gamma \langle e|\dot{e}\rangle\,, \end{aligned} \tag{23}$$

where we have denoted t_a and t_b as the virtual starting and ending time instances 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.

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. (14) and (15)] 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 $\tilde{w}_{ge} = e^{i(\lambda_e-\lambda_g)}w_{ge}$. If we assume that the approximation of adiabatic rates applies for these phase shifted variables, the master equation can be directly used by replacing the original variables with the shifted ones.

If the above assumption fails to be justified, the accuracy can be improved by taking the geometric phase acquired by the basis into account in estimating the power spectra as

$$\begin{aligned} S(\omega_{01}) &\to S(\omega_{01} + w_{ee} - w_{gg}), \\ S(-\omega_{01}) &\to S(-\omega_{01} + w_{gg} - w_{ee}), \\ S(0) &\to S(0). \end{aligned} \tag{24}$$

However, Eq. (24) depends on the local gauge used to define $|g\rangle$ and $|e\rangle$. Thus the local gauge has to be fixed such that w_{gg} and w_{ee} describe the accumulation speed of the geometric phase for open paths, see Ref. [45].

VI. CONCLUSIONS

We deviced 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 non-steered system. We showed that the master equation we obtain 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, 38]. A detailed study of the efficiency of these two approaches is left for future research.

There exists a degree of freedom in the choice of the phases of the basis states during the evolution. We demonstrated a way to choose the phases in an optimal manner which minimizes the local adiabatic parameter and showed that this choice produces basis states that are invariant under a local gauge change. The accumulated phases for the optimally selected basis states are the Berry phases for a closed loop in the parameter space. Altering the phases of the basis states was shown to induce a shift in the diagonal matrix elements of the adiabatic correction operator, w_{gg} and w_{ee}, enabling us to dispose of them in the off-diagonal part of our master equation (15) using the optimal selection. Furthermore, if the approximation of adiabatic rates is not justified for the phase shifted basis states, a frequency shift may appear in the spectral densities.

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Appendix: Non-steered master equation in the two-state basis

We rewrite the derivative of the reduced density matrix in the interaction picture (Redfield equation [44]) as

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

The transformation from the interaction picture to the Schrödinger picture unfolds when we employ

$$\hat{\rho}_S(t) = \hat{U}_S(t,0)\hat{\sigma}_I(t)\hat{U}_S^\dagger(t,0), \tag{A.2}$$

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

$$\begin{aligned}\rho_{gg}(t) &= \sigma_{I,gg}(t),\\ \rho_{ee}(t) &= \sigma_{I,ee}(t),\\ \rho_{ge}(t) &= e^{i\omega_{01}t}\sigma_{I,ge}(t),\\ \rho_{eg}(t) &= e^{-i\omega_{01}t}\sigma_{I,eg}(t).\end{aligned} \tag{A.3}$$

Derivating Eq. (A.2) yields the transformation of the derivative as

$$\frac{d\hat{\rho}_S(t)}{dt} = \frac{i}{\hbar}[\hat{\rho}_S(t), \hat{H}_S(t)] + \hat{U}_S(t,0)\frac{d\hat{\sigma}_I(t)}{dt}\hat{U}_S^{\dagger}(t,0). \tag{A.4}$$

Using Eqs. (A.1) and (A.4), we define the diagonal matrix element

$$\langle g|\frac{d\hat{\rho}_S(t)}{dt}|g\rangle = -\frac{1}{\hbar^2}\int_0^t dt'\mathrm{Tr}_E\{\langle g|[[\hat{\sigma}_I(t)\otimes\hat{\rho}_E, \hat{V}_I(t')], \hat{V}_I(t)]|g\rangle\}, \tag{A.5}$$

and the off-diagonal matrix element

$$\langle g|\frac{d\hat{\rho}_S(t)}{dt}|e\rangle = i\omega_{01}\rho_{ge}(t) - e^{i\omega_{01}t}\frac{1}{\hbar^2}\int_0^t dt'\mathrm{Tr}_E\{\langle g|[[\hat{\sigma}_I(t)\otimes\hat{\rho}_E, \hat{V}_I(t')], \hat{V}_I(t)]|e\rangle\}, \tag{A.6}$$

for the non-steered master equation. Notice that our derivation is based on assuming that the system relaxation time is long compared to the environment correlation time τ_{corr} so that the environment has no memory, i.e., we are in the Markov regime [39]. This allows us to neglect any variation of $\hat{\sigma}_I(t)$ between times t and $t+\tau_{\mathrm{corr}}$. The integral expressions in Eqs. (A.5) and (A.6) simplify to give Eqs. (5) and (6) when we expand the commutators, use the closure relation for the adiabatic basis, and utilize $\mathrm{Tr}_E\{\hat{\rho}_E\hat{X}(t')\hat{X}(t)\} = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}S_X(\omega)e^{-i\omega(t'-t)}$ and Eq. (A.3). 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 assumption leads to neglecting the Lamb shift.

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