Geometric phase for mixed states: Formulation based on a connection on a vector bundle over a Grassmann manifold

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(Received 21 August 2006; revised manuscript received 16 April 2007; published 27 July 2007)

A geometrical description of open quantum systems is presented. This is based on a connection on a vector bundle over a Grassmann manifold, as well as the Anandan geometric phase for pure states [J. Anandan, Phys. Lett. A **133**, 171 (1988)]. The geometric phase proposed here also naturally includes the geometric phase in adiabatic open quantum systems proposed by Sarandy and Lidar [Phys. Rev. A **73**, 062101 (2006)]. The present geometrical description can be applied to all the quantum systems described by time-local master equations for density operators.

DOI: 10.1103/PhysRevA.76.012120 PACS number(s): 03.65.Vf, 02.40.−k, 03.65.Yz, 03.67.Lx

I. INTRODUCTION

The geometric phase is one of the most interesting concepts in quantum physics [1]. Berry first found that a geometrical phase factor appears, in addition to a dynamical phase factor, in an adiabatic and cyclic quantum evolution with a nondegenerate eigenstate of a Hamiltonian [2]. Simon pointed out that the Berry phase can be regarded as a holonomy on a line bundle over a parameter space [3]. The Berry phase was generalized to the case of a degenerate eigenspace by Wilczek and Zee (WZ) [4]. Interestingly, the Berry and WZ phases have the same mathematical structures as *Abelian* and *non-Abelian* gauge field theories, respectively. Aharonov and Anandan (AA) introduced the nonadiabatic (Abelian) geometric phase [5]. Furthermore, Anandan generalized the AA phase to the non-Abelian one [6]. The AA phase has also been generalized to the noncyclic case by Samuel and Bhandari (SB) [7] by applying Pancharatnam's geometric phase for the interference between two polarized light beams [7,8] to quantum interference.

Recently, geometric phases for mixed states have been extensively studied, especially for geometric quantum computations [9,10]. There are mainly three general approaches to the definition of the mixed-state geometric phase which are based on state purification [11,12], quantum trajectories [13], and quantum interferometry (kinematic approach) [14–19], respectively (see Refs. [20–22] for the other approaches). The first approach proposed by Uhlmann defines a parallel transport for a purification of a density operator [12,23]. A connection is defined on a fiber bundle whose fiber and base manifold are a Hilbert-Schmidt space [24,25] and the manifold of all density operators, respectively. This approach has a problem that the geometric phase depends on the evolution of the ancillary part [26]. The second approach proposed by Carollo *et al.* is based on the application of the SB approach (Pancharatnam's phase) to each quantum trajectory [27]. Very recently, a problem of this approach that the geometric phase depends on the type of unraveling (nonphysical parameters) has been pointed out [28]. The third approach is a natural generalization of the SB approach (Pancharatnam's phase) to the mixed-state case. This approach was first based on quantum interferometry assuming unitary evolution and nondegenerate density operators [14]. The geometric phase by this approach has been experimentally observed with nuclear spins [17] and photons [19]. The generalizations to the cases of degenerate density operators [16] and nonunitary evolution [18] have been achieved by kinematic approaches. While the geometric phase by this kinematic approach is well defined, this does not correspond to a generalization of the pure-state non-Abelian geometric phases such as the WZ and Anandan phases [4,6,29]. Recently, the proposals to unify the purification and kinematic approaches have been reported [30,31]. In the case of nonunitary evolution, however, the same problem as the purification approach arises [31]. Very recently, Sarandy and Lidar (SL) have proposed a natural generalization of the WZ phase to the mixed-state case [21], which is based on adiabatic approximation in open quantum systems [32]. In this paper, we propose another formulation of the geometric phase for mixed states, which is a natural generalization of the Anandan phase [6]. The geometric phase proposed here also naturally includes the SL phase.

This paper is organized as follows. In Sec. II, a vector representation for density operators is introduced. In Sec. III, a geometric structure for density operators is defined. The geometric phase for mixed states in the present formulation is also proposed. In Sec. IV, a geometric description of open quantum systems in the present formulation is presented. In Sec. V, a simple example is discussed. This is stimulated Raman adiabatic passage (STIRAP) [10,33,34] with dephasing. The conclusion is presented in Sec. VI.

II. VECTOR REPRESENTATION OF DENSITY OPERATORS

Consider a quantum system described by an N-dimensional complex Hilbert space $\mathcal{H}_N(\mathbf{C})$. The Anandan phase for pure states is based on a connection on a vector bundle over a Grassmann manifold, $G_{n,N}(\mathbf{C})$, where $G_{n,N}(\mathbf{C})$ is the set of n-dimensional subspaces of $\mathcal{H}_N(\mathbf{C})$ [6,35–39]. Each point on $G_{n,N}(\mathbf{C})$ corresponds to a subspace of $\mathcal{H}_N(\mathbf{C})$. The fiber over a point on $G_{n,N}(\mathbf{C})$ is the vector space corresponding to the point. Similarly, our approach is also based

on a connection on a vector bundle over a Grassmann manifold. We use the *Hermitian* Hilbert-Schmidt space [24,25], $\mathcal{H}_{N^2}(\mathbf{R})$, instead of $\mathcal{H}_N(\mathbf{C})$, to describe density operators. $\mathcal{H}_{N^2}(\mathbf{R})$ is an N^2-dimensional *real* Hilbert space spanned by the following Hermitian operators:

$$|k\rangle\rangle \equiv |k\rangle\langle k| \quad \text{for } k = 1,2,\ldots,N,$$

$$|N+1\rangle\rangle \equiv \frac{|1\rangle\langle 2| + |2\rangle\langle 1|}{\sqrt{2}}, \quad |N+2\rangle\rangle \equiv \frac{|1\rangle\langle 2| - |2\rangle\langle 1|}{\sqrt{2}i}, \ldots$$

$$|N^2-1\rangle\rangle \equiv \frac{|N-1\rangle\langle N| + |N\rangle\langle N-1|}{\sqrt{2}},$$

$$|N^2\rangle\rangle \equiv \frac{|N-1\rangle\langle N| - |N\rangle\langle N-1|}{\sqrt{2}i},$$

where $\{|k\rangle | k=1,\ldots,N\}$ is an orthonormal basis of $\mathcal{H}_N(\mathbf{C})$ [40]. The inner product is defined as

$$(w,v) \equiv \langle\langle w|v\rangle\rangle \equiv \mathrm{Tr}[wv], \tag{1}$$

where $w,v \in \mathcal{H}_{N^2}(\mathbf{R})$. $\{|k\rangle\rangle | k=1,2,\ldots,N^2\}$ is an orthonormal basis of $\mathcal{H}_{N^2}(\mathbf{R})$ with respect to the above inner product [41]. Any density operator can be expressed as

$$|\rho\rangle\rangle = \sum_{k=1}^{N^2} \rho_k |k\rangle\rangle, \tag{2}$$

where ρ_k $(k=1,2,\ldots,N^2)$ are real coefficients.

III. GEOMETRIC STRUCTURE FOR DENSITY OPERATORS

We use a Grassmann manifold, $G_{n,N^2}(\mathbf{R})$, which is the set of n-dimensional subspaces of $\mathcal{H}_{N^2}(\mathbf{R})$. We also define a vector bundle, $\mathcal{V}_n$, over $G_{n,N^2}(\mathbf{R})$ whose fiber over a point on $G_{n,N^2}(\mathbf{R})$ is the vector space corresponding to the point. A connection is defined as

$$\nabla |v_k\rangle\rangle \equiv \sum_{j=1}^{n} |v_j\rangle\rangle\langle\langle v_j|d|v_k\rangle\rangle \equiv \sum_{j=1}^{n} |v_j\rangle\rangle \mathcal{A}_{j,k}, \tag{3}$$

where ∇ and d denote the covariant and exterior derivatives, respectively, and $\{|v_k\rangle\rangle | k=1,2,\ldots,n\}$ is an orthonormal basis of $V_n \in G_{n,N^2}(\mathbf{R})$. The one-form $\mathcal{A}_{j,k}$ is regarded as a gauge field in gauge field theory [39]. This type of connection is fundamental from a mathematical point of view [6,36,37,42,43]. The covariant derivative for $|\rho\rangle\rangle = \sum_{j=1}^{n} \alpha_j |v_j\rangle\rangle \in V_n$ is defined as

$$\nabla |\rho\rangle\rangle \equiv \sum_{k=1}^{n} |v_k\rangle\rangle\langle\langle v_k|d|\rho\rangle\rangle = \sum_{j=1}^{n} (d\alpha_j |v_j\rangle\rangle + \alpha_j \nabla |v_j\rangle\rangle). \tag{4}$$

From the definition of $\mathcal{A}_{j,k}$, under a so-called gauge transformation $|v'_k\rangle\rangle = \sum_{j=1}^{n} g_{j,k} |v_j\rangle\rangle$, $\mathcal{A}_{j,k}$ transforms as a gauge field:

$$\mathcal{A}'_{j,k} = \sum_{j',k'=1}^{n} g^{-1}_{j,j'} \mathcal{A}_{j',k'} g_{k',k} + \sum_{j'=1}^{n} g^{-1}_{j,j'} dg_{j',k}, \tag{5}$$

where $\mathcal{A}'_{j,k}$ corresponds to the connection for the new basis. As a result, $\nabla |\rho\rangle\rangle$ is gauge invariant, that is, independent of the choice of the basis. The parallel transport condition is given by $\nabla |\rho\rangle\rangle = 0$. Let $\mathcal{C}$ be a curve represented by $V_n(s)$ on $G_{n,N^2}(\mathbf{R})$. The horizontal lift, $|\rho(s)\rangle\rangle$, of $\mathcal{C}$ is given by

$$|\rho(s)\rangle\rangle = \sum_{j=1}^{n} \alpha_j(s) |v_j(s)\rangle\rangle, \tag{6}$$

$$\vec{\alpha}(s) = P \exp\left[-\int_{\mathcal{C}} \mathcal{A} \right] \vec{\alpha}(0), \tag{7}$$

where $\{|v_j(s)\rangle\rangle\}$ is an orthonormal basis of $V_n(s)$, $\vec{\alpha} = (\alpha_1,\ldots,\alpha_n)^T$ (T denotes transpose), P denotes path ordering, and $\mathcal{A}$ is the matrix-valued one-form whose elements are $\mathcal{A}_{j,k}$. When $\mathcal{C}$ is closed, $P \exp[-\oint_{\mathcal{C}} \mathcal{A}]$ is the holonomy and is gauge invariant. This holonomy is the geometric phase factor for the density operator in the present formulation [44]. In general, the present geometric phase factors are non-Abelian.

IV. GEOMETRIC DESCRIPTION OF OPEN QUANTUM SYSTEMS

Next, we consider the time evolution of a mixed state. In most cases, the evolution of a density operator is determined by a master equation. We consider master equations in the following form:

$$\frac{d}{dt} |\rho(t)\rangle\rangle = \mathcal{L}(t) |\rho(t)\rangle\rangle, \tag{8}$$

with

$$\mathcal{L}(t) \equiv \sum_{k,l} \mathcal{L}_{k,l}(t) |k\rangle\rangle\langle\langle l|, \tag{9}$$

where $\mathcal{L}_{k,l}(t)$ are real numbers. This master equation is local in time in the sense that the time derivative of $\rho(t)$ at any time t is determined by $\rho(t)$, and no time integration is necessary [25,45]. An important example of the time-local master equation is a Lindblad-form master equation [21,25,32,46]. While the Lindblad-form master equations can be applied only to Markovian processes, general time-local master equations can describe non-Markovian processes [25,45]. Here, we consider the case where $|\rho(t)\rangle\rangle$ is confined in a time-dependent n-dimensional subspace $V_n(t)$ of $\mathcal{H}_{N^2}(\mathbf{R})$. Then, $|\rho(t)\rangle\rangle$ can be expressed as $|\rho(t)\rangle\rangle = \sum_{k=1}^{n} \alpha_k(t) |v_k(t)\rangle\rangle$, where $\{|v_k(t)\rangle\rangle\}$ is an orthonormal basis of $V_n(t)$. By applying the projection operator, $\sum_{j=1}^{n} |v_j(t)\rangle\rangle\langle\langle v_j(t)|$, onto $V_n(t)$ to the right-hand and left-hand sides of Eq. (8), we obtain

$$\nabla|\rho\rangle\rangle = dt\sum_{j=1}^{n}|v_j\rangle\rangle\langle\langle v_j|\mathcal{L}|\rho\rangle\rangle, \tag{10}$$

where Eq. (4) has been used. It should be noted that Eq. (10) is obviously gauge invariant. The equation for $\alpha_j(t)$ is given by

$$d\alpha_j + \sum_{k=1}^{n}\mathcal{A}_{j,k}\alpha_k = dt\sum_{k=1}^{n}\langle\langle v_j|\mathcal{L}|v_k\rangle\rangle\alpha_k. \tag{11}$$

$\Sigma_{k=1}^{n}\mathcal{A}_{j,k}\alpha_k$ and $dt\Sigma_{k=1}^{n}\langle\langle v_j|\mathcal{L}|v_k\rangle\rangle\alpha_k$ in Eq. (11) can be regarded as geometrical and dynamical parts, respectively [47]. The formal solution for Eq. (11) is

$$\vec{\alpha}(t) = P\exp\left[-\int\mathcal{A} + \int W(t)dt\right]\vec{\alpha}(0), \tag{12}$$

where $W(t)$ is the matrix whose elements are $\langle\langle v_j(t)|\mathcal{L}(t)|v_k(t)\rangle\rangle$. Thus it is found that if an open quantum system is described by a time-local master equation and is confined in a time-dependent subspace of $\mathcal{H}_{N^2}(\mathbf{R})$, then the time evolution is given by a matrix consisting of the geometrical and dynamical parts. This is the geometrical description of an open quantum system in the present formulation. Since in general $\mathcal{A}$ and $W(t)$ is not commutable with each other, the geometrical and dynamical phase factors cannot be separated from each other. If W is zero or negligible, Eqs. (10) and (12) reduce to $\nabla|\rho\rangle\rangle=0$ (parallel transport condition) and Eq. (7), respectively. Then, the evolution of the open quantum system is purely geometrical and corresponds to the horizontal lift of the curve $V_n(t)$ on $G_{n,N^2}(\mathbf{R})$. Furthermore, if the evolution is cyclic (the curve is closed), the evolution is given by the geometric phase factor (holonomy), $P\exp[-\oint\mathcal{A}]$, proposed here.

As in the case of the Anandan phase [6], we can formulate geometric phases based on a connection on a vector bundle over a parameter space, if a set of parameters $\vec{R}(t)$ determines the subspace $V_n(t)$ of $\mathcal{H}_{N^2}(\mathbf{R})$ in which the state is confined. The vector bundle over the parameter space is naturally induced by $\mathcal{V}_n$ with respect to the mapping $V_n(\vec{R})$ [43]. This formulation based on a connection on the induced bundle is significant for applications to quantum-state manipulation, since we can control quantum states geometrically if the above parameters are controllable. A typical example of this situation is an adiabatic evolution of an open quantum system [21,32]. Thus it turns out that the geometric phase proposed here naturally includes the SL phase [21,22,48].

V. EXAMPLE: STIMULATED RAMAN ADIABATIC PASSAGE WITH DEPHASING

Finally, we discuss a simple example. The example is stimulated Raman adiabatic passage (STIRAP) [10,33,34] in a Λ configuration in the four-level system depicted in Fig. 1. This has been used for the geometric realization of a single-qubit rotation in Ref. [10]. The Hamiltonian is given by

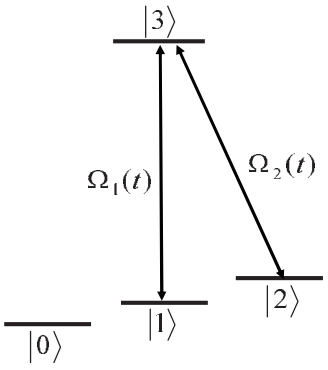

FIG. 1. Four-level system used for the example. $\Omega_j(t)$ $(j=1,2)$ is the Rabi frequency corresponding to the $|j\rangle$-$|3\rangle$ transition.

$$H(t) = i\frac{\hbar}{2}\sum_{j=1,2}[\Omega_j(t)|3\rangle\langle j| - \Omega_j^*(t)|j\rangle\langle 3|], \tag{13}$$

where Ω_1 and Ω_2 are the Rabi frequencies corresponding to the $|1\rangle$-$|3\rangle$ and $|2\rangle$-$|3\rangle$ transitions, respectively, and are set as $\Omega_1=-\Omega e^{\phi}\sin(\theta/2)$ and $\Omega_2=\Omega\cos(\theta/2)$, where Ω is a positive constant. It is assumed that θ varies from $\theta=0$ to $\theta=0$, and the initial state is a superposition of $|0\rangle$ and $|1\rangle$. This Hamiltonian has the following dark state (nontrivial zero-eigenvalue eigenstate): $|D\rangle=\cos(\theta/2)|1\rangle+e^{i\phi}\sin(\theta/2)|2\rangle$. In the pure-state case, the STIRAP process via the dark state provides $|1\rangle$ with the Berry phase factor $e^{i\Theta}$, where $\Theta=i\int\langle D|d|D\rangle=-\int\sin\theta d\theta d\phi$ [10].

To consider the mixed-state case, the dephasing for all the transitions is taken into account [49]. For simplicity, the dephasing rates are assumed to be equal to one another and be much smaller than Ω. The master equation is given by

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] + \frac{\gamma}{6}\left[\sum_{j>k}(\sigma_{j,j}-\sigma_{k,k})\rho(\sigma_{j,j}-\sigma_{k,k}) - 3\rho\right], \tag{14}$$

where γ is the dephasing rate and $\sigma_{k,k}\equiv|k\rangle\langle k|$. The density operator can be expressed as $|\rho\rangle\rangle=\Sigma_{k=1}^{16}\rho_k|k\rangle\rangle$, and then Eq. (14) has the form $\frac{d}{dt}\rho_j=\Sigma_{k=1}^{16}\mathcal{L}_{j,k}\rho_k$. By diagonalizing the matrix $\mathcal{L}$, it is found that $|\rho\rangle\rangle\simeq\Sigma_{k=1}^{6}\alpha_k|v_k\rangle\rangle\in V_6(t)\in G_{6,4^2}(\mathbf{R})$, where

$$|v_1\rangle\rangle = |0\rangle\langle 0|, |v_2\rangle\rangle = \frac{|1\rangle\langle 1|+|2\rangle\langle 2|+|3\rangle\langle 3|}{\sqrt{3}},$$

$$|v_3\rangle\rangle = \frac{3|D\rangle\langle D|-\sqrt{3}|v_2\rangle\rangle}{\sqrt{6}}, \quad |v_4\rangle\rangle = \frac{|D\rangle\langle 0|+|0\rangle\langle D|}{\sqrt{2}},$$

$$|v_5\rangle\rangle = \frac{|D\rangle\langle 0|-|0\rangle\langle D|}{\sqrt{2}i}, \quad |v_6\rangle\rangle = \frac{|3\rangle\langle B|-|B\rangle\langle 0|}{\sqrt{2}i},$$

with $|B\rangle=-e^{-i\phi}\sin(\theta/2)|1\rangle+\cos(\theta/2)|2\rangle$. $\vec{\alpha}(t_f)$ (t_f: the time at which the process finishes) can be expressed as follows under some approximation [50]:

$$\vec{\alpha}(t_f) = M_G M_D \vec{\alpha}(0), \tag{15}$$

with

$$M_G \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos\Theta & \sin\Theta & 0 \\ 0 & 0 & 0 & -\sin\Theta & \cos\Theta & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{16}$$

$$M_D \equiv \mathrm{diag}(1,1,e^{-\Gamma(t_f)},e^{-\gamma t_f},e^{-\gamma t_f},e^{-\gamma t_f}), \tag{17}$$

where Θ is the Berry phase defined above, $\Gamma(t) \equiv \frac{3}{4}\gamma\int_0^t \sin^2\theta(t')dt'$, and $\mathrm{diag}(a_1,\ldots,a_6)$ denotes a 6×6 diagonal matrix whose diagonal elements are $a_1,\ldots,a_6$. M_G and M_D correspond to the geometrical and dynamical phase factors, respectively, in the present formulation. It should be noted that in the present case the geometrical and dynamical phases are commutable, and consequently the evolution of $\vec{\alpha}$ can be given by the product of M_G and M_D. The rotation matrix M_G is exactly equivalent to the Berry phase factor in the pure-state case. This means that the present formulation is a natural generalization of the pure-state geometric phase. On the other hand, M_D induces the decay of the polarization and leads to the uniform distribution of the populations of $|1\rangle$, $|2\rangle$, and $|3\rangle$. Although the present case is similar to adiabatic open quantum systems considered in Refs. [21,22], the simple results derived above may not be naturally obtained from the formulation of Ref. [21] (see Ref. [51] for the reason).

VI. CONCLUSION

We have presented a geometrical description of open quantum systems, which is a generalization of Anandan's formulation for pure states [6] to the mixed-state case. The geometric phase proposed here also naturally includes the geometric phase in adiabatic open quantum systems proposed by Sarandy and Lidar [21], and is expected to be applied to the nonadiabatic case. The geometric description can be applied to all the quantum systems described by time-local master equations in the form of Eq. (8). We have discussed an example using Λ-type STIRAP in a four-level system with dephasing. As a result, the followings have been found: in this case, the mixed-state geometrical and dynamical phase factors in the present formulation are separable from each other; the mixed-state geometric phase factor is equivalent to the Berry phase factor in the pure-state case; and the mixed-state dynamical phase factor induces the decay of the polarization and leads to the uniform distribution of the population. The geometrical description presented here will provide a deeper understanding of the dynamics of open quantum systems.

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[41] $\mathcal{H}_{N^2}(\mathbf{C})$ is the standard Hilbert-Schmidt space, and the inner product on $\mathcal{H}_{N^2}(\mathbf{C})$ is defined by $(w,v)\equiv\mathrm{Tr}[w^\dagger u]$. But here, we use $\mathcal{H}_{N^2}(\mathbf{R})$ instead of $\mathcal{H}_{N^2}(\mathbf{C})$ to remove redundancy. As a result of the use of the real space, the present geometric phase is nontrivial only in multidimensional cases, in contrast to the Anandan phase. [Since the one-dimensional Grassmann manifold, $G_{1,N}$, is the projective space, the famous AA phase is the Anandan phase in the one-dimensional case [6].]
[42] M. S. Narasimhan and S. Ramanan, Am. J. Math. **83**, 563 (1961).
[43] The present connection is related to a universal connection [6,36,37,42]. The Grassmann manifold is more fundamental than the other parameter space in the sense that a connection on some bundle over some parameter space is naturally induced from that on a bundle over the corresponding Grassmann manifold.
[44] It should be noted that the present geometric phase factor depends only on the closed curve on the Grassmann manifold, not on the dynamical details of the system. Also note that a standard phase factor of the form $e^{i\theta}$ is represented by a rotation matrix in the present formulation as a result of the use of a real space. See the example of STIRAP discussed here.
[45] H.-P. Breuer, Phys. Rev. A **70**, 012106 (2004).
[46] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).
[47] It is notable that Eq. (11) has the same form as the classical equation of motion for a charged particle in gravitational and electromagnetic fields in the general theory of relativity [see, for example, L. D. Landau and E. M. Lifschitz, *The Classical Theory of Fields* (Pergamon Press, 1975)], which is given by

$$du^j + (\Gamma^j_{k,l}dx^l)u^k = \frac{e}{mc^2}dsF^{j,k}u_k,$$

where x^j and u^j denote the four-dimensional position and velocity vectors of the particle, respectively, s denotes the proper time, $\Gamma^j{}_{k,l}$ are so-called Christoffel's symbols, F is an electromagnetic tensor, e and m are the charge and mass of the particle, respectively, c is the speed of light in vacuum, and Einstein's rule for the summation of dummy indices has been used.
[48] The present definition for adiabatic evolutions is a little different from that of Ref. [21]. But, this difference may not be essential.
[49] For simplicity, the spontaneous emission from the excited state $|3\rangle$ is ignored.
[50] We have confirmed by numerical calculation that Eq. (15) holds well when $\gamma \ll \Omega$ and the process is sufficiently slow.
[51] In Ref. [21], the case of one-dimensional Jordan blocks with different eigenvalues, which the present case is, was not discussed because this case may not satisfy their adiabatic condition. This point becomes clearer by comparing the present example with the analysis in Ref. [22]. In Ref. [22], only the case of Jordan blocks with the same eigenvalues was discussed.