

Time-convolutionless reduced-density-operator theory of a noisy quantum channel: Two-bit quantum gate for quantum-information processing

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An exact reduced-density-operator for the output quantum states in time-convolutionless form was derived by solving the quantum Liouville equation which governs the dynamics of a noisy quantum channel by using a projection operator method and both advanced and retarded propagators in time. The formalism developed in this work is general enough to model a noisy quantum channel provided specific forms of the Hamiltonians for the system, reservoir, and the mutual interaction between the system and the reservoir are given. Then we apply the formulation to model a two-bit quantum gate composed of coupled spin systems in which the Heisenberg coupling is controlled by the tunneling barrier between neighboring quantum dots. Gate characteristics, including the entropy, fidelity, and the purity, are calculated numerically for both mixed and entangled initial states.

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I. INTRODUCTION

There has been considerable interest in the quantum theory of information and computation for the past several years [1–16]. Especially, quantum-mechanical properties of coding [3,4], noisy channels including error-correcting codes [5–8] and channel fidelity [9], and computation [10–15] have been studied in detail. It was shown [13,14] that any quantum computation procedure can be decomposed into operations on a single-bit gate and a two-bit gate which involves an entanglement operation on two quantum bits or qubits. The presence of decoherence and imperfections causes the operations of these quantum gates away from the ideal ones and as a result one can regard these gates as a part of noisy quantum channels. Detailed analysis of these channels are necessary for the complete understanding of the general quantum information process. Mathematically, the dynamics of quantum channels or generalized quantum gates involves the transformation of input quantum states represented by a density operator ρ into an output state ρ' [16], i.e.,

$$\rho \xrightarrow{\mathcal{E}} \rho' = \mathcal{E}[\rho], \quad (1)$$

where we assume \mathcal{E} is a linear mapping but is not necessarily a unitary transformation if one considers an open system interacting with the reservoir such as noisy quantum channels. A model of noisy quantum channels would involve several Hamiltonians for the system representing qubits, the reservoir, and the mutual interaction between the system and the reservoir that causes the decoherence or noise. The density operator is then governed by the quantum Liouville

equation [17] which is an integro-differential equation and, in general, it is nontrivial to obtain the solution of the form given by Eq. (1). Rather, one is expected to get the solution for the density operator for the output states in a Volterra-type integral equation:

$$\rho(t) = A(t,0)\rho(0) + \int d\tau B(t,\tau)\rho(\tau), \quad (2)$$

where A is a propagator and B is a memory kernel. In general, it is very difficult to solve for the memory kernels of the time-convolution form equation (2) self-consistently and almost always, one must be content with the narrowing limit or the fast modulation limit [20].

Some time ago, the time-convolutionless equations of motion in the Heisenberg picture was suggested by Tokuyama and Mori [18] to overcome the above-mentioned difficulties for problems in nonequilibrium statistical mechanics. These formulations were then developed in the Schrödinger picture by using the projection operator technique [19–21]. One of the authors applied the time-convolutionless formulation to the model of quantum devices for detailed numerical study [22–25]. It was shown that the time-convolutionless formulation can also incorporate both non-Markovian relaxation and renormalization of the memory effects.

Recently, Loss and DiVincenzo [15] made a comprehensive study of the two-bit quantum gate, taking into account the effect of decoherence on the gate operation using the reduced density operator in the time-convolution formulation. Their results indicate that the detailed analysis of the decoherence process is important for the reliable operation of quantum gates which utilize the controlled, nonequilibrium time evolution of solid-state spin systems.

In order to make the reduce-density operator for the output quantum states of the form given by Eq. (1), several approximations, including the Born approximation, were made in their theory. In our opinion, it would be more convenient if there is a way to get the exact solution for the output density-operator in time-convolutionless form given by Eq. (1).

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In this paper we first derive the exact solution for the reduced-density-operator of the output quantum states in time-convolutionless form by solving the quantum Liouville equation for a quantum channel using the projection operator method. The formalism we develop in this paper is general enough to model a realistic quantum channel or a quantum gate. Secondly, we apply the theory to model a two-bit quantum gate composed of coupled spin systems in which the Heisenberg coupling is controlled by the tunneling barrier between neighboring single electron quantum dots.

II. TIME-CONVOLUTIONLESS REDUCED-DENSITY-OPERATOR THEORY OF A QUANTUM SYSTEM INTERACTING WITH A RESERVOIR

In this section we study the quantum Liouville equation for a quantum system which corresponds to a quantum channel or a generalized quantum gate to derive an equation and to solve for a reduced-density-operator of a system coupled to a reservoir. An interaction between the system and the reservoir leads to decoherence. The Hamiltonian of the total system is assumed to be

$$H_T(t) = H_S(t) + H_B + H_{\text{int}}, \quad (3)$$

where $H_S(t)$ is the Hamiltonian of the system representing a quantum gate (or channel), H_B the reservoir and H_{int} the Hamiltonian for the interaction of the system with its reservoir. The evolution of the system might include a coding, transmission, and decoding process. The equation of motion for the density operator $\rho_T(t)$ of the total system is given by a quantum Liouville equation

$$\frac{d}{dt} \rho_T(t) = -i[H_T, \rho_T] = -iL_T \rho_T, \quad (4)$$

where

$$L_T(t) = L_S(t) + L_B + L_{\text{int}}$$

is the Liouville superoperator in one-to-one correspondence with the Hamiltonian. In this work we use a unit where $\hbar = 1$. In order to derive an equation and to solve for a system alone, it is convenient to use the projection operators [26,27] that decompose the total system by eliminating the degrees of freedom for the reservoir. We define time-independent projection operators \underline{P} and \underline{Q} as [19]

$$\underline{P}X = \rho_B \text{tr}_B(X), \quad \underline{Q} = 1 - \underline{P}, \quad (5)$$

for any dynamical variable X . Here tr_B indicates a partial trace over the quantum reservoir. Projection operators satisfy the operator identity $\underline{P}^2 = \underline{P}$, $\underline{Q}^2 = \underline{Q}$, and $\underline{P}\underline{Q} = \underline{Q}\underline{P} = 0$. The information of the system is then contained in the reduced density operator $\rho(t)$ which is defined by

$$\rho(t) = \text{tr}_B \rho_T(t) = \text{tr}_B \underline{P} \rho_T(t). \quad (6)$$

In order to derive a time-convolutionless equation, we first multiply Eq. (4) by \underline{P} and \underline{Q} to obtain coupled equation for $\underline{P}\rho_T(t)$ and $\underline{Q}\rho_T(t)$:

$$\frac{d}{dt} \underline{P}\rho_T(t) = -i\underline{P}L_T \underline{P}\rho_T(t) + i\underline{P}L_T(t)\underline{Q}\rho_T(t), \quad (7)$$

$$\frac{d}{dt} \underline{Q}\rho_T(t) = -i\underline{Q}L_T \underline{Q}\rho_T(t) + i\underline{Q}L_T(t)\underline{P}\rho_T(t). \quad (8)$$

We assume that the channel was turned on at $t=0$ and the input state prepared at $t=0$, $\rho(t=0)$ was isolated with the reservoir at $t=0$, i.e., $\underline{Q}\rho_T(0) = 0$ [19].

The formal solution of (8) is given by [22]

$$\underline{Q}\rho_T(t) = -i \int_0^t d\tau \underline{H}(t, \tau) \underline{Q}L_T(\tau) \underline{P}\rho_T(\tau), \quad (9)$$

where the projected propagator $\underline{H}(t, \tau)$ of the total system is given by

$$\underline{H}(t, \tau) = \underline{T} \exp \left\{ -i \int_{\tau}^t ds \underline{Q}L_T(s) \underline{Q} \right\}. \quad (10)$$

Here \underline{T} denotes the time-ordering operator. Because Eq. (9) is in time-convolution form, we transform the memory kernel in Eq. (9) into time-convolutionless form [22] by substituting the formal solution of Eq. (4)

$$\rho_T(\tau) = \underline{G}(t, \tau) \rho_T(t) \quad (11)$$

into Eq. (9). The antitime evolution operator $\underline{G}(t, \tau)$ of the total system is defined by

$$\underline{G}(t, \tau) = \underline{T}^c \exp \left\{ i \int_{\tau}^t ds L_T(s) \right\},$$

where \underline{T}^c is the antitime-ordering operator. From Eqs. (9) and (11), we obtain

$$\underline{Q}\rho_T(t) = \{\theta(t) - 1\} \underline{P}\rho_T(t) \quad (12)$$

where

$$\theta^{-1}(t) = g(t) = 1 + i \int_0^t d\tau \underline{H}(t, \tau) \underline{Q}L_T(\tau) \underline{P}\underline{G}(t\tau). \quad (13)$$

By substituting Eq. (12) into Eq. (7), we obtain the time-convolutionless equation of motion for $\underline{P}\rho_T(t)$ as

$$\frac{d}{dt} \underline{P}\rho_T(t) = -i\underline{P}L_T(t)\underline{P}\rho_T(t) - i\underline{P}L_T(t)\{\theta(t) - 1\}\underline{P}\rho_T(t). \quad (14)$$

It can be shown that the formal solution of Eq. (14) is given by

$$\begin{aligned} \underline{P}\rho_T &= \underline{U}(t,0)\underline{P}\rho_T(0) - i \int_0^t ds \underline{U}(t,s)\underline{P}L_T(s) \\ &\times \{\theta(s) - 1\}\underline{P}\rho_T(s), \end{aligned} \quad (15)$$

$$\underline{U}(t,\tau) = \underline{T} \exp \left\{ -i \int_0^t ds \underline{P}L_T(s)\underline{P} \right\}. \quad (16)$$

To transform Eq. (15) into time-convolutionless form once again, we substitute

$$\rho_T(s) = \underline{G}(t,s)\rho_T(t) \quad (17)$$

where the projected propagator $\underline{U}(t,\tau)$ of the system is defined by

into (15) to obtain

$$\begin{aligned} \underline{P}\rho_T(t) &= \underline{U}(t,0)\underline{P}\rho_T(0) - i \int_0^t ds \underline{U}(t,s)\underline{P}L_T(s)\{\theta(s) - 1\}\underline{P}\underline{G}(t,s)\rho_T(t) \\ &= \underline{U}(t,0)\underline{P}\rho_T(0) - i \int_0^t ds \underline{U}(t,s)\underline{P}L_T(s)\{\theta(s) - 1\}\underline{P}\underline{G}(t,s)\underline{P}\rho_T(t) - i \\ &\times \int_0^t ds \underline{U}(t,s)\underline{P}L_T(s)\{\theta(s) - 1\}\underline{P}\underline{G}(t,s)\underline{Q}\rho_T(t) \\ &= \underline{U}(t,0)\underline{P}\rho_T(0) - i \int_0^t ds \underline{U}(t,s)\underline{P}L_T(s)\{\theta(s) - 1\}\underline{P}\underline{G}(t,s)\theta(t)\underline{P}\rho_T(t). \end{aligned} \quad (18)$$

By the way,

$$\underline{P}\rho_T(t) = \rho_B \text{tr}_B(\rho_T(t)) = \rho_B \rho(t) \quad (19)$$

and

$$\underline{P}L_T(t)\underline{P} = \underline{P}(L_S(t) + L_B + L_{\text{int}})\underline{P} = \underline{P}L_S(t)\underline{P} = L_S(t)\underline{P}. \quad (20)$$

Then

$$\begin{aligned} \underline{U}(t,0)\underline{P}\rho_T(0) &= \underline{T} \exp \left\{ -i \int_0^t ds \underline{P}L_T(s)\underline{P} \right\} \underline{P}\rho_T(0) \\ &= \underline{T} \exp \left\{ -i \int_0^t ds L_S(s)\underline{P} \right\} \underline{P}\rho_T(0) \\ &= \underline{U}_S(t,0)\underline{P}\rho_T(0) = \underline{U}_S(t,0)\rho_B \rho(t). \end{aligned} \quad (21)$$

Here $\underline{U}_S(t,0)$ denotes the propagator of the system. Likewise,

$$\begin{aligned} &\underline{U}(t,s)\underline{P}L_T(s)\{\theta(s) - 1\}\underline{P}\underline{G}(t,s)\theta(t)\underline{P}\rho_T(t) \\ &= \underline{U}_S(t,s)\rho_B \text{tr}_B[L_T(s)\{\theta(s) - 1\}\rho_B] \\ &\times \text{tr}_B[\underline{G}(t,s)\theta(t)\rho_B]\rho(t) \\ &= \underline{U}_S(t,s)\rho_B \text{tr}_B[L_T(s)\{\theta(s) - 1\}\rho_B] \\ &\times \text{tr}_B[\underline{G}(t,s)\theta(t)\rho_B]\rho(t). \end{aligned} \quad (22)$$

Substituting Eqs. (21) and (22) into Eq. (18), we obtain

$$\begin{aligned} \rho(t) &= \underline{U}_S(t,0)\rho(0) - i \int_0^t ds \underline{U}_S(t,s)\text{tr}_B[L_T(s)\{\theta(s) - 1\}\rho_B] \\ &\times \text{tr}_B[\underline{G}(t,s)\theta(t)\rho_B]\rho(t) \end{aligned} \quad (23)$$

or

$$\rho(t) = \mathcal{E}(t)\rho(0) = \underline{W}^{-1}(t)\underline{U}_S(t,0)\rho(0), \quad (24)$$

with

$$\begin{aligned} \underline{W}(t) &= 1 + i \int_0^t ds \underline{U}_S(t,s)\text{tr}_B[L_T(s)\{\theta(s) - 1\}\rho_B] \\ &\times \text{tr}_B[\underline{G}(t,s)\theta(t)\rho_B] \\ &= 1 + i \int_0^t ds \underline{U}_S(t,s)\text{tr}_B[L_{\text{int}}\underline{\Sigma}(s) \\ &\times \{1 - \underline{\Sigma}(s)\}^{-1}\rho_B]\text{tr}_B[\underline{U}_0(s)\underline{R}(t,s)\underline{U}_0^{-1}(t) \\ &\times \{1 - \underline{\Sigma}(t)\}^{-1}\rho_B]. \end{aligned} \quad (25)$$

Here, we define

$$\underline{\Sigma}(t) = 1 - \theta^{-1}(t), \quad (26)$$

$$\underline{U}_0(t) = e^{-itL_B}\underline{U}_S(t), \quad (27)$$

and

$$\underline{R}(t,\tau) = \underline{T}^c \exp \left\{ i \int_\tau^t ds \underline{U}_0^{-1}(s)L_{\text{int}}\underline{U}_0 \right\}, \quad (28)$$

where $\underline{U}_0(t)$ is the evolution operator of the system with the reservoir and $\underline{R}(t, \tau)$ is the evolution operator [21] of the total system in the interacting picture. In Eq. (25), we use the identities $\underline{P}L_\tau(s)\underline{Q} = \underline{P}L_{\text{int}}\underline{Q}$ and $\underline{H}(t, \tau)\underline{Q} = \underline{Q}\underline{H}(t, \tau)$.

Detailed expression for $\underline{\Sigma}(t)$ becomes

$$\begin{aligned}\Sigma(t) &= 1 - \theta^{-1}(t) = -i \int_0^t d\tau \underline{H}(t, \tau) \underline{Q} L_\tau(\tau) \underline{P} \underline{G}(t, \tau) \\ &= -i \int_0^t d\tau \underline{H}(t, \tau) \underline{Q} L_{\text{int}}(\tau) \underline{P} \underline{G}(t, \tau) \\ &= -i \int_0^t d\tau \underline{U}_0(t) \underline{S}(t, \tau) \underline{U}_0^{-1} \underline{Q} L_{\text{int}} \underline{P} \underline{U}_0(\tau) \\ &\quad \times \underline{R}(t, \tau) \underline{U}_0^{-1}(t),\end{aligned}\quad (29)$$

with

$$\underline{S}(t, \tau) = \underline{T} \exp \left\{ -i \int_\tau^t ds \underline{Q} \underline{U}_0^{-1}(s) L_{\text{int}} \underline{U}_0(s) \underline{Q} \right\}, \quad (30)$$

where $\underline{S}(t, \tau)$ is the projected propagator [21] of the total system in the interaction picture. It is now obvious from (24) and (25), the exact solution $\rho(t)$ for the output quantum state is in time-convolutionless form given by Eq. (1) which is employed in the description of quantum information processing and computation [16].

We now consider the case when the system is interacting weakly with the reservoir and we expand Eq. (25) up to the second order in powers of the interaction Hamiltonian H_{int} . The renormalization of the unperturbed energy of the system and the first order of the interaction H_{int} gives [19–21]

$$\underline{P}L_{\text{int}}\underline{P} = 0. \quad (31)$$

Then in the lowest-order Born approximation, which is valid up to the order $(H_{\text{int}})^2$, we obtain

$$\begin{aligned}\underline{W}^{(2)}(t) &= 1 + i \int_0^t ds \underline{U}_S(t, s) \text{tr}_B [L_{\text{int}} \underline{\Sigma}^{(1)}(s) \rho_B] \\ &\quad \times \text{tr}_B [\underline{U}_0(s) \underline{U}_0^{-1}(t) \rho_B] \\ &= 1 + i \int_0^t ds \underline{U}_S(t, s) \text{tr}_B [L_{\text{int}} \underline{\Sigma}^{(1)}(s) \rho_B] \underline{U}_S^{-1}(t, s),\end{aligned}\quad (32)$$

or

$$\begin{aligned}[\underline{W}^{(2)}(t)]^{-1} &= 1 - i \int_0^t ds \underline{U}_S(t, s) \\ &\quad \times \text{tr}_B [L_{\text{int}} \underline{\Sigma}^{(1)}(s) \rho_B] \underline{U}_S^{-1}(t, s),\end{aligned}\quad (33)$$

and

$$\begin{aligned}\underline{\mathcal{E}}^{(2)} &= \left(1 - i \int_0^t ds \underline{U}_S(t, s) \text{tr}_B [L_{\text{int}} \underline{\Sigma}^{(1)}(s) \rho_B] \underline{U}_S^{-1}(t, s) \right) \\ &\quad \times \underline{U}_S(t, 0).\end{aligned}\quad (34)$$

Here

$$\begin{aligned}\underline{\Sigma}^{(1)}(s) &= -i \int_0^s d\tau \underline{U}_0(s) \underline{U}_0^{-1}(\tau) \underline{Q} L_{\text{int}} \underline{P} \underline{U}_0(\tau) \underline{U}_0^{-1}(s) \\ &= -i \int_0^s d\tau \underline{U}_0(s, \tau) L_{\text{int}} \underline{U}_0^{-1}(s, \tau).\end{aligned}\quad (35)$$

The time-convolutionless form of the output reduced-density operator

$$\rho(t) = \underline{\mathcal{E}}^{(2)}(t) \rho(0), \quad (36)$$

together with Eqs. (32)–(35), can be used in any time scale and is valid up to the second order in powers in the interaction between the system and the reservoir.

In Sec. III the reduced-density operator for the output quantum state is used to study the two-bit quantum gate utilizing a coupled spin system in a nonequilibrium situation.

III. DECOHERENCE OF TWO-BIT QUANTUM GATE

We consider a two-bit quantum gate based on nonequilibrium dynamics of the spin of excess electrons in quantum dots [15]. In this system, the gate operation is controlled by an electrical tunneling between two quantum dots. Projecting out the spatial parts of wave functions of electrons, we model the system by the Hubbard Hamiltonian [28],

$$H_S(t) = J(t) \vec{S}_1 \cdot \vec{S}_2, \quad (37)$$

where $J(t)$ is the time-dependent Heisenberg coupling which involves the energy difference between the spin singlet and triplet states. If we turn on $J(t)$ for $\int dt J(t) = J_0 \tau_s = \pi$, the unitary operator associated with the Hamiltonian (37) gives the swap operation up to the overall phase difference; if $|i, j\rangle$ labels the spin states of two electrons in the S_z basis with $i, j = \uparrow, \downarrow$, then the swap operation U_{swap} on two registers $|i, j\rangle$ gives $U_{\text{swap}} |i, j\rangle = |j, i\rangle$.

In reality, the quantum-dot system of our interest is not a closed system, so we have to take into account the decoherence effects due to the interaction with the environment which is coupled with the system. For the action of the environment during the gate operation, we use a Caldeira-Leggett-type model [29] where a set of harmonic oscillators are coupled linearly to the system spins by

$$H_{\text{int}} = \lambda (\vec{S}_1 \cdot \vec{b}_1 + \vec{S}_2 \cdot \vec{b}_2). \quad (38)$$

Here, $b_i^j = \sum_\alpha g_\alpha (a_{\alpha, i}^j + a_{\alpha, i}^{j \dagger})$ is a fluctuating quantum field whose unperturbed motion is governed by the harmonic-oscillator Hamiltonian,

$$H_B(t) = \sum_\alpha \omega_\alpha a_\alpha^\dagger a_\alpha \quad (39)$$

where a_α^\dagger (a_α) is bosonic creation (annihilation) operator and ω_α are the corresponding frequencies with spectral distribution function $A(\omega) = \pi \sum_\alpha g_\alpha^2 \delta(\omega - \omega_\alpha)$.

For a coupled spin system, the evolution operator $\mathcal{E}^{(2)}$

given by Eq. (34) can be written down explicitly in terms of spin operators. Substituting Eqs. (37)–(39) into definitions for \underline{U}_0 and L_{int} , the integrand of Eq. (34) can be written as

$$\begin{aligned} \text{tr}_B[L_{\text{int}}\Sigma^{(1)}(s)\rho_B]\underline{U}_S^{-1}(t,s)\underline{U}_S(t,0)\rho(0) &= -i \int_0^s d\tau \text{tr}_B[L_{\text{int}}\underline{U}_0(s,\tau)L_{\text{int}}\underline{U}_0^{-1}(s,\tau)\rho_B]\underline{U}_S(s,0)\rho(0) \\ &= -i\lambda^2 \sum_{ijkl} \int_0^s d\tau \{S_i^j, S_k^l(\tau-s)[\underline{U}_S(s,0)\rho(0)]\} \text{tr}_B[b_k^j b_l^i(\tau-s)\rho_B] \\ &\quad + \{[\underline{U}_S(s,0)\rho(0)]S_k^l(\tau-s), S_i^j\} \text{tr}_B[b_k^l(\tau-s)b_i^j\rho_B] \\ &= -i \sum_{ij} \int_0^s d\tau \{S_i^j, S_i^j(\tau-s)[\underline{U}_S(s,0)\rho(0)]\} [\Gamma(\tau-s) - i\Delta(\tau-s)] \\ &\quad + \{[\underline{U}_S(s,0)\rho(0)]S_i^j(\tau-s), S_i^j\} [\Gamma(\tau-s) + i\Delta(\tau-s)], \end{aligned} \quad (40)$$

where the trace over the heat bath is done for the harmonic-oscillator eigenstates,

$$\text{tr}_B[b_k^l(t)b_i^j\rho_B] = \delta_{ik}\delta_{jl} \frac{1}{\pi} \int_0^\infty A(\omega) \left\{ e^{-i\omega t} + \frac{2 \cos(\omega t)}{e^{\omega/k_B T} - 1} \right\} d\omega, \quad (41)$$

and we define $\Gamma(t)$ and $\Delta(t)$ as

$$\Gamma(t) + i\Delta(t) = \lambda^2 \text{Tr}_B[b_i^j(t)b_j^i\rho_B]. \quad (42)$$

Then, Eq. (34) leads to

$$\underline{\mathcal{E}}^{(2)} = \underline{U}_S(t,0) \left[1 - \int_0^t ds \int_0^s d\tau \sum_{ij} \{ [S_i^j(s), S_i^j(\tau)\rho(0)] [\Gamma(\tau-s) - i\Delta(\tau-s)] + [\rho(0)S_i^j(\tau), S_i^j(s)] [\Gamma(\tau-s) + i\Delta(\tau-s)] \} \right]. \quad (43)$$

Now we evaluate the density operator in the multiplet basis representation; $\rho(t) = \sum_{\alpha\beta} \rho_{\alpha\beta}(t) e_{\alpha\beta}$, $e_{\alpha\beta}$ is the basis for the density operators, and in this work we chose $e_{\alpha\beta}$ as the multiplet states, i.e., $e_{\alpha\beta} = |\alpha\rangle\langle\beta|$ with $\alpha, \beta = 1, 2, 3, 4$; $|1\rangle = |\uparrow\uparrow\rangle$, $|2\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$, $|3\rangle = |\downarrow\downarrow\rangle$, and $|4\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. By defining the inner product as $(e_{\alpha\beta}, e_{\gamma\delta}) = \text{tr}[e_{\alpha\beta}^\dagger e_{\gamma\delta}] = \delta_{\alpha\beta}\delta_{\gamma\delta}$, $\rho_{\alpha\beta}(t)$ is obtained as

$$\begin{aligned} \rho_{\alpha\beta} &= (e_{\alpha\beta}, \rho(t)) = (e_{\alpha\beta}, \mathcal{E}^{(2)}\rho(0)) \\ &= \sum_{\gamma\delta} (e_{\alpha\beta}, \mathcal{E}^{(2)}e_{\gamma\delta}) \rho(0)_{\gamma\delta} = \sum_{\gamma\delta} \mathcal{E}_{\alpha\beta|\gamma\delta}^{(2)} \rho(0)_{\gamma\delta}, \end{aligned} \quad (44)$$

where $\rho(0)_{\gamma\delta}$ expansion coefficients of the initial density operator. Without the interaction with the environment, i.e., the absence of the second term in Eq. (43), $\mathcal{E}_{\alpha\beta|\gamma\delta}^{(2)}$ is reduced to $U_S(t)_{\alpha\beta|\gamma\delta}$ and is evaluated on the multiplet basis as

$$(e_{\alpha\beta}, U_S(t)e_{\gamma\delta}) = \delta_{\alpha\beta}\delta_{\gamma\delta} e^{-i\bar{t}(E_\alpha - E_\beta)}, \quad (45)$$

where $E_{1,2,3} = J_0/4$ and $E_4 = -3J_0/4$ are the triplet and singlet energy eigenvalues. Here, \bar{t} has its value $t(\tau_s)$ if t is less (larger) than τ_s . Then, $\underline{U}_S(t)$ becomes the swap operator, $\underline{U}_S(t) = e^{-i\pi/4} \underline{U}_{\text{swap}}$ if $t = \tau_s$.

In order to evaluate $\mathcal{E}^{(2)}$, we first calculate the following matrix elements:

$$\begin{aligned} \left(e_{\alpha\beta}, \sum_{ij} [S_i^j(s), S_i^j(\tau)e_{\gamma\delta}] \right) &= \sum_{ij} \{ \langle \alpha | S_i^j(s) S_i^j(\tau) | \gamma \rangle \langle \delta | \beta \rangle \\ &\quad - \langle \alpha | S_i^j(\tau) | \gamma \rangle \langle \delta | S_i^j(s) | \beta \rangle \} \\ &= \delta_{\delta\beta} \sum_{\kappa} M_{\alpha\kappa\kappa\gamma} e^{i\bar{\tau}\omega_{\kappa\gamma} + i\bar{s}\omega_{\alpha\kappa}} \\ &\quad - M_{\alpha\gamma\delta\beta} e^{i\bar{\tau}\omega_{\alpha\gamma} + i\bar{s}\omega_{\delta\beta}} \end{aligned} \quad (46)$$

and

$$\begin{aligned}
\left(e_{\alpha\beta} \cdot \sum_{ij} [e_{\gamma\delta} S_i^j(\tau), S_i^j(s)] \right) &= \sum_{ij} \{ \langle \delta | S_i^j(\tau) S_i^j(s) | \beta \rangle \langle \alpha | \gamma \rangle \\
&\quad - \langle \alpha | S_i^j(s) | \gamma \rangle \langle \delta | S_i^j(\tau) | \beta \rangle \} \\
&= \delta_{\alpha\gamma} \sum_{\kappa} M_{\delta\kappa\kappa\beta} e^{i\bar{\tau}\omega_{\delta\kappa} + i\bar{s}\omega_{\kappa\beta}} \\
&\quad - M_{\alpha\gamma\delta\beta} e^{i\bar{\tau}\omega_{\delta\beta} + i\bar{s}\omega_{\alpha\gamma}}, \quad (47)
\end{aligned}$$

where $M_{\alpha\beta\gamma\delta} = \sum_{ij} \langle \alpha | S_i^j | \beta \rangle \langle \gamma | S_i^j | \delta \rangle$, $\omega_{\alpha\beta} = E_{\alpha} - E_{\beta}$, and

$$\bar{\tau}(\bar{s}) = \begin{cases} \tau(s) & \text{if } \tau(s) < \tau_s \\ \tau_s & \text{otherwise.} \end{cases}$$

Then, the matrix element of the evolution operator $\mathcal{E}_{\alpha\beta|\gamma\delta}^{(2)}$ is obtained by substituting Eqs. (45)–(47) into Eq. (43),

$$\begin{aligned}
\mathcal{E}_{\alpha\beta|\gamma\delta}^{(2)} &= e^{-i\bar{t}\omega_{\alpha\gamma}} \left[\delta_{\alpha\gamma} \delta_{\beta\delta} - \delta_{\beta\delta} \sum_{\kappa} M_{\alpha\kappa\kappa\gamma} P_{\kappa\kappa|\gamma\alpha}(t) \right. \\
&\quad - \delta_{\alpha\gamma} \sum_{\kappa} M_{\delta\kappa\kappa\beta} P_{\delta\kappa|\gamma\beta}^*(t) + M_{\alpha\gamma\delta\beta} \{ P_{\alpha\beta|\gamma\delta}(t) \\
&\quad \left. + P_{\beta\alpha|\delta\gamma}^*(t) \} \right] \quad (48)
\end{aligned}$$

with the time-dependent term $p_{\alpha\beta|\gamma\delta}(t)$ defined by

$$p_{\alpha\beta|\gamma\delta}(t) = \int_0^t ds e^{-i\bar{s}\omega_{\beta\delta}} \int_0^s d\tau e^{i\bar{\tau}\omega_{\alpha\gamma}} [\Gamma(\tau-s) - i\Delta(\tau-s)]. \quad (49)$$

For numerical calculations, it is more convenient to split the time integrals of the matrix $p_{\alpha\beta|\gamma\delta}(t)$ into three parts,

$$\begin{aligned}
p_{\alpha\beta|\gamma\delta}(t) &= \int_0^{\tau_s} ds e^{-is\omega_{\beta\delta}} \int_0^s d\tau e^{i\tau\omega_{\alpha\gamma}} [\Gamma(\tau-s) - i\Delta(\tau-s)] + \int_{\tau_s}^t ds e^{-i\tau_s\omega_{\beta\delta}} \int_0^{\tau_s} d\tau e^{i\tau\omega_{\alpha\gamma}} [\Gamma(\tau-s) - i\Delta(\tau-s)] \\
&\quad + \int_{\tau_s}^t ds e^{-i\tau_s\omega_{\beta\delta}} \int_{\tau_s}^s d\tau e^{i\tau_s\omega_{\alpha\gamma}} [\Gamma(\tau-s) - i\Delta(\tau-s)] \\
&= \int_0^{\tau_s} ds e^{is(\omega_{\delta\beta} + \omega_{\alpha\gamma})} \int_0^s d\tau e^{i\tau\omega_{\gamma\alpha}} [\Gamma(\tau) + i\Delta(\tau)] + e^{i\tau_s\omega_{\delta\beta}} \int_{\tau_s}^t ds e^{is\omega_{\alpha\gamma}} \int_{s-\tau_s}^s d\tau e^{i\tau\omega_{\gamma\alpha}} [\Gamma(\tau) + i\Delta(\tau)] \\
&\quad + e^{i\tau_s(\omega_{\delta\beta} + \omega_{\alpha\gamma})} \int_{\tau_s}^t ds \int_0^{s-\tau_s} d\tau [\Gamma(\tau) + i\Delta(\tau)]. \quad (50)
\end{aligned}$$

In order to investigate the dynamics of the density operator in a nonequilibrium situation, we calculate Eqs. (44)–(50) numerically, assuming an Ohmic damping for the spectral distribution function $A(\omega) = \eta\omega$ with a cutoff frequency ω_c [30].

IV. NUMERICAL RESULTS AND DISCUSSIONS

We now study the dynamics of the density operator for various initial states. First, we calculate the evolution of the spin states during the swap gate operation and compare our results with those obtained by Loss and DiVincenzo [15]. The initial spin state is chosen to be the spin-up for the second electron while the first electron is unpolarized; $\rho(0) = (|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|)/2$. In the multiplet basis, the initial state is expanded as

$$\rho(0) = \frac{1}{2} |1\rangle\langle 1| + \frac{1}{4} |2\rangle\langle 2| - \frac{1}{4} |2\rangle\langle 4| - \frac{1}{4} |4\rangle\langle 2| + \frac{1}{4} |4\rangle\langle 4|. \quad (51)$$

Figure 1(a) shows the spin polarization calculated using parameters $\lambda^2 \eta = 1.8 \times 10^{-5}$, $T = 300$ K, $\omega_c = 400$ K, and $J_0 = 1$ K (solid lines). For the interval, $0 \leq t \leq \tau_s$ the spin polarization of the first electron $s = 2\langle S_z^1 \rangle = 2 \text{tr}[\rho(t) S_z^1]$

changes to nearly a unity whereas the spin state of the second electron becomes zero (dashed line), demonstrating the feasibility of the swap operation. However, due to the decoherence, we find that a perfect swap operation cannot be achieved. In addition, the perturbing fields cause the monotonic decreases of the spin polarization with the elapse of time after the completion of the swap operation. This means that spin states are becoming thermalized owing to the interaction with the environment, which shows the decoherence of the states. The decoherence would be a fundamental problem in making a reliable quantum logic gate, which puts severe restriction on building the realistic quantum computer. However, there are several quantum error-correction techniques that can compensate for imperfections introduced by the decoherence during and after the gate operation [5–8]. Comparing with the result obtained in the previous work [15] (dotted line), we find that both calculations yield similar results for $t > \tau_s$, except for the value at $t = \tau_s$. We think that the discrepancy at $t = \tau_s$ results from a somewhat simplified evaluation of the evolution operator in Ref. [15] when the swap operation occurs.

In Figs. 1(b) and 1(c) we plot the gate fidelity F and gate purity P which characterize the intrinsic properties of the gate, and they are defined as [31]

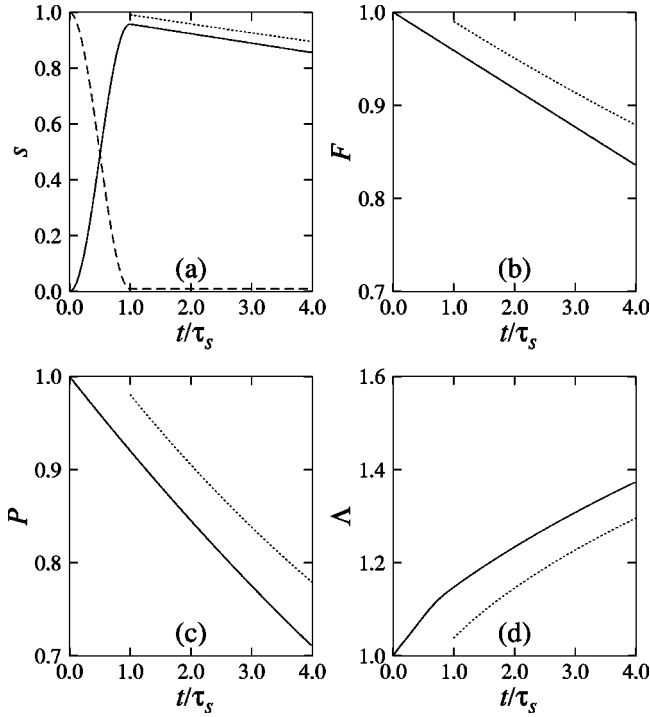


FIG. 1. The calculated spin polarization (s), fidelity (F), purity (P), and entropy (Λ) are plotted as a function of time (solid lines), and compared with those obtained in Ref. [15] (dotted lines). We assume that the first electron is unpolarized on the initial state with the second polarized upward. For $0 \leq t \leq \tau_s$, the swap operation is made by turning on $J(t)$ and, then, $J(t) = 0$.

$$F = \overline{\langle \psi_0 | U_S^\dagger(\bar{t}) \rho(t) | \psi_0 \rangle} \\ = \frac{1}{6} + \frac{1}{24} \left[\sum_{\alpha} \mathcal{E}_{\alpha\alpha}^{(2)} + \sum_{\alpha, \beta} \mathcal{E}_{\alpha\beta}^{(2)} e^{i\bar{t}\omega_{\alpha\beta}} \right], \quad (52)$$

$$P = \overline{\text{tr}[\rho(t)]^2} = \frac{1}{24} \sum_{\alpha, \beta, \gamma} \left[|\mathcal{E}_{\alpha\beta|\gamma\gamma}^{(2)}|^2 \right. \\ \left. + \sum_{\delta} (\mathcal{E}_{\alpha\beta|\gamma\gamma}^{(2)} \mathcal{E}_{\alpha\beta|\delta\delta}^{(2)*} + |\mathcal{E}_{\alpha\beta|\gamma\delta}^{(2)}|^2) \right], \quad (53)$$

where the overbar means an average over all possible initial states $|\psi_0\rangle$ and $U_S(\bar{t})$ is an ideal gate operation that was turned on during the time interval, $0 \leq t \leq \tau_s$. The last equalities in Eqs. (52) and (53) were derived under the condition of both trace and Hermiticity of $\mathcal{E}^{(2)}$ being preserved within our approximation scheme. For an ideal quantum gate, the gate fidelity F and the gate purity P must be equal to one during the gate operation because in that case the evolution operator is unitary. Our calculation shows that both F and P are found to decrease almost linearly as time elapses, which indicates clearly the presence of the decoherence effect. As is the case of the spin polarization, the decreasing rates for F and P are close to those obtained in Ref. [15]; however, its value at

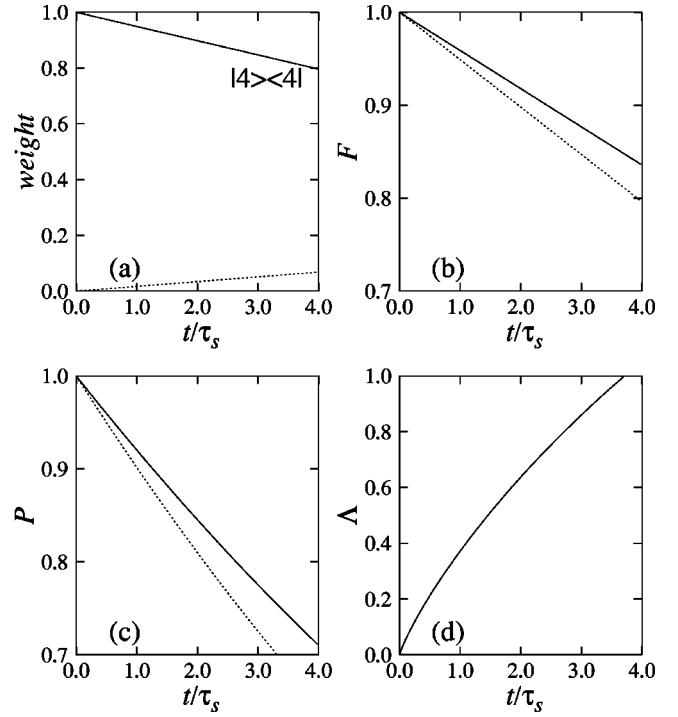


FIG. 2. For the initial density operator ρ_{44} , we show diagonal components of the density operator as time elapses in (a). In this figure ρ_{44} decreases monotonically (solid line) whereas others of diagonal components become larger (dotted lines). In (b) and (c), the fidelity and purity are shown with (solid line) and without (dotted line) an average over the initial states. The evolution of the entropy as plotted in (d) starts from zero because the initial state is pure.

$=\tau_s$ is different and our results show more severe decoherence of the spin state for the same parameters.

Another interesting property of the two-bit gates is the von Neumann entropy Λ defined as $\Lambda = -\text{tr}[\rho(t) \log_2 \rho(t)]$ of a quantum state. In Fig. 1(d), the calculated von Neumann entropy of the spin system is plotted. For the initial density operator of Eq. (51), its entropy is $\Lambda = 1$ (bit) because the eigenvalues of $\rho(0)$ are $\{0, 0, 1/2, 1/2\}$. As time goes on, the entropy becomes larger because the thermalization makes the system reside equally in all states. Eventually, the entropy will reach the maximum value of $\Lambda = 2$ (bits) where all four states are equally probable.

To examine the effect of the perturbing field on an entangled state, we now consider a different initial density operator. We assume that the system is in a pure spin singlet at $t=0$; $|\psi_0\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ and its density operator is $\rho(0) = |\psi_0\rangle\langle\psi_0|$. In Fig. 2(a), we plot the diagonal components of the density operators in the multiplet basis as a function of time. In this figure, ρ_{44} (solid line) loses its coherence linearly to time while other components $\rho_{\alpha\alpha}$ grows as time elapses. This behavior gives rise to an increasing value of the entropy as shown in Fig. 2(d). We also compare the fidelity [$\langle \psi_0 | U_S^\dagger(\bar{t}) \rho(t) | \psi_0 \rangle$] of a given entangled pure state (dotted line) with the gate fidelity (solid line) in Fig. 2(c) and the purity [$\text{tr} \rho(t)^2$] of a given initial entangled state

(dotted line) with gate purity (solid line) in Fig. 2(d). In both quantities, there is a slight difference between the cases of entangled initial state and gate. This implies that although the gate fidelity F and gate purity P define the global characteristics of gate, the fidelity and purity of the gate for a specific input state depends on the input itself.

Now, we discuss the strength of the decoherence which depends on $\Gamma(t)$ and $\Delta(t)$ of Eq. (43)

$$\begin{aligned} \Gamma(t) + i\Delta(t) &= \frac{\lambda^2 \eta}{\pi} \int_0^{\omega_c} \omega \cos \omega t \coth \left[\frac{\omega}{2k_B T} \right] d\omega \\ &\quad - i \frac{\lambda^2 \eta}{\pi} \int_0^{\omega_c} \omega \sin \omega t d\omega. \end{aligned} \quad (54)$$

For a sufficiently high temperature $k_B T \gg \omega_c/2$, $\Gamma(t)$ and $\Delta(t)$ are further simplified to

$$\Gamma(t) + i\Delta(t) = \frac{2\Gamma_0}{\pi\tau_s} \frac{\sin \omega_c t}{t} - i \frac{\Delta_0}{\tau_s} \left[\frac{\sin \omega_c t}{\omega_c t^2} - \frac{\cos \omega_c t}{t} \right] \quad (55)$$

with $\Gamma_0 = \lambda^2 \eta k_B T \tau_s$ and $\Delta_0 = \lambda^2 \eta \omega_c \tau_s / \pi$. Since a typical value of τ_s is 25 psec for $J_0 = 1$ K and, thus $\omega_c \tau_s \gg 1$, $\Gamma(t)$ and $\Delta(t)$ are rapidly oscillating functions. This implies that the dominant contribution to the decoherence can be written as $\Gamma(t) + i\Delta(t) = 2\Gamma_0 \delta(t) / \tau_s$ in the limit of $\omega_c \tau_s \gg 1$. In this approximation we find that $p_{\alpha\beta|\gamma\delta}(t)$ of Eq. (50) is proportional to $\Gamma_0 t$. This behavior is attributed to a linear dependence of various quantities (s, F, P) on time. In addition, we expect that the degradation of the spin polarization is also proportional to $\Gamma_0 t$. For this, we examine the evolution of the spin polarization of the first electron for the initial density operator of Eq. (51) for various values of the coupling constant, $\lambda^2 \eta$, and we plot results in Fig. 3(a). As $\lambda^2 \eta$ increases, we find that more strong decoherence occurs in spin states and its dependence is linear on $\lambda^2 \eta$ as shown in Fig. 3(b). This linear dependence also appears in the fidelity and purity.

In summary, we first derive an exact reduced-density operator for the output quantum states in time-convolutionless form by solving the quantum Liouville equation for a noisy quantum channel. The formalism developed in this paper would be general enough to model a noisy quantum channel if various Hamiltonians for a channel dynamics, environment and an interaction are given. Secondly, we calculated various characteristics including the fidelity, purity, and the change of entropy of a two-bit quantum gate which is based on the spin exchange interaction between two quantum dots. Our calculation shows it is really important to control the decoherence in the quantum gate to protect quantum information against corruption. The decoherence in the quantum logic gate could be a major obstacle to build the realistic quantum computer; however, it is expected that as long as the error rate is below some threshold value, a quantum computer which can give arbitrary accurate answers can be built with a reasonable model of decoherence. In this respect, it will be

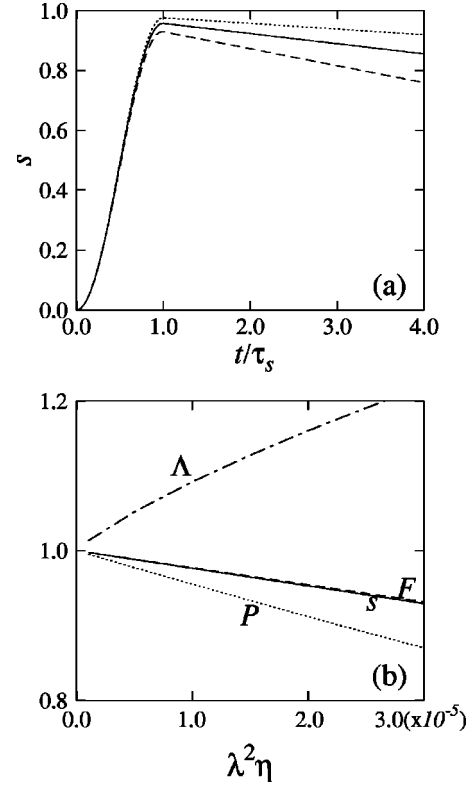


FIG. 3. For various values of the dimensionless coupling constant, $\lambda^2 \eta = 0.5 \times 10^{-5}$ (dotted), 1.8×10^{-5} (solid), and 3.0×10^{-5} (dashed), we show the evolution of the spin polarization of the first electron in (a) for the initial density of Eq. (51). In (b), the degradation of the spin polarization (s), fidelity (F), purity (P), and entropy (Λ) are compared for different parameters $\lambda^2 \eta$ at $t = \tau_s$.

interesting to investigate the implementation of a quantum error correction technique for this model. Another interesting study on the present model is to find an operator sum representation for the evolution operator \mathcal{E} :

$$\mathcal{E}[\rho] = \sum_{\mu} A_{\mu} \rho A_{\mu}^{\dagger}, \quad (56)$$

where A_{μ} is an operator acting on the system alone. With the operator sum representation, we can calculate various information theoretical quantities such as the coherent information, entropy exchange, and the channel capacity [16]. We would like to leave this subject for future work.

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