# Quantitative evaluation of decoherence and applications for quantum-dot charge qubits

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#### Abstract

We review results on evaluation of loss of information in quantum registers due to their interactions with the environment. It is demonstrated that an optimal measure of the level of quantum noise effects can be introduced via the maximal absolute eigenvalue norm of deviation of the density matrix of a quantum register from that of ideal, noiseless dynamics. For a semiconductor quantum dot charge qubits interacting with acoustic phonons, explicit expressions for this measure are derived. For a broad class of environmental modes, this measure is shown to have the property that for small levels of quantum noise it is additive and scales linearly with the size of the quantum register.

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#### 1 Introduction

In recent years, there has been significant progress in quantum computation and design of solid-state quantum information processors [1 - 16]. Quantum computers promise enormous speed-up of computation of certain very important problems, including factorization of large numbers [1] and search [2].

However, practically useful quantum information processing devices have not been made yet. One of the major obstacles to scalability has been decoherence. This is due to the fact that the effect of quantum speed-up is crucially dependent upon the coherence of quantum registers. Therefore, understanding the dynamics of coherence loss has drawn significant experimental and theoretical effort.

In general, decoherence [17 - 38] reveals itself in most experiments with quantum objects. It is a process whereby the quantum coherent physical system of interest interacts with the environment and, because of this interaction, changes its evolution from unperturbed "ideal" dynamics. The change of the dynamics is reflected by the corresponding change of the density matrix [39 - 43] of the system. The time-dependence of the system's density matrix should be evaluated for an appropriate model of the system and its environment. If a multi-particle quantum system is considered then the respective density matrix becomes rather large and difficult to deal with. This occurs even for relatively small quantum registers containing just a few quantum bits (qubits). In this paper, we review evaluation of decoherence effects starting from the system Hamiltonian and followed by the definition and estimation of a decoherence error-measure in a quantum information processing "register" composed of several qubits.

The paper is organized as follows: In Section 2, we consider a specific example of a solid state nanostructure. As a representative model for a qubit, we consider an electron in a semiconductor double quantum dot system. We derive the evolution of the density matrix of the electron, which losses coherence due to interaction with phonons. In Section 3, we define a measure characterizing decoherence and show how to calculate it from the density matrix elements for a semiconductor double quantum dot system introduced earlier. Finally, in Section 4, we establish that the measure of decoherence introduced, is additive for several-qubit registers, i.e., the total "computational error" scales linearly with the number of qubits.

## 2 Semiconductor Quantum Dot Charge Qubit

Solid-state nanostructures attracted much attention recently as a possible basis for large scale quantum information processing [44]. Most stages of their fabrication can be borrowed from existing fabrication steps in microelectronics industry. Also, only microelectronics technology has demonstrated the ability to create and control locally evolution of thousands of nano-objects, which is required for quantum computation. There were sev-

eral proposals for semiconductor qubits, reviewed, e.g., in [24]. In particular, the encoding of quantum information in the position of the electron was investigated in [45 - 49]. In [50] it was argued that an electron in a typical quantum dot will loose coherence very fast which will prevent it from being a good qubit. However, this problem can be resolved with sophisticated designs of quantum-dot arrangements, e.g., arrays of several quantum dots, if properly designed [51], can form a coherent quantum register. It was also shown that a symmetric layout of just two quantum dots can strongly diminish decoherence effects due to phonons and other environmental noises [52 - 54].

Recent successful observations [55 - 59] of spatial evolution of an electron in symmetric semiconductor double dot systems have experimentally confirmed that such a system is capable of maintaining coherence at least on time scales sufficient for observation of several cycles of quantum dynamics. In the above experiments measurements were performed at very low substrate temperatures of few tens of mK, in order to avoid additional thermally activated sources of decoherence. Theoretical results on the influence of the temperature on the first-order phonon relaxation rates in double dot systems were presented in [60, 61].

In view of the above experimental advances, we have chosen a single electron in semiconductor double quantum dot system, whose dynamics is affected by vibrations of the crystal lattice, as a representative example of a quantum coherent system interacting with the environment. In the range of parameters corresponding to experiments [55, 57 - 59] phonons dominate decoherence. Of course, for different systems or for similar systems in different ranges of external conditions some other sources of decoherence may prevail, for example, noise due to hopping of charge carries on nearby traps, studied in [62, 63], or due to the electron-electron interaction [64].

Semiconductor double quantum dot creates three-dimensional double well confinement potential for electron in it. Let us denote the line connecting centers of the dots as the x-axis. Then the electron confining potential along x, is schematically shown in Fig. 1. The nanostructure is composed of two quantum dots with a potential barrier between them. Parameters of the structure are properly adjusted so that two lower energy levels of spatial quantization lie very close to each other compared to the external temperature and to the distances to higher energy levels. Therefore hopping of the electron to higher levels is suppressed. The electron is treated as a superposition of two basis states,  $|0\rangle$  and  $|1\rangle$ , corresponding to "false" and "true" in Boolean logic,

$$\psi = \alpha \psi_0 + \beta \psi_1. \tag{1}$$

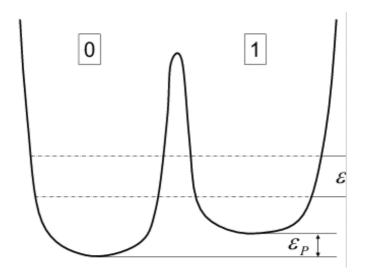


Figure 1: Double well potential.

It should be noted that the states that define the "logical" basis are not the ground and first excited states of the double-dot system. Instead,  $\psi_0$  (the "0" state of the qubit) is chosen to be localized at the first quantum dot and, in a zeroth order approximation, be similar to the ground state of that dot if it were isolated. Similarly,  $\psi_1$  (the "1" state) resembles the ground state of the second dot (if it were isolated). This assumes that the dots are sufficiently (but not necessarily exactly) symmetric. We denote the coordinates of the potential minima of the dots (dot centers) as vectors  $\mathbf{R}_0$  and  $\mathbf{R}_1$ , respectively. The separation between the dot centers is

$$\mathbf{L} = \mathbf{R}_1 - \mathbf{R}_0. \tag{2}$$

The Hamiltonian of an electron interacting with a phonon bath consists of three terms

$$H = H_e + H_p + H_{ep}. (3)$$

The electron term is

$$H_e = -\frac{1}{2}\varepsilon_A(t)\sigma_x - \frac{1}{2}\varepsilon_P(t)\sigma_z,\tag{4}$$

where  $\sigma_x$  and  $\sigma_z$  are Pauli matrices, whereas  $\varepsilon_A(t)$  and  $\varepsilon_P(t)$  can have time-dependence, as determined by unitary single-qubit quantum gate-functions to be implemented for specific quantum algorithm. This can be achieved by

adjusting the potential on the metallic nanogates surrounding the double-dot system. For constant  $\varepsilon_A$  and  $\varepsilon_P$ , the energy splitting between the electron energy levels is

$$\varepsilon = \sqrt{\varepsilon_A^2 + \varepsilon_P^2}. (5)$$

The Hamiltonian term of the phonon bath is described by

$$H_p = \sum_{\mathbf{q},\lambda} \hbar \omega_q b_{\mathbf{q},\lambda}^{\dagger} b_{\mathbf{q},\lambda}, \tag{6}$$

where  $b_{\mathbf{q},\lambda}^{\dagger}$  and  $b_{\mathbf{q},\lambda}$  are the creation and annihilation operators of phonons, respectively, with the wave vector  $\mathbf{q}$  and polarization  $\lambda$ . We approximate the acoustic phonon spectrum as isotropic one with a linear dispersion

$$\omega_q = sq,\tag{7}$$

where s is the speed of sound in the semiconductor crystal.

In the next few paragraphs we show that the electron-phonon interaction can be expressed as

$$H_{ep} = \sum_{\mathbf{q},\lambda} \sigma_z \left( g_{\mathbf{q},\lambda} b_{\mathbf{q},\lambda}^{\dagger} + g_{\mathbf{q},\lambda}^* b_{\mathbf{q},\lambda} \right), \tag{8}$$

with the coupling constants  $g_{\mathbf{q},\lambda}$  determined by the geometry of the doubledot and the properties of the material. The derivation follows [53, 54]. The piezoacoustic electron-phonon interaction [65] is given by

$$H_{ep} = i \sum_{\mathbf{q}, \lambda} \sqrt{\frac{\hbar}{2\rho sqV}} M_{\lambda}(\mathbf{q}) F(\mathbf{q}) (b_{\mathbf{q}} + b_{-\mathbf{q}}^{\dagger}), \tag{9}$$

where  $\rho$  is the density of the semiconductor, V is volume of the sample, and for the matrix element  $M_{\lambda}(\mathbf{q})$ , one can derive

$$M_{\lambda}(\mathbf{q}) = \frac{1}{2q^2} \sum_{ijk} (\xi_i q_j + \xi_j q_i) q_k M_{ijk}.$$
 (10)

Here  $\xi_j$  are the polarization vector components for polarization  $\lambda$ , while  $M_{ijk}$  express the electric field as a linear response to the stress,

$$E_k = \sum_{ij} M_{ijk} S_{ij}. (11)$$

For a crystal with zinc-blende lattice, like GaAs, the tensor  $M_{ijk}$  has only those components non-zero for which all three indexes i, j, k are different; furthermore, all these components are equal,  $M_{ijk} = M$ . Thus, we have

$$M_{\lambda}(\mathbf{q}) = \frac{M}{q^2} (\xi_1 q_2 q_3 + \xi_2 q_1 q_3 + \xi_3 q_1 q_2). \tag{12}$$

The form factor  $F(\mathbf{q})$  accounting for that we are working with electrons which are not usual plane waves, is given by

$$F(\mathbf{q}) = \sum_{j,k} c_j^{\dagger} c_k \int d^3 r \phi_j^*(\mathbf{r}) \phi_k(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}}, \tag{13}$$

where  $c_k$ ,  $c_j^{\dagger}$  are the annihilation and creation operators of the basis states k, j = 0, 1. In quantum dots formed by a repulsive potential of nearby gates, an electron is usually confined near the potential minima, which are approximately parabolic. Therefore the ground states in each dot have Gaussian shape

$$\phi_j(\mathbf{r}) = \frac{e^{-|\mathbf{r} - \mathbf{R}_j|^2/2a^2}}{a^{3/2}\pi^{3/4}},$$
(14)

where 2a is a characteristic size of the dots.

We assume that the distance between the dots,  $L = |\mathbf{L}|$ , is sufficiently large compared to a, and that the different dot wave functions do not strongly overlap,

$$\left| \int d^3 r \phi_j^*(\mathbf{r}) \phi_k(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} \right| \ll 1, \quad \text{for} \quad j \neq k.$$
 (15)

In other words tunneling between the dots is small, as is the case for the recently studied experimental structures [55, 66 - 68], where the splitting due to tunneling, measured by  $\varepsilon_A$ , was just several tens of  $\mu eV$ , while the electron quantization energy in each dot was at least several meV.

For j = k, we obtain

$$\int d^3r \phi_j^*(\mathbf{r}) \phi_j(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} = \frac{1}{a^3 \pi^{3/2}} \int d^3r e^{-|\mathbf{r}-\mathbf{R}_j|^2/a^2} e^{-i\mathbf{q}\cdot\mathbf{r}}$$
$$= e^{-i\mathbf{q}\cdot\mathbf{R}_j} e^{-a^2q^2/4}. \tag{16}$$

The resulting form factor is

$$F(q) = e^{-a^2q^2/4}e^{-i\mathbf{q}\cdot\mathbf{R}}(c_0^{\dagger}c_0e^{i\mathbf{q}\cdot\mathbf{L}/2} + c_1^{\dagger}c_1e^{-i\mathbf{q}\cdot\mathbf{L}/2}), \tag{17}$$

where  $\mathbf{R} = (\mathbf{R}_0 + \mathbf{R}_1)/2$ . Therefore

$$F(q) = e^{-a^2q^2/4}e^{-i\mathbf{q}\cdot\mathbf{R}}\left[\cos(\mathbf{q}\cdot\mathbf{L}/2)I + i\sin(\mathbf{q}\cdot\mathbf{L}/2)\sigma_z\right],\tag{18}$$

where I is the identity operator. Only the last term in (18) represents an interaction affecting the qubit states. It leads to a Hamiltonian term of the form (8), with coupling constants

$$g_{\mathbf{q},\lambda} = -\sqrt{\frac{\hbar}{2\rho q s V}} M e^{-a^2 q^2/4 - i\mathbf{q} \cdot \mathbf{R}} \times (\xi_1 e_2 e_3 + \xi_2 e_1 e_3 + \xi_3 e_1 e_2) \sin(\mathbf{q} \cdot \mathbf{L}/2), \tag{19}$$

where  $e_k = q_k/q$ .

The general form of qubit evolution controlled by the Hamiltonian term (4) is time dependent. Decoherence estimates for some solid-state systems with certain shapes of time dependence of the system Hamiltonian were reported recently [38, 69, 70]. However, such estimations are rather sophisticated. To avoid this difficulty we observe that all single-qubit rotations which are required for quantum algorithms can be successfully performed by using two constant-Hamiltonian gates without loss of quantum speed-up, e.g., by amplitude rotation gate and phase shift gate [71]. To implement these gates one can keep the Hamiltonian term (4) constant during the implementation of each gate, adjusting the parameters  $\varepsilon_A$  and  $\varepsilon_P$  as appropriate for each gate and for the idling qubit in between gate functions. In the next paragraph we initiate our consideration of decoherence during the implementation of the NOT amplitude gate. Then consider  $\pi$ -phase shift gate later in the section.

The quantum NOT gate is a unitary operator which transforms the states  $|0\rangle$  and  $|1\rangle$  into each other. Any superposition of  $|0\rangle$  and  $|1\rangle$  transforms accordingly,

$$NOT (\alpha |0\rangle + \beta |1\rangle) = \beta |0\rangle + \alpha |1\rangle.$$
 (20)

The NOT gate can be implemented by properly choosing  $\varepsilon_A$  and  $\varepsilon_P$  in the Hamiltonian term (4). Specifically, with constant

$$\varepsilon_A = \varepsilon$$
 (21)

and

$$\varepsilon_P = 0,$$
 (22)

the "ideal" NOT gate function is carried out, with these interaction parameters, over the time interval

$$\tau = \frac{\pi\hbar}{\varepsilon}.\tag{23}$$

The major source of quantum noise for double-dot qubit subject to the NOT-gate type coupling, is relaxation involving energy exchange with the phonon bath (i.e., emission and absorption of phonons). Here it is more convenient to study the evolution of the density matrix in the energy basis,  $\{|+\rangle, |-\rangle\}$ , where

$$|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}.$$
 (24)

Then, assuming that the time interval of interest is  $[0, \tau]$ , the qubit density matrix can be expressed [41] in the energy basis as

$$\rho(t) = \begin{pmatrix} \rho_{++}^{th} + \left[\rho_{++}(0) - \rho_{++}^{th}\right] e^{-\Gamma t} & \rho_{+-}(0)e^{-(\Gamma/2 - i\varepsilon/\hbar)t} \\ \rho_{-+}(0)e^{-(\Gamma/2 + i\varepsilon/\hbar)t} & \rho_{--}^{th} + \left[\rho_{--}(0) - \rho_{--}^{th}\right] e^{-\Gamma t} \end{pmatrix}. (25)$$

This is a standard Markovian approximation for the evolution of the density matrix. For large times, this type of evolution would in principle result in the thermal state, with the off-diagonal density matrix elements decaying to zero, while the diagonal ones approaching the thermal values proportional to the Boltzmann factors corresponding to the energies  $\pm \varepsilon/2$ . However, here we are only interested in such evolution for a relatively short time interval,  $\tau$ , of a NOT gate. The rate parameter  $\Gamma$  is simply the sum [41] of the phonon emission rate,  $W^e$ , and absorption rate,  $W^a$ ,

$$\Gamma = W^e + W^a. \tag{26}$$

The probability for the absorption of a phonon due to excitation from the ground state to the upper level is

$$w^{\lambda} = \frac{2\pi}{\hbar} |\langle f | H_{ep} | i \rangle|^2 \delta(\varepsilon - \hbar sq), \qquad (27)$$

where  $|i\rangle$  is the initial state with the extra phonon with energy  $\hbar sq$  and  $|f\rangle$  is the final state,  $\mathbf{q}$  is the wave vector, and  $\lambda$  is the phonon polarization. Thus, we have to calculate

$$W^{a} = \sum_{\mathbf{q}, \lambda} w^{\lambda} = \frac{V}{(2\pi)^{3}} \sum_{\lambda} \int d^{3}q \, w^{\lambda}. \tag{28}$$

For the interaction (8) one can derive

$$w^{\lambda} = \frac{2\pi}{\hbar} |g_{\mathbf{q},\lambda}|^2 N^{th} \delta(\varepsilon - \hbar sq), \tag{29}$$

where

$$N^{th} = \frac{1}{\exp(\hbar sq/k_B T) - 1} \tag{30}$$

is the phonon occupation number at temperature T, and  $k_B$  is the Boltzmann constant.

The coupling constant in (19) depends on the polarization if the interaction is piezoelectric. For longitudinal phonons, the polarization vector has Cartesian components, expressed in terms of the spherical-coordinate angles,

$$\xi_1^{\parallel} = e_1 = \sin \theta \cos \phi, \quad \xi_2^{\parallel} = e_2 = \sin \theta \sin \phi, \quad \xi_3^{\parallel} = e_3 = \cos \theta,$$
 (31)

where  $e_j = q_j/q$ . For transverse phonons, it is convenient to define the two polarization vectors  $\xi_i^{\perp 1}$  and  $\xi_i^{\perp 2}$  to have

$$\xi_1^{\perp 1} = \sin \phi, \quad \xi_2^{\perp 1} = -\cos \phi, \quad \xi_3^{\perp 1} = 0,$$
 (32)

$$\xi_1^{\perp 2} = -\cos\theta\cos\phi, \quad \xi_2^{\perp 2} = -\cos\theta\sin\phi, \quad \xi_3^{\perp 2} = \sin\theta.$$
 (33)

Then for longitudinal phonons, one obtains [54]

$$w^{\parallel} = \frac{\pi}{\rho s V q} M^2 e^{-a^2 q^2/4}$$

$$\times 9 \sin^4 \theta \cos^2 \theta \sin^2 \phi \cos^2 \phi \sin^2 (qL \cos \theta/2).$$
(34)

For transverse phonons, one gets

$$w^{\perp 1} = \frac{\pi}{\rho s V q} M^2 e^{-a^2 q^2/4} (-2\sin\theta\cos^2\theta\sin\phi\cos\phi + \sin^3\theta\cos\phi\sin\phi)^2 \sin^2(qL\cos\theta/2), \tag{35}$$

$$w^{\perp 2} = \frac{\pi}{\rho s V q} M^2 e^{-a^2 q^2/4} (-2\sin\theta\cos\theta\cos^2\phi + \sin\theta\cos\theta\sin^2\phi)^2 \sin^2(qL\cos\theta/2). \tag{36}$$

By combining these contributions and substituting them in (28), one can obtain the probability of absorption of a phonon for all polarizations,

$$W_{\text{piezo}}^{a} = \frac{M^{2}}{20\pi\rho s^{2}\hbar L^{5}k^{4}} \frac{\exp\left(-\frac{a^{2}k^{2}}{2}\right)}{\exp\left(\frac{\hbar sk}{k_{B}T}\right) - 1} \times \left\{ (kL)^{5} + 5kL\left[2(kL)^{2} - 21\right]\cos(kL) + 15\left[7 - 3(kL)^{2}\right]\sin(kL) \right\},$$
(37)

where

$$k = \frac{\varepsilon}{\hbar s} \tag{38}$$

is the wave-vector of the absorbed phonon.

Finally, the expressions for the phonon emission rates,  $W^e$ , can be obtained by multiplying the above expression, (37), by  $(N_{th} + 1)/N_{th}$ .

The  $\pi$  phase gate is a unitary operator which does not change the absolute values of the probability amplitudes of a qubit in the superposition of the  $|0\rangle$  and  $|1\rangle$  basis states. instead it increases the relative phase between the probability amplitudes by  $\pi$  angle. Consequently, superposition of  $|0\rangle$  and  $|1\rangle$  transforms according to

$$\Pi\left(\alpha|0\rangle + \beta|1\rangle\right) = \alpha|0\rangle - \beta|1\rangle. \tag{39}$$

Over a time interval  $\tau$ , the  $\pi$  gate can be carried out with constant interaction parameters,

$$\varepsilon_A = 0 \tag{40}$$

and

$$\varepsilon_P = \varepsilon = \frac{\pi\hbar}{\tau}.\tag{41}$$

Charge qubit dynamics during implementation of phase gates was investigated in [53]. The relaxation dynamics is suppressed during the  $\pi$  gate, because there is no tunneling between the dots. The main quantum noise then results due to pure dephasing. It leads to the decay of the off-diagonal qubit density matrix elements, while keeping the diagonal density matrix elements unchanged. The qubit density matrix can be represented in this regime as [72, 73]

$$\rho(t) = \begin{pmatrix} \rho_{00}(0) & \rho_{01}(0)e^{-B^2(t) + i\varepsilon t/\hbar} \\ \rho_{10}(0)e^{-B^2(t) - i\varepsilon t/\hbar} & \rho_{11}(0) \end{pmatrix}, \tag{42}$$

with the spectral function.

$$B^{2}(t) = \frac{8}{\hbar^{2}} \sum_{\mathbf{q},\lambda} \frac{|g_{\mathbf{q},\lambda}|^{2}}{\omega_{q}^{2}} \sin^{2} \frac{\omega_{q}t}{2} \coth \frac{\hbar\omega_{q}}{2k_{B}T}$$

$$= \frac{V}{\hbar^{2}\pi^{3}} \int d^{3}q \sum_{\lambda} \frac{|g_{\mathbf{q},\lambda}|^{2}}{q^{2}s^{2}} \sin^{2} \frac{qst}{2} \coth \frac{\hbar qs}{2k_{B}T}. \tag{43}$$

For the piezoelectric interaction, the coupling constant  $g_{\mathbf{q},\lambda}$  was obtained in (19), and expression for the spectral function is

$$B_{\text{piezo}}^{2}(t) = \frac{M^{2}}{2\pi^{3}\hbar\rho s^{3}} \int_{0}^{\infty} q^{2}dq \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{2\pi} d\varphi$$

$$\times \sum_{\lambda} \frac{(\xi_{1}^{\lambda}e_{2}e_{3} + \xi_{2}^{\lambda}e_{1}e_{3} + \xi_{3}^{\lambda}e_{1}e_{2})^{2}}{q^{3}} \exp(-a^{2}q^{2}/2)$$

$$\times \sin^{2}(qL\cos\theta) \sin^{2}\frac{qst}{2} \coth\frac{\hbar qs}{2k_{B}T}.$$
(44)

In summary, in this section we obtained the leading-order expressions for the semiconductor double-dot qubit density matrix in the presence of decoherence due to piezoelectric interaction with acoustic phonons during implementation of amplitude and phase gates.

### 3 Quantification of Decoherence

Quantum information processing at the level of qubits and few-qubit registers, assumes near coherent evolution, which is at best achievable at short to intermediate times. Therefore attention has recently shifted from large-time system dynamics in the regime of onset of thermalization, to almost perfectly coherent dynamics at shorter times. Since many quantum systems proposed as candidates for qubits for practical realizations of quantum computing require estimation of their coherence, quantitative characterization of decoherence is crucially important for quantum information processing [4 - 6, 46 - 50, 52, 55, 60, 61, 66 - 68, 71, 74 - 102]. A single measure characterizing decoherence is highly desirable for comparison of different qubit designs. Besides the evaluation of single qubit performance one also has to analyze scaling of decoherence as the register size (the number of qubits involved) increases. Direct quantitative calculations of decoherence of even few-qubit quantum registers are not feasible. Therefore, a practical approach has been to explore quantitative measures of decoherence [100], develop techniques to

calculate such measures at least approximately for realistic one- and twoqubit systems [53, 54], and then establish scaling (additivity) [101, 102] for several-qubit quantum systems.

In this section, we outline different approaches to define and quantify decoherence. We argue that a measure based on a properly defined as a certain operator norm of deviation of the density matrix from ideal, is the most appropriate for quantifying decoherence in quantum registers.

We consider several approaches to generally quantifying the degree of decoherence due to interactions with environment. We first mention the approach based on the asymptotic relaxation time scales. The entropy and idempotency-defect measures are then reviewed. The fidelity measure of decoherence is considered next. Finally, we introduce our operator norm measure of decoherence. Furthermore, we discuss an approach to eliminate the initial-state dependence of the decoherence measures.

Markovian approximation schemes typically yield exponential approach to the limiting values of the density matrix elements for large times [40 - 42]. For a two-state system, this defines the time scales  $T_1$  and  $T_2$ , associated, respectively, with the approach by the diagonal (thermalization) and off-diagonal (dephasing, decoherence) density-matrix elements to their limiting values. More generally, for large times we approximate deviations from stationary values of the diagonal and off-diagonal density matrix elements as

$$\rho_{kk}(t) - \rho_{kk}(\infty) \propto e^{-t/T_{kk}},\tag{45}$$

$$\rho_{jk}(t) \propto e^{-t/T_{jk}} \qquad (j \neq k).$$
(46)

The shortest time among  $T_{kk}$  is often identified as  $T_1$ . Similarly,  $T_2$  can be defined as the shortest time among  $T_{n\neq m}$ . These definitions yield the characteristic times of thermalization and decoherence (dephasing).

Unfortunately the exponential behavior of the density matrix elements in the energy basis is applicable only for large times, whereas for quantum computing applications, the short-time behavior is usually relevant [31]. Moreover, while the energy basis is natural for large times, the choice of the preferred basis is not obvious for short and intermediate times [31, 72]. Therefore, the time scales  $T_1$  and  $T_2$  have limited applicability for evaluating coherence in quantum computing.

An alternative approach is based on the calculation of the entropy [39] of the system,

$$S(t) = -\text{Tr}\left(\rho \ln \rho\right),\tag{47}$$

or the first order entropy (idempotency defect) [103 - 105],

$$s(t) = 1 - \operatorname{Tr}\left(\rho^2\right). \tag{48}$$

Both expressions are basis independent, have a minimum at pure states and effectively describe the degree of the state's "purity." Any deviation from a pure state leads to the deviation from the minimal values, 0, for both measures,

$$S_{\text{pure state}}(t) = s_{\text{pure state}}(t) = 0.$$
 (49)

Unfortunately, entropy measures the deviation from pure-state evolution rather than deviation from a specific ideal evolution.

The fidelity measure, considered presently, has been widely used. If the Hamiltonian of the system and environment is

$$H = H_S + H_B + H_I, (50)$$

where  $H_S$  is the internal system dynamics,  $H_B$  gives the evolution of environment (bath), and  $H_I$  describes system-bath interaction, then the fidelity measure [106, 107] can be defined as,

$$F(t) = \operatorname{Tr}_{S} \left[ \rho_{\text{ideal}}(t) \rho(t) \right]. \tag{51}$$

Here the trace is over the system degrees of freedom, and  $\rho_{\text{ideal}}(t)$  represents the pure-state evolution of the system under  $H_S$  only, without interaction with the environment ( $H_I = 0$ ). In general, the Hamiltonian term  $H_S$  governing the system dynamics can be time dependent. For the sake of simplicity throughout this review we consider constant  $H_S$  over time intervals of quantum gates, cf. Section 2. In this case

$$\rho_{\text{ideal}}(t) = e^{-iH_S t} \rho(0) e^{iH_S t}. \tag{52}$$

More sophisticated scenarios with qubits evolving under time dependent  $H_S$  were considered in [38, 69, 70].

The fidelity provides a measure of decoherence in terms of the difference between the "real," environmentally influenced evolution,  $\rho(t)$ , and the "ideal" evolution,  $\rho_{\text{ideal}}(t)$ . It will attain its maximal value, 1, only provided  $\rho(t) = \rho_{\text{ideal}}(t)$ . This property relies on the added assumption the  $\rho_{\text{ideal}}(t)$  remains a projection operator (pure state) for all times  $t \geq 0$ .

As an simple example consider a two-level system decaying to the ground state, when there is no internal system dynamics,

$$\rho_{\text{ideal}}(t) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{53}$$

$$\rho(t) = \begin{pmatrix} 1 - e^{-\Gamma t} & 0\\ 0 & e^{-\Gamma t} \end{pmatrix},\tag{54}$$

and the fidelity is monotonic,

$$F(t) = e^{-\Gamma t}. (55)$$

Note that the requirement that  $\rho_{\text{ideal}}(t)$  is a pure-state (projection operator), excludes, in particular, any T>0 thermalized state as the initial system state. Consider the application of the fidelity measure for the infinite-temperature initial state of our two level system. We get

$$\rho(0) = \rho_{\text{ideal}}(t) = \begin{pmatrix} 1/2 & 0\\ 0 & 1/2 \end{pmatrix}, \tag{56}$$

which is not a projection operator. The spontaneous-decay density matrix is then

$$\rho(t) = \begin{pmatrix} 1 - (e^{-\Gamma t}/2) & 0\\ 0 & e^{-\Gamma t}/2 \end{pmatrix}.$$
 (57)

The fidelity remains constant

$$F(t) = 1/2, \tag{58}$$

and it does not provide any information of the time dependence of the decay process.

Let us now consider the operator norms [108] that measure the deviation of the system from the ideal state, to quantify the degree of decoherence, as proposed in [100 - 102]. Such measures do not require the initial density matrix to be pure-state. We define the deviation according to

$$\sigma(t) \equiv \rho(t) - \rho_{\text{ideal}}(t). \tag{59}$$

We can use, for instance, the eigenvalue norm [108],

$$\|\sigma\|_{\lambda} = \max_{i} |\lambda_{i}|, \tag{60}$$

or the trace norm,

$$\|\sigma\|_{\text{Tr}} = \sum_{i} |\lambda_{i}|,\tag{61}$$

etc., where  $\lambda_i$  are the eigenvalues of the deviation operator (59). Since density operators are Hermitian and bounded, their norms, as well the norm of the deviation, can be always defined and evaluated by using the expressions

shown, avoiding the more formal mathematical definitions. We also note that ||A|| = 0 implies that A = 0.

The calculation of these norms is sometimes simplified by the observation that  $\sigma(t)$  is traceless. Specifically, for two-level systems, we get

$$\|\sigma\|_{\lambda} = \sqrt{|\sigma_{00}|^2 + |\sigma_{01}|^2} = \frac{1}{2} \|\sigma\|_{\text{Tr}}.$$
 (62)

For our example of the two-level system undergoing spontaneous decay, the norm is

$$\|\sigma\|_{\lambda} = 1 - e^{-\Gamma t}.\tag{63}$$

The measures considered above quantify decoherence of a system provided that its initial state is given. However, in quantum computing, it is impractical to keep track of all the possible initial states for each quantum register, that might be needed for implementing a particular quantum algorithm. Furthermore, even the preparation of the initial state can introduce additional noise. Therefore, for evaluation of fault-tolerance (scalability), it will be necessary to obtain an upper-bound estimate of decoherence for an arbitrary initial state.

To characterize decoherence for an arbitrary initial state, pure or mixed, we proposed [100] to use the maximal norm, D, which is determined as an operator norm maximized over all the initial density matrices (the worst case scenario error estimate),

$$D(t) = \sup_{\rho(0)} \left( \|\sigma(t, \rho(0))\|_{\lambda} \right). \tag{64}$$

For realistic two-level systems coupled to various types of environmental modes, the expressions of the maximal norm are surprisingly elegant and compact. They are usually monotonic and contain no oscillations due to the internal system dynamics. Most importantly, in the next section we will establish the *additivity* property of the maximal norm of deviation measure.

Here we conclude by presenting the expressions for this measure for the two gates for the semiconductor double-dot system introduced in preceding section. The qubit error measure, D, was obtained from the density matrix deviation from the "ideal" evolution by using the operator norm approach [100]. After lengthy calculations, one gets [53] relatively simple expressions for the NOT gate,

$$D_{\text{NOT}} = \frac{1 - e^{-\Gamma \tau}}{1 + e^{-\varepsilon/k_B T}},\tag{65}$$

and for the  $\pi$  gate,

$$D_{\pi} = \frac{1}{2} \left[ 1 - e^{-B^2(\tau)} \right], \tag{66}$$

where all the parameters were defined in Section 2. A realistic "general" noise estimate per typical quantum-gate cycle time  $\tau$ , could be taken as the larger of these two expressions.

### 4 Additivity of the Decoherence Measure

In the study of decoherence of several-qubit systems, one has to consider the degree to which noisy environments of different qubits are correlated [73, 101, 109]. Furthermore, if all constituent qubits are interacting with the same bath, then there are methods to reduce decoherence without quantum error correction, by instead encoding the state of one logical qubit in a decoherence-free subspace of the states of several physical qubits [51, 73, 110 - 112]. In this section, we will consider several-qubit system and assume the "worst case scenario," i.e., that the qubits experience uncorrelated noise, and each is coupled to a separate bath. Since analytical calculations for several qubits are impractical, we have to find some "additivity" properties that will allow us to estimate the error measure for the whole system from the error measures of the constituent qubits. For a general class of decoherence processes, including those occurring in semiconductor qubits considered in Section 2, we argue that maximal deviation norm measure introduced in Section 3 is additive.

The decoherence dynamics of a multiqubit system is rather complicated. The loss of quantum coherence results also in the loss of two-particle and several-particle entanglements in the system. The higher order (multi-qubit) entanglements are "encoded" in the far off-diagonal elements of the multi-qubit register density matrix, and therefore these quantum correlations will decay at least as fast as the products of the decay factors for the qubits involved, as exemplified by several explicit calculations [36, 113 - 115]. This observation supports the conclusion that at large times the *rates* of decay of coherence of the qubits will be additive.

However, here we seek a different result. We look for additivity property which is valid not in the regime of the asymptotic large-time decay of quantum coherence, but for short times,  $\tau$ , of quantum gate functions, when the noise level, namely the value of the measure  $D(\tau)$  for each qubit, is relatively small. In this regime, we will establish [101]: even for strongly entangled qubits—which are important for the utilization of the power of

quantum computation—the error measures D of the individual qubits in a quantum register are additive. Thus, the error measure for a register made of similar qubits, scales up linearly with their number, consistent with other theoretical and experimental observations [106, 116, 117].

Thus, to characterize decoherence for an arbitrary initial state, pure or mixed, we use the maximal norm, D, which was defined (64) as an operator norm maximized over all the possible initial density matrices. One can show that  $0 \le D(t) \le 1$ . This measure of decoherence will typically increase monotonically from zero at t = 0, saturating at large times at a value  $D(\infty) \le 1$ . The definition of the maximal decoherence measure D(t) looks rather complicated for a general multiqubit system. However, it can be evaluated in closed form for short times, appropriate for quantum computing, for a single-qubit (two-state) system. We then establish an approximate additivity that allows us to estimate D(t) for several-qubit systems as well.

The evolution of the reduced density operator of the system (51) and the one for the ideal density matrix (52) can be formally expressed [71, 96, 97] in the superoperator notation as

$$\rho(t) = T(t)\rho(0),\tag{67}$$

$$\rho^{(i)}(t) = T^{(i)}(t)\rho(0), \tag{68}$$

where T,  $T^{(i)}$  are linear superoperators. The deviation matrix can be expressed as

$$\sigma(t) = \left[ T(t) - T^{(i)}(t) \right] \rho(0). \tag{69}$$

The initial density matrix can decomposed as follows,

$$\rho(0) = \sum_{j} p_{j} |\psi_{j}\rangle\langle\psi_{j}|, \tag{70}$$

where  $\sum_{j} p_{j} = 1$  and  $0 \leq p_{j} \leq 1$ . Here the wavefunction set  $|\psi_{j}\rangle$  is not assumed to have any orthogonality properties. Then, we get

$$\sigma(t, \rho(0)) = \sum_{i} p_{j} \left[ T(t) - T^{(i)}(t) \right] \left| \psi_{j} \right\rangle \left\langle \psi_{j} \right|. \tag{71}$$

The deviation norm can thus be bounded,

$$\|\sigma(t,\rho(0))\|_{\lambda} \leq \left\| \left[ T(t) - T^{(i)}(t) \right] |\phi\rangle\langle\phi| \right\|_{\lambda}. \tag{72}$$

Here  $|\phi\rangle$  is defined according to

$$\left\| \left[ T - T^{(i)} \right] |\phi\rangle\langle\phi| \right\|_{\lambda} = \max_{i} \left\| \left[ T - T^{(i)} \right] |\psi_{j}\rangle\langle\psi_{j}| \right\|_{\lambda}. \tag{73}$$

For any initial density operator which is a statistical mixture, one can always find a density operator which is pure-state,  $|\phi\rangle\langle\phi|$ , such that  $||\sigma(t,\rho(0))||_{\lambda} \le ||\sigma(t,|\phi\rangle\langle\phi|)||_{\lambda}$ . Therefore, evaluation of the supremum over the initial density operators in order to find D(t), see (64), can be done over only pure-state density operators,  $\rho(0)$ .

Consider briefly strategies of evaluating D(t) for a single qubit. We can parameterize  $\rho(0)$  as

$$\rho(0) = U \begin{pmatrix} P & 0 \\ 0 & 1 - P \end{pmatrix} U^{\dagger}, \tag{74}$$

where  $0 \le P \le 1$ , and U is an arbitrary  $2 \times 2$  unitary matrix,

$$U = \begin{pmatrix} e^{i(\alpha+\gamma)}\cos\theta & e^{i(\alpha-\gamma)}\sin\theta \\ -e^{i(\gamma-\alpha)}\sin\theta & e^{-i(\alpha+\gamma)}\cos\theta \end{pmatrix}.$$
 (75)

Then, one should find a supremum of the norm of deviation (60) over all the possible real parameters P,  $\alpha$ ,  $\gamma$  and  $\theta$ . As shown above, it suffices to consider the density operator in the form of a projector and put P=1. Thus, one should search for the maximum over the remaining three real parameters  $\alpha$ ,  $\gamma$  and  $\theta$ .

Another parameterization of the pure-state density operators,  $\rho(0) = |\phi\rangle\langle\phi|$ , is to express an arbitrary wave function  $|\phi\rangle = \sum_{j} (a_j + ib_j)|j\rangle$  in some convenient orthonormal basis  $|j\rangle$ , where j = 1, ..., N. For a two-level system,

$$\rho(0) = \begin{pmatrix} a_1^2 + b_1^2 & (a_1 + ib_1)(a_2 - ib_2) \\ (a_1 - ib_1)(a_2 + ib_2) & a_2^2 + b_2^2 \end{pmatrix}, \tag{76}$$

where the four real parameters  $a_{1,2}$ ,  $b_{1,2}$  satisfy  $a_1^2 + b_1^2 + a_2^2 + b_2^2 = 1$ , so that the maximization is again over three independent real numbers. The final expressions (65) and (66) for D(t), for our selected single-qubit systems considered in Section 2, are actually quite compact and tractable.

In quantum computing, the error rates can be significantly reduced by using several physical qubits to encode each logical qubit [51, 110, 111]. Therefore, even before active quantum error correction is incorporated [87-95], evaluation of decoherence of several qubits is an important, but formidable task. Here our aim is to prove the approximate additivity of  $D_q(t)$ ,

including the case of the initially *entangled* qubits, labeled by q, whose dynamics is governed by

$$H = \sum_{q} H_q = \sum_{q} (H_{Sq} + H_{Bq} + H_{Iq}), \qquad (77)$$

where  $H_{Sq}$  is the Hamiltonian of the qth qubit itself,  $H_{Bq}$  is the Hamiltonian of the environment of the qth qubit, and  $H_{Iq}$  is corresponding qubitenvironment interaction. We consider a more complicated (for actual evaluation) diamond norm [71, 96, 97], as an auxiliary quantity used to establish the additivity of the more easily calculable operator norm D(t).

The establishment of the upper-bound estimate for the maximal deviation norm of a multiqubit system, involves several steps. We first derive a bound for this norm in terms of the diamond norm. Actually, for single qubits, in several models the diamond norm can be expressed via the corresponding maximal deviation norm. At the same time, the diamond norm for the whole quantum system is bounded by sum of the norms of the constituent qubits by using a certain specific stability property of the diamond norm, K(t). This norm is defined as

$$K(t) = \|T - T^{(i)}\|_{\diamond} = \sup_{\varrho} \|\{[T - T^{(i)}] \otimes I\} \varrho\|_{\text{Tr}}.$$
 (78)

The superoperators T,  $T^{(i)}$  characterize the actual and ideal evolutions according to (67), (68). Here I is the identity superoperator in a Hilbert space G whose dimension is the same as that of the corresponding space of the superoperators T and  $T^{(i)}$ , and  $\varrho$  is an arbitrary density operator in the product space of twice the number of qubits.

The diamond norm has an important stability property, proved in [71, 96, 97],

$$||B_1 \otimes B_2||_{\diamond} = ||B_1||_{\diamond} ||B_2||_{\diamond}.$$
 (79)

Note that (79) is a property of the superoperators rather than that of the operators.

Consider a composite system consisting of two subsystems  $S_1$ ,  $S_2$ , with the noninteracting Hamiltonian

$$H_{S_1S_2} = H_{S_1} + H_{S_2}. (80)$$

The evolution superoperator of the system will be

$$T_{S_1S_2} = T_{S_1} \otimes T_{S_2}, \tag{81}$$

and the ideal one

$$T_{S_1S_2}^{(i)} = T_{S_1}^{(i)} \otimes T_{S_2}^{(i)}. \tag{82}$$

The diamond measure for the system can be expressed as

$$\begin{split} K_{S_{1}S_{2}} &= \|T_{S_{1}S_{2}} - T_{S_{1}S_{2}}^{(i)}\|_{\diamond} = \|(T_{S_{1}} - T_{S_{1}}^{(i)}) \otimes T_{S_{2}} + T_{S_{1}}^{(i)} \otimes (T_{S_{2}} - T_{S_{2}}^{(i)})\|_{\diamond} \\ &\leq \|(T_{S_{1}} - T_{S_{1}}^{(i)}) \otimes T_{S_{2}}\|_{\diamond} + \|T_{S_{1}}^{(i)} \otimes (T_{S_{2}} - T_{S_{2}}^{(i)})\|_{\diamond}. \end{split} \tag{83}$$

By using the stability property (79), we get

$$K_{S_{1}S_{2}} \leq \|(T_{S_{1}} - T_{S_{1}}^{(i)}) \otimes T_{S_{2}}\|_{\diamond} + \|T_{S_{1}}^{(i)} \otimes (T_{S_{2}} - T_{S_{2}}^{(i)})\|_{\diamond} =$$

$$\|T_{S_{1}} - T_{S_{1}}^{(i)}\|_{\diamond} \|T_{S_{2}}\|_{\diamond} + \|T_{S_{1}}^{(i)}\|_{\diamond} \|T_{S_{2}} - T_{S_{2}}^{(i)}\|_{\diamond} =$$

$$\|T_{S_{1}} - T_{S_{1}}^{(i)}\|_{\diamond} + \|T_{S_{2}} - T_{S_{2}}^{(i)}\|_{\diamond} = K_{S_{1}} + K_{S_{2}}.$$

$$(84)$$

The inequality

$$K \le \sum_{q} K_q, \tag{85}$$

for the diamond norm K(t) has thus been obtained. Let us emphasize that the subsystems can be initially entangled. This property is particularly useful for quantum computing, the power of which is based on qubit entanglement. However, even in the simplest case of the diamond norm of one qubit, the calculations are extremely cumbersome. Therefore, the use of the measure D(t) is preferable for actual calculations.

For short times, of quantum gate functions, we can use (85) as an approximate inequality for order of magnitude estimates of decoherence measures, even when the qubits are interacting. Indeed, for short times, the interaction effects will not modify the quantities entering both sides significantly. The key point is that while the interaction effects are small, this inequality can be used for *strongly entangled* qubits.

The two deviation-operator norms considered are related by the following inequality

$$\|\sigma\|_{\lambda} \le \frac{1}{2} \|\sigma\|_{\text{Tr}} \le 1. \tag{86}$$

Here the left-hand side follows from

$$\operatorname{Tr} \sigma = \sum_{\mathbf{i}} \lambda_{\mathbf{j}} = 0. \tag{87}$$

Therefore the  $\ell$ th eigenvalue of the deviation operator  $\sigma$  that has the maximum absolute value,  $\lambda_{\ell} = \lambda_{\text{max}}$ , can be expressed as

$$\lambda_{\ell} = -\sum_{j \neq \ell} \lambda_j. \tag{88}$$

Thus, we have

$$\|\sigma\|_{\lambda} = \frac{1}{2} (2|\lambda_{\ell}|) \le \frac{1}{2} \left( |\lambda_{\ell}| + \sum_{j \ne \ell} |\lambda_{j}| \right) = \frac{1}{2} \left( \sum_{j} |\lambda_{j}| \right) = \frac{1}{2} \|\sigma\|_{\text{Tr}}.$$
 (89)

The right-hand side of (86) then also follows, because any density matrix has trace norm 1,

$$\|\sigma\|_{\mathrm{Tr}} = \|\rho - \rho^{(i)}\|_{\mathrm{Tr}} \le \|\rho\|_{\mathrm{Tr}} + \|\rho^{(i)}\|_{\mathrm{Tr}} = 2. \tag{90}$$

From the relation (90) it follows that

$$K(t) \le 2. \tag{91}$$

By taking the supremum of both sides of the relation (89) we get

$$D(t) = \sup_{\rho(0)} \|\sigma\|_{\lambda} \le \frac{1}{2} \sup_{\rho(0)} \|\sigma\|_{\text{Tr}} \le \frac{1}{2} K(t), \tag{92}$$

where the last step involves technical derivation details [101] not reproduced here. In fact, for a single qubit, calculations for typical qubit models [101] give

$$D_q(t) = \frac{1}{2}K_q(t). (93)$$

Since D is generally bounded by (or equal to) K/2, it follows that the multiqubit norm D is approximately bounded from above by the sum of the single-qubit norms even for the *initially entangled* qubits,

$$D(t) \le \frac{1}{2}K(t) \le \frac{1}{2}\sum_{q}K_{q}(t) = \sum_{q}D_{q}(t),$$
 (94)

where q labels the qubits.

For specific models of decoherence of the type encountered in Section 2, as well as those formulated for general studies of short-time decoherence [100], a stronger property has been demonstrated by deriving additional bounds not reviewed here [101], namely that the noise measures are actually equal, for low levels of noise,

$$D(t) = \sum_{q} D_q(t) + o\left(\sum_{q} D_q(t)\right). \tag{95}$$

Thus, in this section we considered the maximal operator norm suitable for evaluation of decoherence for a quantum register consisting of qubits immersed in noisy environments. We established the approximate additivity property of this measure of decoherence for multi-qubit registers at short times, for which the level of quantum noise is low, and the qubit-qubit interaction effects are small, but without any limitation on the initial entanglement of the qubit register.

In conclusion, we surveyed the theory of evaluation of quantum noise effects for quantum registers. Maximal deviation norm was proposed for error estimation and its expressions were presented for a realistic model of semiconductor double-dot qubit interacting with acoustic phonons. Maximal deviation norm has a unique additivity property which facilitates error rate estimation for several-qubit registers.

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