Vol 18 No 2, February 2009
1674-1056/2009/18(02)/0430-05

Chinese Physics B

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Decoherence of qubits: results beyond Markovian approximation*

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(Received 17 April 2008; revised manuscript received 26 May 2008)

In this paper the master equation method is used to calculate the relaxation and decoherence times of a qubit. The results are beyond Markovian approximation, where the noise spectrum is assumed to be wide-band, so that they are valid for not only the wide- but also the narrow-band noises, which may be the main decoherence source in solid-state qubits. Moreover, for some special cases, analytical results can be achieved, which are consistent with those derived by others.

Keywords: qubit, decoherence, master equation
PACC: 0367

1. Introduction

Early proposals for quantum computers were mainly based on quantum optical systems.[1,2] These systems are well isolated from their environment and thus have a relatively long decoherence time. Because the scalability of quantum computer architectures to many qubits is also of central importance for realizing quantum computers of practical use, considerable efforts have recently been devoted to solid-state qubits.[3−10] However, in such qubits, decoherence is much more severe, and various noise sources take effect, such as fluctuations originating from the surrounding circuit, quasiparticle tunnelling, fluctuating background charge and flux noise.

Usually, one of the main steps in calculating the decoherence time via the master equation method is to take the Markovian approximation, where the environment is assumed to have a wide-band noise spectrum, so that the qubit and the environment could lose their entanglement on a very short time scale. However, in a solid-state qubit, not only the wide band noise, but also the narrow band noise may induce strong decoherence. For instance, in a superconducting Josephson-junction qubit, the main source of decoherence can be $1/f$ noise, which has a narrow band. In this case, the Markovian approximation becomes unsuitable.

In this paper, we employ the master equation method to calculate the relaxation time (T_1) and decoherence time (T_2) of a qubit beyond the Markovian approximation. As will be shown below, we can obtain T_1 and T_2 by solving three equations through using the parameters of the qubit and the noise (no matter whether it is wide-band or not). Moreover, for the narrow-band noise, we are able to derive analytical expressions for the short-time behaviour of the quantum dynamics. For the wide-band noise, in which Markovian approximation is valid, analytical results are also derived for both short- and long-time behaviours.

2. Master equation method

For a qubit coupled with an environment, the entire system, i.e. the qubit and the reservoir, can be characterized by the spin-boson model

$$H = H_0 + H_{\rm I} = H_{\rm s} + H_{\rm r} + H_{\rm I}, \qquad (1)$$

*Project supported by the SRFDP, the PCSIRT, the NFRPC (Grant No 2006CB921205), the National Natural Science Foundation of China (Grant Nos 10534060 and 10625416) and the State Key Program for Basic Research of China (Grant Nos 2006CB921801 and 2006CB921106).

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where

$$H_{\rm r}=\sum_j\left(\frac{p_j^2}{2m_j}+\frac{1}{2}m_j\omega_j^2x_j^2\right)=\sum_j\hbar\omega_jb_j^+b_j \quad (2)$$

is the Hamiltonian of the reservoir modelled as a bath of bosons with a spectral distribution of ω_j;

$$H_{\rm s}=\epsilon\sigma_z-\mu\sigma_x\equiv\hbar\Omega\rho_z \quad (3)$$

is the Hamiltonian of the qubit, where

$$\hbar\Omega\equiv E=\sqrt{\epsilon^2+\mu^2}, \quad (4)$$

and

$$\rho_z=|+\rangle\langle+|-|-\rangle\langle-| \quad (5)$$

with $|+\rangle$ and $|-\rangle$ being the eigen-states of the qubit. For instance, for the superconducting charge qubit, $\epsilon=(2n_g-1){\rm e}^2/C_\Sigma$ and $\mu=E_J/2$,[10] while $\epsilon=-I_{\rm P}\left(\phi_x-\frac{\phi_0}{2}\right)$ and $\mu=\frac{\Delta}{2}$ for the superconducting flux qubit, where Δ is the minimum energy level splitting.[8]

For the interaction Hamiltonian $H_{\rm I}$, we consider the typical longitudinal and transverse interactions: σ_zX and σ_xX, where $X=\sum_j\lambda_jx_j$ characterizes the coupling strength due to the bath. Generally, we can write $H_{\rm I}$ as

$$H_{\rm I}=(A\rho_x+B\rho_z)\sum_j\hbar k_j(b_j^++b_j), \quad (6)$$

where

$$\begin{cases}A=\dfrac{\mu}{E}, & B=\dfrac{\epsilon}{E} \quad \text{for} \quad \sigma_zX,\\ A=\dfrac{\epsilon}{E}, & B=-\dfrac{\mu}{E} \quad \text{for} \quad \sigma_xX,\end{cases} \quad (7)$$

and $\hbar k_j=\frac{1}{2}\lambda_j\sqrt{\frac{\hbar}{2m_j\omega_j}}$.

The quantum-mechanical behaviour of the entire system can be described by using its density matrix $\rho_{\rm sr}(t)$, which obeys the equation of motion

$$\dot\rho_{\rm sr}=-\frac{\rm i}{\hbar}[H,\rho_{\rm sr}]. \quad (8)$$

Suppose that the qubit and reservoir are brought into contact at the time $t=0$, then at the beginning, there will be no entanglement between the qubit and the reservoir, and the initial state of the system is

$$\rho_{\rm sr}(0)=\rho_s(0)\rho_{\rm r}(H_{\rm r}), \quad (9)$$

where $\rho_{\rm s}(0)$ is the density matrix $\rho_{\rm s}(t)$ of the qubit at $t=0$, and $\rho_{\rm r}$ is density matrix of the reservoir, which does not depend on t.

To reveal the effect of the reservoir on the qubit, we trace out the degrees of freedom of the reservoir to obtain an equation of motion, i.e. the master equation, of the qubit $\rho_{\rm s}={\rm Tr}_{\rm r}(\rho_{\rm sr})$. For simplicity, we use the interaction picture where the free evolution is eliminated.[11]

In the interaction picture, the equation of motion for the system is

$$\dot P_{\rm sr}(t)=-\frac{\rm i}{\hbar}[H_{\rm I}(t),P_{\rm sr}], \quad (10)$$

where all operators are related to those in Schrödinger picture by

$$P_{\rm sr}(t)={\rm e}^{{\rm i}H_0(t)/\hbar}\rho_{\rm sr}(t){\rm e}^{-{\rm i}H_0(t)/\hbar},$$

and

$$H_{\rm I}(t)={\rm e}^{{\rm i}H_0(t)/\hbar}H_{\rm I}{\rm e}^{-{\rm i}H_0(t)/\hbar}. \quad (11)$$

We can approximately derive $P_{\rm sr}(t)$ by solving Eq.(10) to second order in the perturbation theory. Then the density matrix of the qubit is

$$\rho(t)={\rm Tr}_{\rm r}(P_{\rm sr}(t)). \quad (12)$$

The exponential attenuations of the diagonal and off-diagonal matrix elements of $\rho(t)$ give two characteristic times, i.e. T_1 and T_2.

Now, we consider a time interval τ, in which no significant change occurs for the qubit. Thus, we have

$$\dot\rho(t)\simeq\frac{\rho(\tau)-\rho(0)}{\tau}, \quad (13)$$

where $0\le t\le\tau$. From Eqs.(10), (12) and (13) we obtain

$$\begin{aligned}\dot\rho(t)\simeq&-\frac{\rm i}{\hbar\tau}\int_0^\tau{\rm d}\tau'{\rm Tr}_{\rm r}\big(H_{\rm I}(\tau')P_{\rm sr}(0)\big)-\frac{1}{\hbar^2\tau}\int_0^\tau{\rm d}\tau'\int_0^{\tau'}{\rm d}\tau''{\rm Tr}_{\rm r}[H_{\rm I}(\tau')H_{\rm I}(\tau'')P_{\rm sr}(0)-H_{\rm I}(\tau')P_{\rm sr}(0)H_{\rm I}(\tau'')]+{\rm H.C.}\\ =&-\frac{1}{\tau}\int_0^\tau{\rm d}\tau'\int_0^{\tau'}{\rm d}\tau''\big(G(\tau')G(\tau'')\rho(t)\langle F(\tau')F(\tau'')\rangle-G(\tau')\rho(t)G(\tau'')\langle F(\tau'')F(\tau')\rangle+{\rm H.C.}\big),\end{aligned} \quad (14)$$

where

$$F(\tau)=\sum_j k_j\Big[b_j^+ \mathrm{e}^{\mathrm{i}\omega_j\tau}+b_j\mathrm{e}^{-\mathrm{i}\omega_j\tau}\Big],$$

and

$$G(\tau)=A[\rho_x\cos(\Omega\tau)-\rho_y\sin(\Omega\tau)]+B\rho_z. \quad (15)$$

We can simplify this equation and calculate the matrix elements of $\dot\rho(t)$. With the relation $\rho_{++}(t)+\rho_{--}(t)=1$ and $\dot\rho_{++}(t)+\dot\rho_{--}(t)=0$, we have the final form of the master equation

$$\begin{pmatrix}\dot\rho_{++}(t)\\ \dot\rho_{-+}(t)\\ \dot\rho_{+-}(t)\end{pmatrix}=\boldsymbol{M}\begin{pmatrix}\rho_{++}(t)\\ \rho_{-+}(t)\\ \rho_{+-}(t)\end{pmatrix}+\boldsymbol{N}, \quad (16)$$

where $\rho_{++}=\langle+|\rho(t)|+\rangle$, $\rho_{-+}=\langle-|\rho(t)|+\rangle$, $\rho_{+-}=\langle+|\rho(t)|-\rangle$ and $\rho_{--}=\langle-|\rho(t)|-\rangle$. The elements of matrices $\boldsymbol{M}$ and $\boldsymbol{N}$ are given in the appendix. Note that the Markovian approximation has not been used till now. Equation (16) is valid for all kinds of noises, no matter whether they are wide-band or narrow-band. In general, we can use the parameters of the qubit and the noise and then solve Eq.(16) to obtain T_1 and T_2. For some special cases, we can even acquire analytical expressions for T_1 and T_2. Below we show two examples in detail.

2.1. Short-time behaviour

When τ is small, the matrix $\boldsymbol{M}$ has only real elements, and the three matrix elements of $\boldsymbol{N}$ are $\boldsymbol{N}_1=2A^2W_1$, $\boldsymbol{N}_2=\boldsymbol{N}_3=-2ABW_5$. The solution of Eq.(16) is

$$\begin{aligned}\rho_{++}(t)=&\frac{1}{2}+\frac{1}{2X_3}\Big\{\big[(\rho_{++}(0)-\frac{1}{2})(X_3+X_2)-(\rho_{-+}(0)+\rho_{+-}(0))ABW_3\big]\mathrm{e}^{(-4A^2W_1+2X_2-2X_3)t}\\&+\big[(\rho_{++}(0)-\frac{1}{2})(X_3-X_2)+(\rho_{-+}(0)+\rho_{+-}(0))ABW_3\big]\mathrm{e}^{(-4A^2W_1+2X_2+2X_3)t}\Big\},\\ \rho_{-+}(t)=&\frac{1}{4X_3}\Big\{[-(\rho_{++}(0)-\frac{1}{2})4ABW_5+(\rho_{-+}(0)+\rho_{+-}(0))(X_3-X_2)]\mathrm{e}^{(-4A^2W_1+2X_2-2X_3)t}\\&+[(\rho_{++}(0)-\frac{1}{2})4ABW_5+(\rho_{-+}(0)+\rho_{+-}(0))(X_3+X_2)]\mathrm{e}^{(-4A^2W_1+2X_2+2X_3)t}\\&+[(\rho_{-+}(0)-\rho_{+-}(0))2X_3]\mathrm{e}^{4(-B^2W_7-A^2W_8)t}\Big\}, \quad (17)\end{aligned}$$

and

$$\begin{aligned}\rho_{+-}(t)=&\frac{1}{4X_3}\Big\{[-(\rho_{++}(0)-\frac{1}{2})4ABW_5+(\rho_{-+}(0)+\rho_{+-}(0))(X_3-X_2)]\mathrm{e}^{(-4A^2W_1+2X_2-2X_3)t}\\&+[(\rho_{++}(0)-\frac{1}{2})4ABW_5+(\rho_{-+}(0)+\rho_{+-}(0))(X_3+X_2)]\mathrm{e}^{(-4A^2W_1+2X_2+2X_3)t}\\&-[(\rho_{-+}(0)-\rho_{+-}(0))2X_3]\mathrm{e}^{4(-B^2W_7-A^2W_8)t}\Big\},\end{aligned}$$

where

$$\begin{aligned}X_1=&A^2B^2W_3W_5,\\ X_2=&-B^2W_7+A^2W_8,\end{aligned}$$

and

$$X_3=\sqrt{4X_1+X_2^2}. \quad (18)$$

Obviously, there are three (instead of two) characteristic times:

$$\begin{aligned}\frac{1}{\tau_1}=&4A^2W_1+2B^2W_7-2A^2W_8\\&+2\sqrt{4A^2B^2W_3W_5+(-B^2W_7+A^2W_8)^2},\\ \frac{1}{\tau_2}=&4A^2W_1+2B^2W_7-2A^2W_8\\&-2\sqrt{4A^2B^2W_3W_5+(-B^2W_7+A^2W_8)^2},\end{aligned}$$

and

$$\frac{1}{\tau_3}=4(B^2W_7+A^2W_8). \quad (19)$$

Generally, the attenuations of ρ_{++} and ρ_{--} are characterized by two characteristic times τ_1 and τ_2; the shorter one has a larger effect on the state relaxation of the qubit. However, ρ_{-+} and ρ_{+-} are characterized by three times, i.e. τ_1,τ_2, and τ_3, with the decoherence of the quantum state most affected by the shortest one.

For special cases, the results can become much simplified. For instance, in the case of pure dephasing with $A = 0$ and $B = 1$, we have

$$\rho_{++}(t) = \rho_{++}(0),$$
$$\rho_{-+}(t) = \rho_{-+}(0)\mathrm{e}^{-4W_7 t},$$

and

$$\rho_{+-}(t) = \rho_{+-}(0)\mathrm{e}^{-4W_7 t}.$$

It is clear that the qubit does not relax but only decoheres. This pure dephasing gives a decoherence time T_2:

$$\frac{1}{T_2} = 4W_7 = 2\int \mathrm{d}\omega S(\omega)\frac{\sin^2\frac{\omega}{2}\tau}{\pi\tau\omega^2}. \tag{20}$$

Because $\tau \to 0$ and $0 \le t \le \tau$, we could simply replace τ in Eq.(20) with t. Thus, ρ_{-+} and ρ_{+-} behave as $\mathrm{e}^{-\eta(t)}$, where

$$\eta(t) = 2\int \mathrm{d}\omega S(\omega)\frac{\sin^2\frac{\omega}{2}t}{\pi\omega^2}. \tag{21}$$

This is the exact result derived by Duan and Guo.[12]

In the case of $A = 1$ and $B = 0$, we have

$$\rho_{++}(t) = \frac{1}{2} + (\rho_{++}(0) - \frac{1}{2})\mathrm{e}^{-4W_1 t},$$
$$\rho_{-+}(t) = \frac{1}{2}\big[(\rho_{-+}(0) + \rho_{+-}(0))\mathrm{e}^{(-4W_1+4W_8)t} + (\rho_{-+}(0) - \rho_{+-}(0))\mathrm{e}^{-4W_8 t}\big],$$

and

$$\rho_{+-}(t) = \frac{1}{2}\big[(\rho_{-+}(0) + \rho_{+-}(0))\mathrm{e}^{(-4W_1+4W_8)t} - (\rho_{-+}(0) - \rho_{+-}(0))\mathrm{e}^{-4W_8 t}\big].$$

It is clear that there are only one relaxation time and two decoherence times.

2.2. Long-time behaviour

When τ is large, this method is valid only when the Markovian approximation is applied, i.e. on the assumption that the noise spectrum is wide-band. Now, equation (16) is simplified into

$$\dot{\rho}_{++}(t) = -\frac{1}{2}A^2 S(\Omega)\rho_{++}(t) + \frac{1}{4}A^2\big[S(\Omega) - J(\Omega)\big],$$
$$\dot{\rho}_{-+}(t) = [-\frac{A^2}{4}S(\Omega) - B^2 S(0)]\rho_{-+}(t),$$

and

$$\dot{\rho}_{+-}(t) = [-\frac{A^2}{4}S(\Omega) - B^2 S(0)]\rho_{+-}(t),$$

which give the following relaxation and decoherence times:

$$\frac{1}{T_1} = \frac{1}{2}A^2 S(\Omega),$$

and

$$\frac{1}{T_2} = \frac{1}{4}A^2 S(\Omega) + B^2 S(0) = \frac{1}{2T_1} + B^2 S(0). \tag{22}$$

In the case of $\sigma_z X$-type interaction, these results are the same as those given in Ref.[9].

3. Conclusion

We have used the master equation method to calculate the relaxation and decoherence times of a qubit coupled to an environment. If the short-time behaviour of the quantum dynamics is considered, by solving the equations, we can calculate T_1 and T_2 of a qubit, no matter whether the noise spectrum is either wide-band or narrow-band. In some special cases, we can derive more analytical expressions for T_1 and T_2, which are identical with the results previously derived by others.

Appendix: Elements of matrices $\boldsymbol{M}$ and $\boldsymbol{N}$

For explicitness, the elements of matrices $\boldsymbol{M}$ and $\boldsymbol{N}$ in Eq.(16) are given below:

$$\begin{aligned}
\boldsymbol{M}_{11} &= -4A^2 W_1,\\
\boldsymbol{M}_{12} &= AB(2W_3 + \mathrm{i}2W_4),\\
\boldsymbol{M}_{13} &= AB(2W_3 - \mathrm{i}2W_4),\\
\boldsymbol{M}_{21} &= AB(4W_5 - \mathrm{i}4W_6),\\
\boldsymbol{M}_{22} &= -2A^2 W_1 - 4B^2 W_7 + \mathrm{i}2A^2 W_2,\\
\boldsymbol{M}_{23} &= -2A^2(W_1 - 2W_8 + \mathrm{i}W_2 + \mathrm{i}2W_9),\\
\boldsymbol{M}_{31} &= AB(4W_5 + \mathrm{i}4W_6),\\
\boldsymbol{M}_{32} &= -2A^2(W_1 - 2W_8 - \mathrm{i}W_2 - \mathrm{i}2W_9),\\
\boldsymbol{M}_{33} &= -2A^2 W_1 - 4B^2 W_7 - \mathrm{i}2A^2 W_2,\\
\boldsymbol{N}_1 &= 2A^2(W_1 + W_{10}),\\
\boldsymbol{N}_2 &= -AB(2W_5 + 2W_{12} - 2W_{14} - \mathrm{i}2W_6 + \mathrm{i}2W_{11} - \mathrm{i}2W_{13}),
\end{aligned}$$

and

$$\boldsymbol{N}_3 = -AB(2W_5 + 2W_{12} - 2W_{14} + \mathrm{i}2W_6 - \mathrm{i}2W_{11} + \mathrm{i}2W_{13}),$$

where

$$W_1 = \frac{1}{16\pi}\int \mathrm{d}\omega S(\omega)\tau\left[\mathrm{Sa}^2\left(\frac{\Omega-\omega}{2}\tau\right) + \mathrm{Sa}^2\left(\frac{\Omega+\omega}{2}\tau\right)\right],$$

$$W_2 = \frac{1}{4\pi}\int \mathrm{d}\omega S(\omega)\frac{\Omega}{\Omega^2-\omega^2} - \frac{1}{8\pi}\int \mathrm{d}\omega S(\omega)\left[\frac{\mathrm{Sa}(\Omega+\omega)\tau}{\Omega+\omega} + \frac{\mathrm{Sa}(\Omega-\omega)\tau}{\Omega-\omega}\right],$$

$$W_3 = \frac{1}{16\pi}\int \mathrm{d}\omega S(\omega)\tau\left[\frac{\Omega+\omega}{\omega}\mathrm{Sa}^2\left(\frac{\Omega+\omega}{2}\tau\right) - \frac{\Omega-\omega}{\omega}\mathrm{Sa}^2\left(\frac{\Omega-\omega}{2}\tau\right)\right],$$

$$W_4 = \frac{1}{8\pi}\int \mathrm{d}\omega S(\omega)\frac{1}{\omega}\left[\mathrm{Sa}(\Omega-\omega)\tau - \mathrm{Sa}(\Omega+\omega)\tau\right],$$

$$W_5 = \frac{1}{8\pi}\int \mathrm{d}\omega S(\omega)\frac{\tau}{\Omega^2-\omega^2}\left[\Omega^2\mathrm{Sa}^2\left(\frac{\Omega}{2}\tau\right) - \omega^2\mathrm{Sa}^2\left(\frac{\omega}{2}\tau\right)\right],$$

$$W_6 = \frac{1}{4\pi}\int \mathrm{d}\omega S(\omega)\frac{\Omega}{\Omega^2-\omega^2}\left[\mathrm{Sa}(\omega\tau) - \mathrm{Sa}(\Omega\tau)\right],$$

$$W_7 = \frac{1}{8\pi}\int \mathrm{d}\omega S(\omega)\tau\mathrm{Sa}^2\left(\frac{\omega}{2}\tau\right),$$

$$W_8 = \frac{1}{16\pi}\int \mathrm{d}\omega S(\omega)\tau\left[-\frac{\omega}{\Omega-\omega}\mathrm{Sa}^2\left(\frac{\Omega+\omega}{2}\tau\right) + \frac{\omega}{\Omega+\omega}\mathrm{Sa}^2\left(\frac{\Omega-\omega}{2}\tau\right) + \frac{2\Omega^2}{\Omega^2-\omega^2}\mathrm{Sa}^2(\Omega\tau)\right],$$

$$W_9 = \frac{1}{8\pi}\int \mathrm{d}\omega S(\omega)\left[\frac{\Omega}{\Omega^2-\omega^2}\mathrm{Sa}(\Omega+\omega)\tau + \frac{\Omega}{\Omega^2-\omega^2}\mathrm{Sa}(\Omega-\omega)\tau - \frac{\Omega}{\Omega^2-\omega^2} - \frac{\Omega}{\Omega^2-\omega^2}\mathrm{Sa}(2\Omega\tau)\right],$$

$$W_{10} = \frac{1}{16\pi}\int \mathrm{d}\omega J(\omega)\tau\left[\mathrm{Sa}^2\left(\frac{\Omega+\omega}{2}\tau\right) - \mathrm{Sa}^2\left(\frac{\Omega-\omega}{2}\tau\right)\right],$$

$$W_{11} = \frac{1}{8\pi}\int \mathrm{d}\omega J(\omega)\frac{1}{\omega}\left[\mathrm{Sa}(\Omega+\omega)\tau + \mathrm{Sa}(\Omega-\omega)\tau - 2\mathrm{Sa}(\Omega\tau)\right],$$

$$W_{12} = \frac{1}{16\pi}\int \mathrm{d}\omega J(\omega)\tau\left[\frac{\Omega+\omega}{\omega}\mathrm{Sa}^2\left(\frac{\Omega+\omega}{2}\tau\right) + \frac{\Omega-\omega}{\omega}\mathrm{Sa}^2\left(\frac{\Omega-\omega}{2}\tau\right) - \frac{2\Omega}{\omega}\mathrm{Sa}^2\left(\frac{\Omega}{2}\tau\right)\right],$$

$$W_{13} = \frac{1}{4\pi}\int \mathrm{d}\omega J(\omega)\frac{\omega}{\Omega^2-\omega^2}\left[\mathrm{Sa}(\Omega\tau) - \mathrm{Sa}(\omega\tau)\right],$$

and

$$W_{14} = \frac{1}{8\pi}\int \mathrm{d}\omega J(\omega)\frac{\Omega\omega}{\Omega^2-\omega^2}\tau\left[\mathrm{Sa}^2\left(\frac{\Omega}{2}\tau\right) - \mathrm{Sa}^2\left(\frac{\omega}{2}\tau\right)\right]$$

with

$$\mathrm{Sa}(x) = \frac{\sin(x)}{x},$$
$$J(\omega) = 4\pi\sum_i k_i^2\delta(\omega-\omega_i),$$

and

$$S(\omega) = [2\bar{n}(\omega)+1]J(\omega),$$

where $S(\omega)$ is the density spectrum of the noise and $\bar{n}(\omega) = 1/(\exp(\hbar\omega/k_\mathrm{B}T)-1)$ is the Bose–Einstein distribution.

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