

# Non-Markovian dynamics of a dissipative two-level system: Nonzero bias and sub-Ohmic bath

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The quantum dynamics of the dissipative two-level system with nonzero bias and sub-Ohmic bath is studied by means of the perturbation approach based on a unitary transformation. It has been shown that for the sub-Ohmic bath it is necessary to use the non-Markovian approach, especially for the short time behavior of the coupled system and environment. The nonequilibrium correlation  $P(t)$  has been calculated to show that a finite bias may favor the short time coherence. The spectrum of the susceptibility  $\chi''(\omega)$  of the sub-Ohmic case may have a double peak structure in the range of  $\omega > 0$  when the coupling  $\alpha$  is relatively strong. Besides, the coherence-decoherence transition point  $\alpha_c$  is determined for different  $0 < s \leq 1$  by the condition of  $\chi''(\omega=0) = \infty$  when  $\alpha = \alpha_c$ . Finally, we show that Shiba's relation is exactly satisfied in our results.

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## I. INTRODUCTION

The physics of a quantum two-level system coupled to dissipative bosonic environment [spin-boson model (SBM)] has attracted considerable attention in last years because it provides a universal model for numerous physical and chemical processes [1,2]. The Hamiltonian of SBM reads (throughout this paper we set  $\hbar=1$ )

$$H = -\frac{1}{2}\Delta\sigma_x + \frac{1}{2}\epsilon\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \frac{1}{2} \sum_k g_k (b_k^\dagger + b_k) \sigma_z, \quad (1)$$

where  $b_k^\dagger$  ( $b_k$ ) is the creation (annihilation) operator of boson mode with frequency  $\omega_k$  and  $\sigma_x$  and  $\sigma_z$  are Pauli matrices to describe the two-level system.  $\epsilon$  is the bias,  $\Delta$  is the bare tunneling, and  $g_k$  is the coupling between spin and environment.

The essential physics contained in SBM is the competition between the coherent quantum dynamics of the two-level system [the Rabi oscillation described by the first two term of Eq. (1)] and the dissipative effect of the environment which tends to make the dynamics decoherent. The main theoretical interest is to understand how the environment influences the dynamics of the two-level system and, in particular, how dissipation destroys quantum coherence [1-4]. Both the nonequilibrium and equilibrium dynamics are of interest for the different experimental realizations of two-level systems. When the system can be prepared in one of the two states by applying a strong bias for times  $t < 0$  and then let it evolve for  $t > 0$  in a finite bias  $\epsilon \neq 0$ , the nonequilibrium correlation function  $P(t)$  is of primary interest [1,5]. When the initial state preparation is not realizable, the interest then lies in the susceptibility  $\chi(\omega)$  [2,3]. Moreover, the real and imaginary parts of  $\chi(\omega)$  should satisfy Shiba's relation [3,6-8].

The effect of the bosonic environment is characterized by a spectral density  $J(\omega) = \sum_k g_k^2 \delta(\omega - \omega_k) = 2\alpha\omega^s \omega_c^{1-s} \theta(\omega_c - \omega)$  with the dimensionless coupling strength  $\alpha$  and the hard upper cutoff  $\omega_c$  [ $\theta(\omega_c - \omega)$  is the usual step function] [9]. The index  $s$  accounts for various physical situations:  $s=1$  is the Ohmic bath [1,2] but  $s < 1$  stands for the sub-Ohmic bath

[1,2,10-13]. There are suggestions to model a lossy resistor-inductor-capacitor transmission line or the  $1/f$  noise found in experiments by the  $s < 1$  sub-Ohmic bath [14,15].

In this paper, we focus on the sub-Ohmic SBM ( $0 < s < 1$ ) since, in terms of the renormalization group approach, the sub-Ohmic coupling represents a relevant perturbation. In last a few years, the numerical renormalization group method [15-19] and the quantum Monte Carlo method [20] are used for the sub-Ohmic SBM, and their main interest is to study the properties of the delocalized-localized quantum phase transition. But our main interest is different from theirs, that is, our purpose is to understand how the sub-Ohmic bath influences the dynamics of the two-level system and destroys the quantum coherence. Moreover, based on the noninteracting blip approximation [1] there are claims that the two-level system might be always localized in the sub-Ohmic case for zero temperature, thus there should be no coherent dynamics for the sub-Ohmic bath. However, in a previous paper [21] we studied the unbiased ( $\epsilon=0$ ) sub-Ohmic SBM to show that a finite coherence-decoherence transition point exists for all  $0 < s \leq 1$ . Due to technical difficulties, little result about quantum dynamics of  $s < 1$  sub-Ohmic bath at zero temperature with finite bias is known.

In this work the analytical approach in Ref. [21] is extended to calculate the non-Markovian dynamics of SBM with sub-Ohmic bath  $0 < s \leq 1$  and finite bias  $\epsilon \neq 0$ . Our results will show that for the sub-Ohmic bath a nonzero bias plays an important role in the quantum dynamics and the Markovian approximation is not good, especially for the short time behavior of the coupled system and environment.

## II. UNITARY TRANSFORMATION

Here we present a treatment based on the unitary transformation approach. A unitary transformation [22,23] is applied to  $H$ ,  $H' = \exp(S)H \exp(-S)$ , and the purpose of the transformation is to take into account the correlation between the spin and bosons, where

$$S = \sum_k \frac{g_k}{2\omega_k} (b_k^\dagger - b_k) [\xi_k \sigma_z + (1 - \xi_k) \sigma_0]. \quad (2)$$

Here we introduce in  $S$  a constant  $\sigma_0$  and a  $k$ -dependent function  $\xi_k$ ; their form will be determined later.

The transformation can be done to the end and the result is

$$H' = H'_0 + H'_1 + H'_2, \quad (3)$$

$$H'_0 = -\frac{1}{2}\eta\Delta\sigma_x + \frac{1}{2}\epsilon\sigma_z + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k} \xi_k(2 - \xi_k) - \sum_k \frac{g_k^2}{4\omega_k} \sigma_0^2(1 - \xi_k)^2, \quad (4)$$

$$H'_1 = \frac{1}{2} \sum_k g_k(1 - \xi_k)(b_k^\dagger + b_k)(\sigma_z - \sigma_0) - \frac{1}{2}\eta\Delta i\sigma_y \sum_k \frac{g_k}{\omega_k} \xi_k(b_k^\dagger - b_k), \quad (5)$$

$$H'_2 = -\sum_k \frac{g_k^2}{2\omega_k} \sigma_0(1 - \xi_k)^2(\sigma_z - \sigma_0) - \frac{1}{2}\Delta\sigma_x \left( \cosh \left\{ \sum_k \frac{g_k}{\omega_k} \xi_k(b_k^\dagger - b_k) \right\} - \eta \right) - \frac{1}{2}\Delta i\sigma_y \left( \sinh \left\{ \sum_k \frac{g_k}{\omega_k} \xi_k(b_k^\dagger - b_k) \right\} - \eta \sum_k \frac{g_k}{\omega_k} \xi_k(b_k^\dagger - b_k) \right), \quad (6)$$

where

$$\eta = \exp \left[ -\sum_k \frac{g_k^2}{2\omega_k^2} \xi_k^2 \right]. \quad (7)$$

Obviously,  $H'_0$  can be solved exactly because the spin and bosons are decoupled.  $H'_0$  can be diagonalized by a unitary matrix  $U$ ,

$$U = \begin{pmatrix} u & v \\ v & -u \end{pmatrix}, \quad (8)$$

$$u = \frac{1}{\sqrt{2}} \left( 1 - \frac{\epsilon}{W} \right)^{1/2}, \quad v = \frac{1}{\sqrt{2}} \left( 1 + \frac{\epsilon}{W} \right)^{1/2}, \quad (9)$$

where  $W = [\epsilon^2 + \eta^2 \Delta^2]^{1/2}$ .

The diagonalized  $H'_0$  is

$$\tilde{H}_0 = U^\dagger H'_0 U = -\frac{1}{2}W\sigma_z + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k} \xi_k(2 - \xi_k) - \sum_k \frac{g_k^2}{4\omega_k} \sigma_0^2(1 - \xi_k)^2. \quad (10)$$

The eigenstate of  $\tilde{H}_0$  is a direct product:  $|s\rangle\{|n_k\rangle\}$ , where  $|s\rangle$  is the eigenstate of  $\sigma_z$ ,  $|s_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  or  $|s_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , and  $\{|n_k\rangle\}$  is the eigenstate of bosons with  $n_k$  phonons for mode  $k$ . In particular,  $\{|0_k\rangle\}$  is the vacuum state in which  $n_k=0$  for every  $k$ . The ground state of  $\tilde{H}_0$  is

$$|g_0\rangle = |s_1\rangle\{|0_k\rangle\}, \quad (11)$$

with ground state energy

$$E_g = -\frac{1}{2}W - \sum_k \frac{g_k^2}{4\omega_k} \xi_k(2 - \xi_k) - \sum_k \frac{g_k^2}{4\omega_k} \sigma_0^2(1 - \xi_k)^2. \quad (12)$$

$H'_1$  is transformed as follows:

$$\tilde{H}_1 = U^\dagger H'_1 U = -\frac{1}{2} \sum_k g_k(1 - \xi_k)(b_k^\dagger + b_k) \left[ \frac{\epsilon}{W} \sigma_z + \sigma_0 \right] + \frac{\eta\Delta}{2W} \sigma_x \sum_k g_k(1 - \xi_k)(b_k^\dagger + b_k) + \frac{1}{2} \eta\Delta i\sigma_y \sum_k \frac{g_k}{\omega_k} \xi_k(b_k^\dagger - b_k). \quad (13)$$

$\tilde{H}_1$  and  $\tilde{H}_2 = U^\dagger H'_2 U$  are treated as perturbation and they should be as small as possible. For this purpose  $\sigma_0$  and  $\xi_k$  are determined in such a way

$$\sigma_0 = -\frac{\epsilon}{W}, \quad (14)$$

$$\xi_k = \frac{\omega_k}{\omega_k + W}, \quad (15)$$

which

$$\begin{aligned} \tilde{H}_1 &= \frac{1}{2} \sum_k g_k(1 - \xi_k)(b_k^\dagger + b_k) \frac{\epsilon}{W} [1 - \sigma_z] \\ &+ \frac{1}{2} \eta\Delta \sum_k \frac{g_k}{\omega_k} \xi_k [b_k^\dagger(\sigma_x + i\sigma_y) + b_k(\sigma_x - i\sigma_y)] \\ &= \frac{1}{2}(1 - \sigma_z) \sum_k Q_k(b_k^\dagger + b_k) \\ &+ \frac{1}{2} \sum_k V_k [b_k^\dagger(\sigma_x + i\sigma_y) + b_k(\sigma_x - i\sigma_y)], \end{aligned} \quad (16)$$

where  $Q_k = \lambda_k \epsilon$ ,  $V_k = \lambda_k \eta \Delta$ , and  $\lambda_k = g_k / (\omega_k + W)$ . Note that  $\tilde{H}_1|g_0\rangle = 0$  and this is the key point in our approach. Thus  $E_g$  in Eq. (12) is the ground state energy of  $\tilde{H}$ ,

$$E_g = -\frac{1}{2}W - \sum_k \frac{g_k^2}{4\omega_k} \left[ 1 - \left( \frac{\eta\Delta}{\omega_k + W} \right)^2 \right]. \quad (17)$$

The original Hamiltonian can be solved exactly in two limits: one is the weak-coupling limit  $\alpha \rightarrow 0$  with  $E_g(\alpha \rightarrow 0) = -\frac{1}{2}\sqrt{\Delta^2 + \epsilon^2}$  and the other is the zero tunneling limit  $\Delta \rightarrow 0$  with  $E_g(\Delta \rightarrow 0) = -\frac{1}{2}|\epsilon| - \sum_k g_k^2 / 4\omega_k$ . It is easily to check that  $E_g$  in Eq. (17) goes to the correct ground state energy in these two limits.

$\eta$  in Eq. (7) is the renormalized factor for the tunneling,

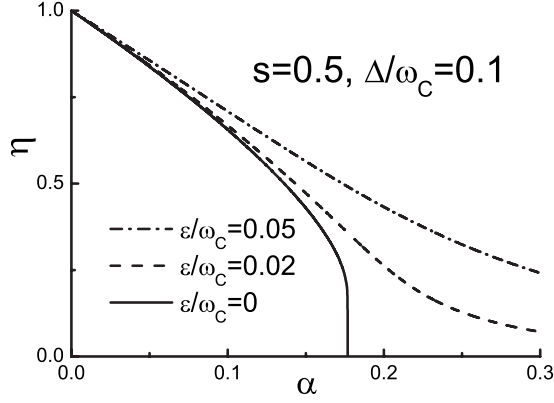


FIG. 1. The renormalized tunneling  $\eta$  vs  $\alpha$  relations for different biases:  $\epsilon/\omega_c=0$  (solid line), 0.02 (dashed line), and 0.05 (dashed-dotted line).

$$\eta = \exp \left[ -\alpha \int_0^1 \frac{x^s dx}{(x+W')^2} \right], \quad (18)$$

where  $W'=W/\omega_c$ . For some special  $s$  values the integration can be done easily, e.g., for  $s=1$   $\eta = \exp(-\alpha \{\ln[(1+W')/W'] - 1/(1+W')\})$  and for  $s=1/2$   $\eta = \exp\{-\alpha [\tan^{-1}(1/\sqrt{W'})/\sqrt{W'} - 1/(1+W')]\}$ . For unbiased case  $\epsilon=0$ , there is a delocalized-localized quantum phase transition [21]. Figure 1 shows that this transition point for  $s=1/2$  is at  $\alpha_t=0.177$ . But for the biased case  $\epsilon \neq 0$  the system is always in the delocalized phase with finite  $\eta > 0$  (see Fig. 1 for  $\epsilon=0.02$  and 0.05). We note that this is one of the most important differences between the biased and unbiased cases.

In the following, the transformed Hamiltonian is approximated as  $\tilde{H} \approx \tilde{H}_0 + \tilde{H}_1$  since  $\langle g_0 | \tilde{H}_2 | g_0 \rangle = 0$  [because of the definition for  $\eta$  [Eq. (7)] and the terms in  $\tilde{H}_2$  are related to the multiboson nondiagonal transition (like  $b_k b_{k'}$  and  $b_k^\dagger b_{k'}^\dagger$ )]. The contributions of these nondiagonal terms to the physical quantities are  $O(g_k^4)$ . For zero temperature case the contribution from these multiboson nondiagonal transitions may be dropped safely.

### III. DENSITY OPERATOR AND MASTER EQUATION

The density operator in Schrödinger representation is  $\rho_{SB}(t)$  with Hamiltonian  $H$ , where the subscript  $SB$  indicates that it is density operator for the coupled two-level system and bath. For transformed Hamiltonian  $\tilde{H}$  the density operator is  $\tilde{\rho}_{SB}(t) = U^\dagger e^S \rho_{SB}(t) e^{-S} U$ . We treat  $\tilde{H}_0$  as the unperturbed Hamiltonian and the density operator in the interaction representation is [24]

$$\tilde{\rho}_{SB}^J(t) = \exp(i\tilde{H}_0 t) \tilde{\rho}_{SB}(t) \exp(-i\tilde{H}_0 t). \quad (19)$$

The equation of motion for  $\tilde{\rho}_{SB}^J(t)$  is

$$\frac{d}{dt} \tilde{\rho}_{SB}^J(t) = -i[\tilde{H}_1(t), \tilde{\rho}_{SB}^J(t)]. \quad (20)$$

$\tilde{H}_1(t)$  is the perturbation  $\tilde{H}_1$  in the interaction representation,

$$\begin{aligned} \tilde{H}_1(t) = & \frac{1}{2}(1 - \sigma_z) \sum_k Q_k (b_k^\dagger e^{i\omega_k t} + b_k e^{-i\omega_k t}) \\ & + \frac{1}{2} \sum_k V_k [b_k^\dagger (\sigma_x + i\sigma_y) e^{i(\omega_k - W)t} \\ & + b_k (\sigma_x - i\sigma_y) e^{-i(\omega_k - W)t}]. \end{aligned} \quad (21)$$

We assume

$$\tilde{\rho}_{SB}^J(t) = \tilde{\rho}_S^J(t) \rho_B, \quad (22)$$

where  $\tilde{\rho}_S^J(t) = \text{Tr}_B \tilde{\rho}_{SB}^J(t)$  is the reduced density operator. Then we get the master equation [24] for  $\tilde{\rho}_S^J(t)$ ,

$$\frac{d}{dt} \tilde{\rho}_S^J(t) = - \int_0^t \text{Tr}_B \{ \tilde{H}_1(t), [\tilde{H}_1(t'), \tilde{\rho}_S^J(t') \rho_B] \} dt', \quad (23)$$

where we neglect all higher order (than  $g_k^2$ ) terms.

Because the density operator is Hermitian, i.e.,  $[\tilde{\rho}_S^J(t)]^\dagger = \tilde{\rho}_S^J(t)$ , we can consider only two terms  $\tilde{\rho}_{22}^J(t)$  and  $\tilde{\rho}_{21}^J(t)$ . Starting from Eq. (23), for zero temperature we can reach the following equations for them:

$$\frac{d}{dt} \tilde{\rho}_{22}^J(t) = - \int_0^t dt' \sum_k V_k^2 [e^{-i(\omega_k - W)(t-t')} + e^{i(\omega_k - W)(t-t')}] \tilde{\rho}_{22}^J(t'), \quad (24)$$

$$\frac{d}{dt} \tilde{\rho}_{21}^J(t) = - \int_0^t dt' \sum_k [Q_k^2 e^{-i\omega_k(t-t')} + V_k^2 e^{-i(\omega_k - W)(t-t')}] \tilde{\rho}_{21}^J(t'). \quad (25)$$

Here the higher order terms are dropped. From Eq. (19) we have

$$\begin{pmatrix} \tilde{\rho}_{11}(t) & \tilde{\rho}_{12}(t) \\ \tilde{\rho}_{21}(t) & \tilde{\rho}_{22}(t) \end{pmatrix} = \begin{pmatrix} \tilde{\rho}_{11}^J(t) & \tilde{\rho}_{12}^J(t) e^{iWt} \\ \tilde{\rho}_{21}^J(t) e^{-iWt} & \tilde{\rho}_{22}^J(t) \end{pmatrix}, \quad (26)$$

then

$$\frac{d}{dt} \tilde{\rho}_{22}(t) = - \int_0^t dt' \sum_k V_k^2 [e^{i(\omega_k - W)(t-t')} + e^{-i(\omega_k - W)(t-t')}] \tilde{\rho}_{22}(t'), \quad (27)$$

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}_{21}(t) = & -iW \tilde{\rho}_{21}(t) - \int_0^t dt' \sum_k [Q_k^2 e^{-i(\omega_k + W)(t-t')} \\ & + V_k^2 e^{-i\omega_k(t-t')}] \tilde{\rho}_{21}(t'). \end{aligned} \quad (28)$$

These equations can be solved by means of the Laplace transformation,

$$\tilde{\rho}_{22}(p) = \frac{\tilde{\rho}_{22}(0)}{p + \sum_k V_k^2 \left[ \frac{1}{p - i(\omega_k - W)} + \frac{1}{p + i(\omega_k - W)} \right]}, \quad (29)$$

$$\tilde{\rho}_{21}(p) = \frac{\tilde{\rho}_{21}(0)}{p + iW + \sum_k \left[ \frac{Q_k^2}{p + i(\omega_k + W)} + \frac{V_k^2}{p + i\omega_k} \right]}. \quad (30)$$

Then, the inverse Laplace transformation is performed with the so-called Bromwich path  $\int_B$ ,

$$\tilde{\rho}_{22}(t) = \frac{1}{2\pi i} \int_B dp \exp(pt) \tilde{\rho}_{22}(p) = \frac{\tilde{\rho}_{22}(0)}{2\pi} \int_{-\infty}^{\infty} \frac{i \exp(-i\omega t) d\omega}{\omega - [R(W + \omega) - R(W - \omega)] + i[\gamma(W + \omega) + \gamma(W - \omega)]} \quad (31)$$

and

$$\begin{aligned} \tilde{\rho}_{21}(t) &= \frac{1}{2\pi i} \int_B dp \exp(pt) \tilde{\rho}_{21}(p) \\ &= \frac{\tilde{\rho}_{21}(0)}{2\pi} \int_{-\infty}^{\infty} \frac{i \exp(-i\omega t) d\omega}{\omega - W - \Sigma(\omega) + i\Gamma(\omega)}. \end{aligned} \quad (32)$$

Here the integration on the Bromwich path has been changed to that on the real axis  $-\infty < \omega < \infty$  by the transform  $p = 0^+ - i\omega$ , with  $0^+$  as a positive infinitesimal.  $R(\omega)$  and  $\gamma(\omega)$  are real and imaginary parts of  $\sum_k V_k^2 / (\omega - i0^+ - \omega_k)$ ,

$$\begin{aligned} R(\omega) &= (\eta\Delta)^2 \sum_k \frac{\lambda_k^2}{(\omega - \omega_k)} \\ &= (\eta\Delta)^2 \int_0^{\infty} d\omega' \frac{J(\omega')}{(\omega - \omega')(\omega' + W)^2}, \end{aligned} \quad (33)$$

$$\gamma(\omega) = \pi(\eta\Delta)^2 \sum_k \lambda_k^2 \delta(\omega - \omega_k) = \frac{\pi J(\omega)(\eta\Delta)^2}{(\omega + W)^2}, \quad (34)$$

where  $J(\omega)$  is the spectral density. The following abbreviation has been used:

$$\Gamma(\omega) = \gamma(\omega) + \frac{\epsilon^2}{\eta^2 \Delta^2} \gamma(\omega - W), \quad (35)$$

$$\Sigma(\omega) = R(\omega) + \frac{\epsilon^2}{\eta^2 \Delta^2} R(\omega - W). \quad (36)$$

The initial density operator,  $\tilde{\rho}_{21}(0)$  and  $\tilde{\rho}_{22}(0)$ , of the coupled system and its surrounding at  $t=0$  is  $\rho_{SB}(0) = e^{-S} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \rho_B e^S$ , and the corresponding initial reduced density operator for  $\tilde{H} \approx \tilde{H}_0 + \tilde{H}_1$  is

$$\tilde{\rho}_S(0) = \frac{1}{2} \begin{pmatrix} 1 - \epsilon/W & \eta\Delta/W \\ \eta\Delta/W & 1 + \epsilon/W \end{pmatrix}. \quad (37)$$

#### IV. NONEQUILIBRIUM CORRELATION

One of our purpose is to calculate the nonequilibrium correlation  $P(t)$ , which is defined as  $P(t) = \text{Tr}_S \{ \text{Tr}_B [ \rho_{SB}(t) \sigma_z ] \}$ , where  $\rho_{SB}(t)$  is the density operator for the original Hamiltonian. Because of the unitary transforms, it can be calculated as

$$\begin{aligned} P(t) &= \text{Tr}_S \{ \text{Tr}_B [ e^{-S} U \tilde{\rho}_{SB}(t) U^\dagger e^S \sigma_z ] \} \\ &= \text{Tr}_S \left( \tilde{\rho}_S(t) \left[ -\frac{\epsilon}{W} \sigma_z + \frac{\eta\Delta}{W} \sigma_x \right] \right) \\ &= \frac{\epsilon}{W} [2\tilde{\rho}_{22}(t) - 1] + \frac{2\eta\Delta}{W} \text{Re}[\tilde{\rho}_{21}(t)]. \end{aligned} \quad (38)$$

Thus, Eqs. (31) and (32) are to be calculated to get  $P(t)$  by numerical integration with sub-Ohmic spectral density.

The Markovian approximation is equivalent to approximate the integration by the residue theorem with the simple pole of the integrand of Eq. (31) at  $-2i\gamma_0$  and that of Eq. (32) at  $\omega_0 - i\gamma_0$ , which leads to

$$\begin{aligned} P(t) &= \frac{\epsilon}{W} \left\{ \left( \frac{\epsilon}{W} + 1 \right) \exp[-2\gamma_0 t] - 1 \right\} \\ &\quad + \frac{\eta^2 \Delta^2}{W^2} \cos(\omega_0 t) \exp[-\gamma_0 t], \end{aligned} \quad (39)$$

where  $\gamma_0 = \gamma(W)$  is the Weisskopf-Wigner approximation for the decay rate,

$$\gamma(W) = \frac{1}{2} \pi \alpha \omega_c^{1-s} W^s \frac{(\eta\Delta)^2}{W^2}, \quad (40)$$

and  $\omega_0 = W + \Sigma(W)$  [ $\Sigma(W)$  is the level shift]. Figure 2(a) shows comparison between Eqs. (38) and (39) for weak-coupling case  $\alpha=0.02$  ( $s=1/2$ ,  $\Delta/\omega_c=0.1$ , and  $\epsilon/\omega_c=0.05$ ), where our non-Markovian dynamics [Eq. (38)] is nearly the same as that of the Markovian approximation [Eq. (39)]. However, for strong-coupling case  $\alpha=0.1$ , Fig. 2(b) shows a big difference of our non-Markovian dynamics from that of the Markovian one, especially for the short time oscillating

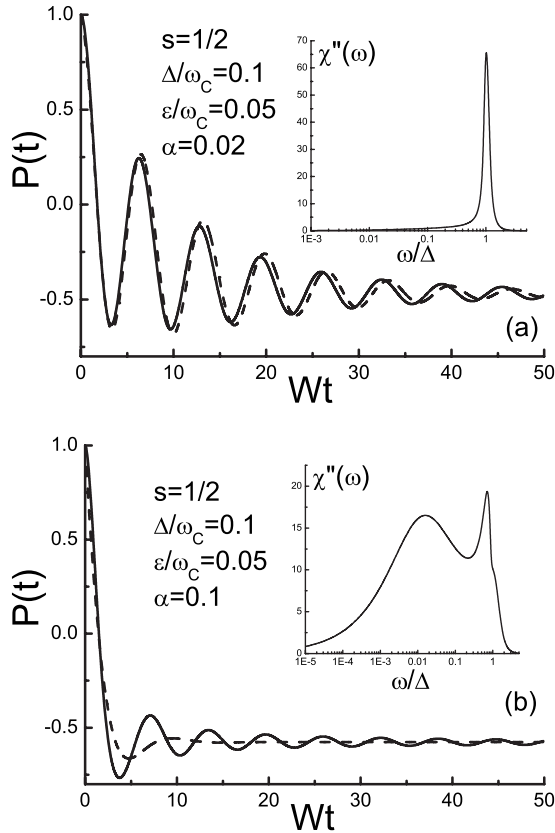


FIG. 2. Nonequilibrium correlation  $P(t)$  for (a) weak-coupling case  $\alpha=0.02$  and (b) strong-coupling case  $\alpha=0.1$ . The dashed lines are the Markovian approximation [Eq. (39)]. The insets show the susceptibility  $\chi''(\omega)$  vs  $\omega$  relations.

behavior which has been smeared out in Markovian approximation. The insets are for the susceptibility  $\chi''(\omega)$  which will be calculated in Sec. V. Here we note that for weak-coupling case [Fig. 2(a)] the susceptibility has one sharp peak only and the Markovian approximation may be a good one; for strong-coupling case [Fig. 2(b)] the susceptibility has two peaks and the Markovian approximation is not good at least for the short time behavior.

A nonzero bias plays an important role in the quantum dynamics of the two-level system coupled with a sub-Ohmic bath. Figure 3 shows the nonequilibrium correlation  $P(t)$  for zero and nonzero biases. One can see that, apart from the effect of bias on the behavior of long time limit [ $P(t \rightarrow \infty) = -\epsilon/W$ ], a nonzero bias enhances the quantum coherence as the decay rate of the Rabi oscillation for the case of  $\epsilon/\omega_c = 0.05$  is obviously lower than that of  $\epsilon=0$ .

Figure 4 compares the nonequilibrium correlation  $P(t)$  for different couplings for  $s=1/2$  with nonzero bias  $\epsilon/\omega_c=0.02$ . For weak coupling  $\alpha=0.01$  (dashed-dotted line), the quantum coherence may be kept for a longer time, but for the moderate coupling  $\alpha=0.04$  (solid line), the Rabi oscillation proceeds for a shorter time. For the strong coupling  $\alpha=0.091$  (dashed line), the Rabi oscillation is quite weak. We note that for  $s=1/2$  and  $\epsilon/\omega_c=0.02$  the coherence-decoherence transition point is at  $\alpha_c=0.0917$ , which will be determined in Sec. V.

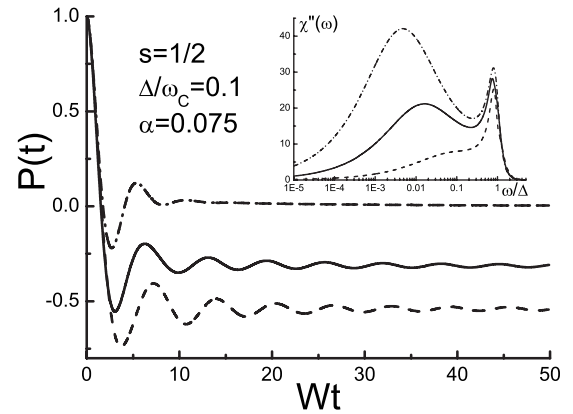


FIG. 3. Nonequilibrium correlation  $P(t)$  for different biases:  $\epsilon/\omega_c=0$  (dashed-dotted line), 0.025 (solid line), and 0.05 (dashed line). The inset shows the susceptibility  $\chi''(\omega)$  vs  $\omega$  relations for different biases.

In our approach two approximations have been made: one is the omission of  $\tilde{H}_2$  and the other is the usual Born approximation for deriving the master equation [Eq. (23)]. Hence, the validity of our approach should be checked and one check may be the sum rule  $P(t=0)=1$  for Eq. (38). It has been checked and is satisfied exactly for all the cases we calculated.

## V. SUSCEPTIBILITY AND COHERENCE-DECOHERENCE TRANSITION

The retarded Green's functions [25] are

$$G(t) = -i\theta(t)Z^{-1} \text{Tr}\{\exp(-\beta H)[\exp(iHt)\sigma_z \exp(-iHt), \sigma_z]\}, \quad (41)$$

where  $[A, B] = AB - BA$  and  $Z = \text{Tr}[\exp(-\beta H)]$ . The Fourier transformation  $G(\omega)$  is obtained in the Appendix. The imaginary part of  $G(\omega)$  is

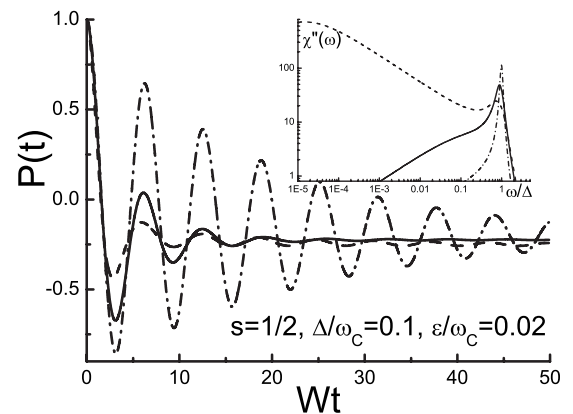


FIG. 4. Nonequilibrium correlation  $P(t)$  for different couplings:  $\alpha=0.01$  (dashed-dotted line), 0.04 (solid line), and 0.091 (dashed line). The inset shows the susceptibility  $\chi''(\omega)$  vs  $\omega$  relations for different couplings. The coherence-decoherence transition point is at  $\alpha_c=0.0917$ .



TABLE I. Shiba's relation is checked for nonzero bias and sub-Ohmic cases.  $R = \lim_{\omega \rightarrow 0} S(\omega) / \frac{\pi}{4} [\chi'(\omega)]^2$ , where  $S(\omega) = \chi''(\omega) / J(\omega)$ .

$s$	$\Delta / \omega_C$	$\epsilon / \omega_C$	$\alpha$	$\chi'(\omega)$	$\lim_{\omega \rightarrow 0} S(\omega)$	$R$
1/4	0.1	0	0.01	34.495979	934.60225	1.0
1/4	0.1	0.05	0.03	121.46668	11587.889	1.0000004
1/4	0.1	0.1	0.05	23.147908	420.84016	1.0000088
1/2	0.1	0	0.05	51.586893	2090.1075	1.0
1/2	0.1	0.05	0.1	73.517115	4244.8999	1.0000015
1/2	0.1	0.1	0.2	19.755668	306.53734	1.0000232
3/4	0.1	0	0.1	43.000554	1452.2386	1.0
3/4	0.1	0.05	0.3	78.204433	4803.4538	1.0000023
3/4	0.1	0.1	0.5	11.44906	102.95554	1.0000465
1	0.1	0	0.5	3072.9597	7416578.9	1.0
1	0.1	0.01	0.5	694.5864	378915.56	1.0
1	0.1	0.02	0.5	205.86769	33286.362	1.0000002

$$\text{Im } G(\omega) = -\frac{(\eta\Delta)^2 \langle \sigma_z \rangle_{\tilde{H}_0}}{W^2} \left\{ \frac{\Gamma(\omega)\theta(\omega)}{[\omega - W - \Sigma(\omega)]^2 + \Gamma^2(\omega)} - \frac{\Gamma(-\omega)\theta(-\omega)}{[\omega + W + \Sigma(-\omega)]^2 + \Gamma^2(-\omega)} \right\}. \quad (42)$$

$\langle \sigma_z \rangle_{\tilde{H}_0} = 1$ , which is the average value of  $\sigma_z$  in the ground state of  $\tilde{H}_0$ .  $\Sigma(\omega)$  and  $\Gamma(\omega)$  are those in Eqs. (35) and (36).

The susceptibility  $\chi(\omega) = -G_-(\omega)$  and its imaginary part is

$$\begin{aligned} \chi''(\omega) &= \int_{-\infty}^{\infty} dt \exp(i\omega t) \frac{1}{2} \text{Tr} \{ \exp(-\beta H) [\sigma_z(t)\sigma_z - \sigma_z\sigma_z(t)] \} / Z \\ &= \frac{(\eta\Delta)^2}{W^2} \left\{ \frac{\Gamma(\omega)\theta(\omega)}{[\omega - W - \Sigma(\omega)]^2 + \Gamma^2(\omega)} - \frac{\Gamma(-\omega)\theta(-\omega)}{[\omega + W + \Sigma(-\omega)]^2 + \Gamma^2(-\omega)} \right\}. \end{aligned} \quad (43)$$

The real part of static susceptibility  $\chi'(\omega=0)$  can be obtained by the following integral:

$$\chi'(\omega=0) = \frac{2}{\pi} \int_0^{\infty} \frac{\chi''(\omega)}{\omega} d\omega. \quad (44)$$

Another check for our approach is Shiba's relation [3,6,7],

$$\lim_{\omega \rightarrow 0} \frac{\chi''(\omega)}{J(\omega)} = \frac{\pi}{4} [\chi'(\omega=0)]^2, \quad (45)$$

which should be satisfied for the two-level system coupled to a heat bath. Table I shows that Shiba's relation is exactly satisfied for  $s \leq 1$  in our calculations.

Generally speaking,  $\chi''(\omega)$  is an even function of  $\omega$ ,  $\chi''(-\omega) = \chi''(\omega)$ . For the Ohmic bath ( $s=1$ ) with zero bias, it is well known [1,2] that  $\chi''(\omega)$  has a peak at  $\omega = \Delta_r$  for  $\alpha < \alpha_c = 1/2$ , where  $\Delta_r$  is the renormalized tunneling. Besides,

$\chi''(\omega=0) = 0$  when  $\alpha < \alpha_c = 1/2$ . At  $\alpha = \alpha_c$ , the peak moves to  $\omega = 0$  with  $\chi''(\omega=0) = \infty$ .  $\alpha_c$  is the coherence-decoherence transition point [1,2].

For the Ohmic bath ( $s=1$ ) with zero bias ( $\epsilon=0$ ) our result is exactly the same, that is,  $\chi''(\omega)$  has a peak at  $\omega \approx \omega_p$  for  $\alpha < \alpha_c$  with  $\alpha_c = \frac{1}{2}(1 + \eta\Delta/\omega_c)$  [13,23], where  $\omega_p$  is the solution of following equation:

$$\omega_p - W - \Sigma(\omega_p) = 0. \quad (46)$$

But for nonzero bias and sub-Ohmic bath, which is the main focus of this work, the spectrum of  $\chi''(\omega)$  becomes more complicated. When coupling is weak (smaller  $\alpha$ ),  $\chi''(\omega)$  has one peak only at  $\omega \approx \omega_p$  [see the inset of Fig. 2(a)]. For stronger coupling,  $\chi''(\omega)$  has two peaks in the range  $\omega > 0$ , one is at  $\omega \approx \omega_p$  [the solution of Eq. (46)] and the other at the place much lower than  $\omega_p$  [see the inset of Fig. 2(b)].

The inset of Fig. 3 shows the effect of a nonzero bias on the susceptibility  $\chi''(\omega)$ . When  $\epsilon/\omega_c$  increases, the double peak structure of the susceptibility  $\chi''(\omega)$  for  $\epsilon=0$  changes gradually to a single peak structure for  $\epsilon/\omega_c = 0.05$ . Besides, the inset of Fig. 4 shows the effect of different couplings on the susceptibility  $\chi''(\omega)$  for  $s=1/2$  and nonzero bias  $\epsilon/\omega_c = 0.02$ . For weak coupling  $\alpha=0.01$  (dashed-dotted line), the quantum coherence can be kept for a longer time and the susceptibility has a sharp single peak. But for the moderate coupling  $\alpha=0.04$  (solid line), the second peak with lower frequency emerges. For the strong coupling  $\alpha=0.091$  (dashed line), the second peak with lower frequency approaches  $\omega \approx 0$  with higher peak height.

At  $\alpha = \alpha_c$ , the second peak is at  $\omega=0$  with infinite height  $\chi''(\omega=0) = \infty$  since  $\Gamma(\omega) \sim \omega^s$  for  $\omega \rightarrow 0$ . That means, at  $\alpha = \alpha_c$ , the lower peak moves to  $\omega=0$  while the higher peak may still exist. Here, as in the case of zero bias and Ohmic bath, we define  $\alpha_c$  as the coherence-decoherence transition point for nonzero bias and sub-Ohmic bath. Mathematically,  $\alpha_c$  is determined as the solution of

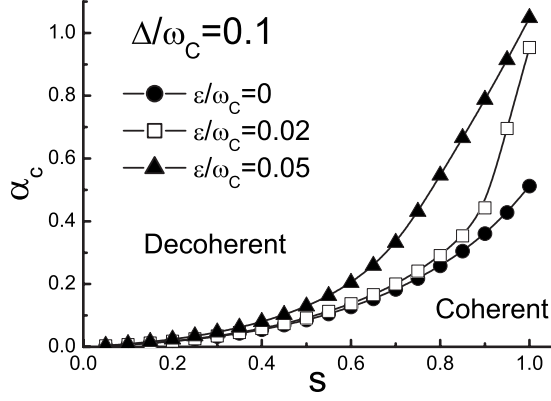


FIG. 5. The coherent-decoherent transition point  $\alpha_c$  vs the index of sub-Ohmic bath  $s$  relations for different biases:  $\epsilon/\omega_c=0$  (solid circles), 0.02 (empty squares), and 0.05 (solid triangles).

$$-W - \Sigma(0) = 0 \quad (47)$$

because this is the condition for  $\chi''(\omega=0)=\infty$ . For  $s < 1$  the formula for  $\alpha_c$  is quite complicated, but for nonzero bias with Ohmic bath ( $s=1$ ) it is

$$\alpha_c = \frac{1}{2} \left[ \frac{(\eta\Delta)^2}{W^2} \frac{\omega_c}{\omega_c + W} + \frac{1}{2} \frac{\epsilon^2}{W^2} \frac{\omega_c^2}{(\omega_c + W)^2} \right]^{-1}, \quad (48)$$

which leads to the transition point for zero bias ( $\epsilon=0$ ):  $\alpha_c = \frac{1}{2}(1 + \eta\Delta/\omega_c)$  [23].

Figure 5 shows the coherence-decoherence transition point  $\alpha_c$  as functions of the index of sub-Ohmic bath  $s$ , which may be treated as a “phase diagram” with the area of  $\alpha < \alpha_c$  as the “coherent phase” but that of  $\alpha > \alpha_c$  the “decoherent phase.”

## VI. CONCLUDING REMARKS

The non-Markovian dynamics of the dissipative two-level system coupled to the sub-Ohmic bath ( $0 < s \leq 1$ ) with non-

zero bias has been studied by means of the perturbation approach based on a unitary transformation. It has been shown that the Markovian approximation may be not good for the case of sub-Ohmic bath and the non-Markovian approach should be used especially for the short time behavior of the coupled system and environment. The nonequilibrium correlation  $P(t)$  has been calculated to show that a finite bias may favor the short time coherence. The spectrum of the susceptibility  $\chi''(\omega)$  of the sub-Ohmic case may have a double peak structure in the range of  $\omega > 0$  when the coupling  $\alpha$  is relatively strong. Besides, the coherence-decoherence transition point  $\alpha_c$  is determined for different  $0 < s \leq 1$  by the condition of  $\chi''(\omega=0)=\infty$  when  $\alpha = \alpha_c$ . Our results have been checked by showing that Shiba's relation is exactly satisfied for  $0 < s \leq 1$  with nonzero bias.

The key point of our treatment is the unitary transformation with generator equation [Eq. (2)], where a parameter  $\xi_k$  is introduced. After the transformation a perturbation expansion has been performed. If  $\xi_k=0$  for all  $k$ , that is, without the transformation, the perturbation expansion would be similar to the standard weak-coupling expansion (Bloch-Redfield theory). Besides, if  $\xi_k=1$  for all  $k$ , then our transformation is the usual polaronic transformation and the perturbation expansion is for the small parameter  $\Delta$  which is equivalent to the non-interacting blip approximation [26]. Our choice for  $0 < \xi_k < 1$  [Eq. (15)] is in between and thus is an improvement on the analytical methods.

## ACKNOWLEDGMENT

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## APPENDIX

The retarded Green's functions are

$$\begin{aligned} G(t) &= -i\theta(t)Z^{-1} \text{Tr}\{\exp(-\beta H)[\exp(iHt)\sigma_z \exp(-iHt), \sigma_z]\} \\ &= -i\theta(t)Z^{-1} \text{Tr}\{\exp(-\beta H')[\exp(iH't)\sigma_z \exp(-iH't), \sigma_z]\} \\ &= -i\theta(t)Z^{-1} \text{Tr}\{\exp(-\beta \tilde{H})[\exp(i\tilde{H}t)U^\dagger \sigma_z U \exp(-i\tilde{H}t), U^\dagger \sigma_z U]\} \\ &= -i\theta(t)Z^{-1} \text{Tr}\left\{ \exp(-\beta \tilde{H}) \left( \frac{\epsilon^2}{W^2} [\sigma_z(t), \sigma_z] + \frac{(\eta\Delta)^2}{W^2} [\sigma_x(t), \sigma_x] - \frac{\epsilon\eta\Delta}{W^2} [\sigma_z(t), \sigma_x] - \frac{\epsilon\eta\Delta}{W^2} [\sigma_x(t), \sigma_z] \right) \right\}, \quad (A1) \end{aligned}$$

where

$$Z = \text{Tr}[\exp(-\beta H)] = \text{Tr}[\exp(-\beta \tilde{H})],$$

$[A, B] = AB - BA$ , and  $\sigma_{z(x)}(t) = \exp(i\tilde{H}t)\sigma_{z(x)}\exp(-i\tilde{H}t)$  is in the Heisenberg picture of  $\tilde{H}$ . The Fourier transformation of  $G(t)$  is denoted as  $G(\omega)$ ,

$$\begin{aligned} G(\omega) &= \frac{\epsilon^2}{W^2} \langle\langle \sigma_z; \sigma_z \rangle\rangle + \frac{(\eta\Delta)^2}{W^2} \langle\langle \sigma_x; \sigma_x \rangle\rangle - \frac{\epsilon\eta\Delta}{W^2} \langle\langle \sigma_z; \sigma_x \rangle\rangle \\ &\quad - \frac{\epsilon\eta\Delta}{W^2} \langle\langle \sigma_x; \sigma_z \rangle\rangle, \end{aligned}$$

where

$$\langle\langle A; B \rangle\rangle = -i\theta(t)Z^{-1} \text{Tr}\{\exp(-\beta\tilde{H})[\exp(i\tilde{H}t)A \exp(-i\tilde{H}t), B]\}$$

denotes the retarded Green's function which satisfies the following equation of motion:

$$\omega\langle\langle A; B \rangle\rangle = \langle[A, B]\rangle + \langle\langle[A, \tilde{H}]; B\rangle\rangle,$$

$$\langle[A, B]\rangle = Z^{-1} \text{Tr}\{\exp(-\beta\tilde{H})[A, B]\}.$$

Thus, we can get the following equation chain:

$$\begin{aligned} \omega\langle\langle\sigma_x; \sigma_x\rangle\rangle &= W\langle\langle i\sigma_y; \sigma_x\rangle\rangle + \sum_k Q_k\langle\langle i\sigma_y(b_k^\dagger + b_k); \sigma_x\rangle\rangle \\ &\quad - \sum_k V_k\langle\langle\sigma_z(b_k^\dagger - b_k); \sigma_x\rangle\rangle, \end{aligned} \quad (\text{A2})$$

$$\begin{aligned} \omega\langle\langle i\sigma_y; \sigma_x\rangle\rangle &= 2\langle\sigma_z\rangle + W\langle\langle\sigma_x; \sigma_x\rangle\rangle + \sum_k Q_k\langle\langle\sigma_x(b_k^\dagger + b_k); \sigma_x\rangle\rangle \\ &\quad + \sum_k V_k\langle\langle\sigma_z(b_k^\dagger + b_k); \sigma_x\rangle\rangle, \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \omega\langle\langle\sigma_x(b_k^\dagger + b_k); \sigma_x\rangle\rangle &= -\omega_k\langle\langle\sigma_x(b_k^\dagger - b_k); \sigma_x\rangle\rangle + W\langle\langle i\sigma_y(b_k^\dagger \\ &\quad + b_k); \sigma_x\rangle\rangle + Q_k\langle\langle i\sigma_y; \sigma_x\rangle\rangle, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} \omega\langle\langle\sigma_x(b_k^\dagger - b_k); \sigma_x\rangle\rangle &= -\omega_k\langle\langle\sigma_x(b_k^\dagger + b_k); \sigma_x\rangle\rangle + W\langle\langle i\sigma_y(b_k^\dagger \\ &\quad - b_k); \sigma_x\rangle\rangle - Q_k\langle\langle\sigma_x; \sigma_x\rangle\rangle, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} \omega\langle\langle i\sigma_y(b_k^\dagger + b_k); \sigma_x\rangle\rangle &= -\omega_k\langle\langle i\sigma_y(b_k^\dagger - b_k); \sigma_x\rangle\rangle + W\langle\langle\sigma_x(b_k^\dagger \\ &\quad + b_k); \sigma_x\rangle\rangle + Q_k\langle\langle\sigma_x; \sigma_x\rangle\rangle, \end{aligned} \quad (\text{A6})$$

$$\begin{aligned} \omega\langle\langle i\sigma_y(b_k^\dagger - b_k); \sigma_x\rangle\rangle &= -\omega_k\langle\langle i\sigma_y(b_k^\dagger + b_k); \sigma_x\rangle\rangle + W\langle\langle\sigma_x(b_k^\dagger \\ &\quad - b_k); \sigma_x\rangle\rangle - Q_k\langle\langle i\sigma_y; \sigma_x\rangle\rangle, \end{aligned} \quad (\text{A7})$$

where  $V_k = \eta\Delta g_k \xi_k / \omega_k$  and  $Q_k = \epsilon g_k \xi_k / \omega_k$ . We already made the cutoff approximation for the equation chain at the second order of  $g_k$ . Besides, until the second order of  $g_k$  we have  $\langle\langle\sigma_z; \sigma_x\rangle\rangle = 0$ ,  $\langle\langle\sigma_z; \sigma_z\rangle\rangle = 0$ , and  $\langle\langle\sigma_x; \sigma_z\rangle\rangle = 0$ . So the solution for  $G(\omega)$  is

$$\begin{aligned} G(\omega) &= \frac{(\eta\Delta)^2}{W^2} \\ &\quad \times \left( \frac{\langle\sigma_z\rangle}{\omega - W - \sum_k V_k^2/(\omega - \omega_k) - \sum_k Q_k^2/(\omega - W - \omega_k)} \right. \\ &\quad \left. - \frac{\langle\sigma_z\rangle}{\omega + W - \sum_k V_k^2/(\omega + \omega_k) - \sum_k Q_k^2/(\omega + W + \omega_k)} \right). \end{aligned} \quad (\text{A8})$$

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