# Localization breakdown as a joint effect of nonlinear and quantum dissipation

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We evaluate the time evolution of $\sigma_x$, the transverse component of a spin-$\frac{1}{2}$ dipole coupled to an Ohmic bath, using a theory balancing the quantum-mechanical fluctuations of the bath, as depicted by the noninteracting-blip approximation, with the nonlinear dynamics of the discrete nonlinear Schrödinger equation. As a relevant effect of the joint action of these two ingredients, we find that the time evolution of the system does not lead to the localization predicted by some equilibrium analyses. More precisely, starting from an eigenstate of $\sigma_x$, the spin system will never asymptotically reach a broken-symmetry state.

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## I. INTRODUCTION

The well known "spin-boson Hamiltonian" [1]

$$H=-\frac{\omega_0}{2}\sigma_z+gx\sigma_x+\sum_i \omega_i b_i^\dagger b_i \ , \tag{1.1}$$

where

$$x\equiv\sum_i x_i, \quad x_i\equiv\Gamma_i(b_i+b_i^\dagger) \tag{1.2}$$

is the simplest model used to describe the influence of the environment on the dynamics of a quantum system. The two-level system (equivalent to a spin-$\frac{1}{2}$ magnetic dipole in a magnetic field) is the quantum system of interest. The coupling between the system of interest and the set of quantum-mechanical oscillators introduces a mechanism of fluctuation and dissipation within a fully Hamiltonian picture. The number of oscillators is assumed to be infinite with the corresponding frequencies distributed over a continuum. Because of its simplicity, the model Hamiltonian of Eq. (1.1) has been studied in many different areas, to name a few, solid-state physics, chemical physics [2], and the foundation of quantum mechanics [3].

Usually all these studies refer to the time evolution of $\langle\sigma_x(t)\rangle$ starting from the initial condition [1]

$$\rho(0)\propto|+\rangle_x\langle+|_x\exp\left[-\beta\left[\sum_i \omega_i b_i^\dagger b_i+gx\right]\right], \tag{1.3}$$

where $\beta\equiv 1/k_BT$. This means that at the initial time the spin-$\frac{1}{2}$ dipole is polarized along the positive direction of the $x$ axis, i.e., it is in the eigenstate $|+\rangle_x$ defined by $\sigma_x|+\rangle_x=|+\rangle_x$. The initial statistical distribution of the oscillators is canonical with respect to the correspondingly shifted harmonic potential.

It is well known [4] that a reliable simulation of a fluctuation-dissipation process implies a proper treatment of the so-called reaction field, i.e., the influence that the system of interest exerts on its own "bath." It has been shown [5] that the approximation proposed by Leggett and co-workers [1] to study this problem, i.e, the noninteracting-blip approximation (NBA) [1], is actually equivalent to neglecting the reaction field. For this reason, in a preceding paper [6] two of the authors tried to improve the NBA theory and devoted a great deal of attention to the role of the reaction field. The theory developed in [6] is based on the adoption of a coordinate transformation reminiscent of the polaronic transformation [7], but well distinct from it and termed pseudopolaronic transformation (PPT). For the sake of concision we shall refer to the theory of Ref. [6] as the PPT theory. The main prediction of this theory [6] is the following equation of motion for $\langle\sigma_x(t)\rangle$:

$$\langle\dot\sigma_x(t)\rangle=-\omega_0^2\int_0^t ds\langle\sigma_x(s)\rangle\mathrm{Re}\left[\exp\left[-4g^2\int_0^{t-s}dt_1\int_0^{t_1}dt_2\langle\bar x^{(0)}(t_2)\bar x^{(0)}(0)\rangle\right]e^{-4i\Delta(t-s)}\right.$$
$$\left.\times\exp\left[4ig^2\int_s^t d\tau\int_0^\tau d\tau'\sum_i\Gamma_i^2\sin[\omega_i(\tau-\tau')][1-\langle\sigma_x(\tau')\rangle]\right]\right] \tag{1.4}$$

(the coordinate $\bar x^{(0)}$ refers to the unperturbed motion of the bath of oscillators while the parameter $\Delta$ will be defined later on). This equation generalizes the NBA theory through the third exponential term of the kernel, which makes it nonlinear. Remarkably this nonlinear term, triggered by the reaction field, is proved [6] to be *closely related* to the nonlinear term of the discrete nonlinear Schrödinger equation (DNSE) for the two-site case

 

[8–10]. In Ref. [6] it has been stressed indeed that if the thermal and quantum fluctuations are neglected, then Eq. (1.4) becomes equivalent to the theory developed by Kenkre and Wu (KW), who applied the DNSE to the case of the "nonadiabatic dimer" [11]. The striking consequences of the reaction field are widely discussed in Refs. [12–14] under strong semiclassical assumptions.

In this paper we shall study the dynamics predicted by Eq. (1.4) in the case of Ohmic bath, i.e., when the bath is described by the spectral density:

$$J(\omega)\equiv g^2\sum_i \Gamma_i^2\delta(\omega-\omega_i)=g^2\omega\exp(-\omega/\omega_c)\ . \quad (1.5)$$

We shall focus our attention especially on the intriguing phenomenon of localization. The authors of Ref. [15], with a static analysis have shown that at $T=0$ and in the Ohmic case, the spin $\frac{1}{2}$ can partially localize in one site, i.e., $\langle\sigma_x\rangle_{eq}\neq 0$, provided that the coupling $g$ is sufficiently strong. However, it is not yet clearly assessed if and how this localization dynamically develops from the initial condition of Eq. (1.3). To shed light on this key issue, it is convenient to illustrate the predictions of the NBA and KW theory on the problem of dynamical localization.

The NBA theory [16] results in a satisfactory agreement with the equilibrium predictions of Ref. [15]. According to these theories localization takes place at

$$g=\frac{1}{\sqrt{2}} \quad (1.6a)$$

(note that the parameter $\alpha$ of Refs [1,16] in our notations corresponds to $2g^2$) and beyond it, the NBA theory predicts the following asymptotic mean value for the $x$ component of the dipole [16]:

$$\langle\sigma_x(\infty)\rangle=\frac{1}{1+(\omega_0/\omega_c)^2[1/(4g^2-1)(4g^2-2)]} \quad (1.6b)$$

Also the KW theory predicts the existence of an asymptotic-time symmetry breaking. In fact, taking into account the correspondence rules given in [6] between the spin-boson model of Eq. (1.1) and the phenomenological KW model (actually the bath of Kenkre and Wu [11] corresponds to a single classical and overdamped oscillator) it turns out that the transition to localization takes place at

$$g=\frac{1}{2}\left[\frac{\omega_0}{\omega_c}\right]^{1/2} \quad (1.7a)$$

and the corresponding expression for $\langle\sigma_x(\infty)\rangle$ is

$$\langle\sigma_x(\infty)\rangle=\left[1-\left[\frac{\omega_0}{4g^2\omega_c}\right]^2\right]^{1/2}\ . \quad (1.7b)$$

The PPT theory recovers under specific conditions both the NBA and the KW theories, each of them leading to localization. Thus one would be tempted to conclude that the PPT theory also implies localization with perhaps a different threshold. The main result of this paper is that this intuitive conclusion is wrong and that the initial condition of Eq. (1.3) does not lead to any localization within the context of the PPT theory. The joint action of the reaction field and quantum-mechanical fluctuations leads to the localization breakdown, in spite of the fact that their separate action would support localization.

Section II is devoted to a further derivation of Eq. (1.4) which makes more transparent the role of the reaction field. In Sec. III we shall evaluate the long-time prediction of the PPT theory and we will prove that it does not admit localization. Section IV will illustrate with numerical results how the dynamical evolution driven by Eq. (1.4) departs from the NBA predictions to adhere to the long-time theoretical predictions of Sec. III. Section V is devoted to comparing the predictions of the PPT theory to those of the current literature on this subject and to transparent physical arguments explaining why the joint action of the reaction field and quantum fluctuations provokes the localization breakdown.

## II. TREATMENT OF THE REACTION FIELD

This section is devoted to the derivation of Eq. (1.4) with an approach which is slightly different from that used in Ref. [6] and makes it easier to understand the approximation on which the PPT theory rests.

From the Hamiltonian of Eq. (1.1), we get the following Heisenberg equations:

$$\begin{aligned}&\dot\sigma_x(t)=\omega_0\sigma_y(t)\ ,\\ &\dot\sigma_y(t)=-\omega_0\sigma_x(t)-2gx(t)\sigma_z(t)\ ,\\ &\dot\sigma_z(t)=2gx(t)\sigma_y(t)\ ,\\ &\ddot x_i(t)+\omega_i^2x_i(t)=-2\omega_i g\Gamma_i^2\sigma_x(t)\ .\end{aligned} \quad (2.1)$$

Because of the initial condition of Eq. (1.3), the unperturbed motion of the collective coordinate $x(t)$, which will be denoted with $x^{(0)}(t)$, is such that $\langle x^{(0)}(t)\rangle\neq 0$. Then it is convenient to shift the reference frame so as to make the mean value of the new unperturbed coordinate, $\tilde x^{(0)}(t)$, vanish. This condition is fulfilled by adopting the new $b$ and $x$ operators defined by

$$\tilde b_i\equiv b_i+\frac{g\Gamma_i}{\omega_i}\ , \quad (2.2a)$$

$$\tilde x_i\equiv\Gamma_i(\tilde b_i+\tilde b_i^\dagger),\quad \tilde x\equiv\sum_i\tilde x_i\ . \quad (2.2b)$$

The initial condition of Eq. (1.3) expressed in terms of the new operators is

$$\rho(0)\propto|+\rangle_x\langle+|_x\exp\left[-\beta\left[\sum_i\omega_i\tilde b_i^\dagger\tilde b_i\right]\right]\ . \quad (2.3)$$

As a consequence of adopting the new reference framework, the collective and unperturbed coordinate $\tilde x^{(0)}(t)$ is a Gaussian stochastic operator, with vanishing mean value that is completely defined by the two-time correlation function; in fact we have

$$\langle \bar{x}^{(0)}(t_1)\cdots\bar{x}^{(0)}(t_{2n+1})\rangle = 0 \,, \tag{2.4a}$$

$$\langle \bar{x}^{(0)}(t_1)\cdots\bar{x}^{(0)}(t_{2n})\rangle = \sum_{\text{pair}} \langle \bar{x}^{(0)}(t_{i_1})\bar{x}^{(0)}(t_{i_2})\rangle \cdots \langle \bar{x}^{(0)}(t_{i_{2n-1}})\bar{x}^{(0)}(t_{i_{2n}})\rangle \tag{2.4b}$$

with order preserved [17].

In the new reference system the set of equations of (2.1) becomes

$$\begin{aligned}
&\dot{\sigma}_x(t) = \omega_0 \sigma_y(t) \,, \\
&\dot{\sigma}_y(t) = -\omega_0 \sigma_x(t) + 4\Delta\sigma_z(t) - 2g\bar{x}(t)\sigma_z(t) \,, \\
&\dot{\sigma}_z(t) = -4\Delta\sigma_y(t) + 2g\bar{x}(t)\sigma_y(t) \,, \\
&\ddot{\bar{x}}_i(t) + \omega_i^2 \bar{x}_i(t) = -2\omega_i g \Gamma_i^2 [\sigma_x(t) - 1] \,,
\end{aligned} \tag{2.5}$$

where

$$\Delta \equiv g^2 \sum_i \frac{\Gamma_i^2}{\omega_i} \,. \tag{2.6}$$

Formally solving the second and the third equations of Eq. (2.5) and inserting the solution in the first one, we get

$$\begin{aligned}
\dot{\sigma}_x(t) = {} & \frac{\omega_0}{2} \left[ T \exp\left[ 2ig \int_0^t d\tau \bar{x}(\tau) \right] \exp(-4i\Delta t)\sigma_+(0) + \text{H.c.} \right] \\
& - \frac{\omega_0^2}{2} \int_0^t ds \left[ T \exp\left[ 2ig \int_s^t d\tau \bar{x}(\tau) \right] \exp[-4i\Delta(t-s)]\sigma_x(s) + \text{H.c.} \right] \,,
\end{aligned} \tag{2.7}$$

where

$$\sigma_\pm \equiv \sigma_y \pm i\sigma_z \tag{2.8}$$

and $T$ exp denotes the time-ordered exponential. Note that $\bar{x}(t)$ reads

$$\bar{x}(t) = \bar{x}^{(0)}(t) + R(t) \,. \tag{2.9}$$

It consists of the sum of the unperturbed time evolution of the collective bath coordinate $\bar{x}^{(0)}(t)$, the explicit expression of which is

$$\bar{x}^{(0)}(t) = \sum_i \Gamma_i (\tilde{b}_i e^{-i\omega_i t} + \tilde{b}_i^\dagger e^{i\omega_i t}) \,, \tag{2.10}$$

and of the term $R(t)$, depending on the state of the system,

$$R(t) \equiv 2g \int_0^t d\tau \sum_i \Gamma_i^2 \sin\omega_i(t-\tau)[1 - \sigma_x(\tau)] \,. \tag{2.11}$$

This term takes into account the influence exerted by the state of the spin-$\frac{1}{2}$ system on the bath. From now on we shall refer to it as the reaction field [4,18].

In order to determine the evolution of $\langle \sigma_x(t)\rangle$, we have now to average Eq. (2.7) using the initial condition given by Eq. (1.3), which is actually a prohibitive task because of the presence of the reaction field $R(t)$. This is where approximations are necessary. The NBA is recovered [5,6] by averaging Eq. (2.7) with the key assumption that $R(t) \approx 0$. The PPT theory [6] is recovered by replacing the $R(t)$ with its mean value. This will be proved later in this section. First, let us discuss the physical reasons for the key assumption that $R(t)$ can be replaced by $\langle R(t)\rangle$.

From a general point of view, the motion of the two-level system can be seen as a superposition of three processes with distinct time scales. First of all there is a slow and systematic process. In the weak-coupling limit this is a damped oscillatory motion with frequency $\approx\omega_0$. In the strong-coupling limit this motion becomes much slower [1]. Thus we can say that the time scale of the systematic motion of the spin is comparable to $\omega_0^{-1}$ or else larger. The second process characterizing the dynamics of the spin system is due to the interaction with the bath of oscillators. This interaction, in addition to heavily affecting the free oscillations with frequency $\omega_0$, also makes the system fluctuate with approximately the same time scale as that of the bath. The third and fastest process concerns the merely quantum-mechanical fluctuations of the system.

The "bath coordinate" $\bar{x}$ certainly is affected by the first process, since this is much slower than its own dynamics. In principle, the coordinate $\bar{x}$ can also be influenced by the second process, with precisely its own time scale. As to the quantum fluctuations of the spin system, on the contrary, these must be imagined as being an infinitely fast process stemming from the uncertainty principle itself of quantum mechanics, and the dynamics of the coordinate $\bar{x}$ can be safely imagined as being independent of them. This would lead us to the following sound assumption:

$$\bar{x}(t)\approx\langle\bar{x}(t)\rangle_S\ , \tag{2.12}$$

where we adopt the following definition:

$$\langle A(t)\rangle_S\equiv\mathrm{Tr}_S[A(t)\rho_S(0)] \tag{2.13}$$

and $\rho_s(0)=|+\rangle_x\langle+|_x$ is the density matrix describing the initial condition of the spin-$\frac{1}{2}$ dipole. This means that in (2.7) and (2.8) the following assumption should be adopted:

$$R(t)=\langle R(t)\rangle_S\ . \tag{2.14}$$

Averaging over Eq. (2.7), we then obtain

$$\langle\dot{\sigma}_x(t)\rangle=-\omega_0^2\int_0^t ds\ \mathrm{Re}\left[\left\langle T\exp\left[2ig\int_s^t d\tau[\bar{x}^{(0)}(\tau)+\langle R(\tau)\rangle_S]\right]\sigma_x(s)\right\rangle_B e^{-4i\Delta(t-s)}\right] \tag{2.15}$$

where $\langle\cdots\rangle_B$ stands for $\mathrm{Tr}_B\{\cdots\rho_B\}$ and $\rho_B$ is the initial condition for the bath [see Eq. (1.3)]. Note that with the symbol $\langle\ \rangle$ we denote averaging on both $S$ and $B$. Equation (2.15) is supposed to be the best possible approximation because it only sets equal to zero the "time scale" of the quantum fluctuations, which are therefore thought of as "instantaneous." Unfortunately this scheme involves the moments of $\sigma_x$ at all orders. To get a closed equation for $\langle\sigma_x(t)\rangle$ alone we must have recourse to the less accurate approximation

$$R(t)\approx\langle R(t)\rangle\ , \tag{2.16}$$

which is a sort of "mean-field approximation." This is equivalent to saying that the dynamics of the coordinate $\bar{x}$ is affected only by the systematic part of the spin motion, but not by the thermal and quantum fluctuations around it. This is not a completely correct physical assumption, since the thermal fluctuations of the spin system have the same time scale as that of the bath, which therefore should be affected by them.

However, we believe that keeping the mean value of the reaction field is certainly a better approximation than neglecting it completely (as is done by the NBA). The PPT theory departs from the NBA theory as a consequence of this nonvanishing mean value. This discrepancy can be significant also in the case where the NBA theory predicts localization. In this case the reaction field, weak in the short-time region, becomes increasingly important upon an increase of time [see Eq. (2.11)] and produces a striking discrepancy between PPT and NBA theory in the long-time limit. According to this "physical" argument, we think that our treatment means a significant improvement over the NBA theory.

Using the Gaussian properties of $\bar{x}^{(0)}(t)$, utilizing Eq. (2.7), (2.8), (2.10), (2.15), and factorizing $\langle\sigma_x(s)\rangle$ within the integrand, we then obtain

$$\langle\dot{\sigma}_x(t)\rangle=-\omega_0^2\int_0^t ds\langle\sigma_x(s)\rangle\mathrm{Re}\left[\exp\left[-4g^2\int_0^{t-s}dt_1\int_0^{t_1}dt_2\langle\bar{x}^{(0)}(t_2)\bar{x}^{(0)}(0)\rangle\right]e^{-4i\Delta(t-s)}\right.$$
$$\left.\times\exp\left[4ig^2\int_s^t d\tau\int_0^\tau d\tau'\sum_i\Gamma_i^2\sin[\omega_i(\tau-\tau')][1-\langle\sigma_x(\tau')\rangle]\right]\right]\ , \tag{2.17}$$

which is precisely the central equation discussed in Sec. I [Eq. (1.4)], with $\Delta$ defined by Eq. (2.6).

This is nothing but the PPT theory [6]. In Ref. [6] this equation was indeed derived by adopting the pseudopolaronic transformation rather than the traditional polaronic transformation [7]. Equation (2.17) has the same integro-differential form as the equation stemming from the NBA [1], but with a different kernel. The PPT kernel is obtained from the NBA kernel by inclusion of the third exponential appearing on the right-hand side (2.17). *This makes the dynamics of the system nonlinear and nonstationary.*

Remarkably, the nonlinear terms produced by the reaction field in Eq. (2.17) turn out to account for the nonlinear coupling of the DNSE in the two-site case [6,19]. The advocates of the DNSE [10,11] usually do not answer the basic question of whether or not the physical manifestations of the nonlinear structure of the DNSE survive the quantum-mechanical fluctuations of the phonon bath (whereas the PPT theory in principle does). The theory of the coherent transport of excitations along molecular chains, the so-called Davydov solitons [8,9], rests on the DNSE. On the basis of numerical calculations it has been shown that the Schrödinger equation of the Hamiltonian behind the DNSE does not support the existence of the Davydov solution as a persistent localized entity [20]. This suggests that the quantum-mechanical fluctuations of the bath might have a crucial role in determining the ultimate behavior of the system, which would widely depart from the prediction of the DNSE. Nevertheless this would not imply a diminished importance of the reaction field, and the importance of

the PPT theory is reinforced, not weakened, by the remark that the DNSE is recovered from the PPT theory under the assumption of neglecting the bath quantum-mechanical fluctuations.

## III. ASYMPTOTIC ANALYSIS

This section is devoted to the analysis of the predictions of the PPT theory in the asymptotic-time limit. We rewrite Eq. (2.17) in the following form:

$$\langle \dot{\sigma}_x(t)\rangle = -\omega_0^2 \int_0^t ds \langle \sigma_x(s)\rangle \times \mathrm{Re}\left[ M(t-s)\exp\left[ i\int_s^t d\tau\, G(\tau)\right]\right], \tag{3.1}$$

where the function $G(t)$ is given by

$$G(t)=\int_0^t d\tau K(\tau)[1-\langle \sigma_x(t-\tau)\rangle]. \tag{3.2}$$

The next step consists of expressing this theoretical prediction in the Ohmic case, namely, in terms of the spectral density of Eq. (1.5). Using Eqs. (2.6) and (2.10), we express the functions $M(t)$ and $K(t)$ under the respective forms

$$M(t)=\left\{(1+i\omega_c t)\prod_{n=1}^{\infty}\left[1+\left[\frac{\omega_c t}{1+n\beta\omega_c}\right]^2\right]\right\}^{-4g^2} \tag{3.3}$$

and

$$K(t)=\frac{8g^2\omega_c^3 t}{(1+\omega_c^2 t^2)^2}. \tag{3.4}$$

Let us now analyze the asymptotic properties of Eq. (3.1) by assuming that $\langle \sigma_x(t)\rangle$ tends to a well-defined limit, $\langle \sigma_x(\infty)\rangle$. This implies that

$$\lim_{t\to\infty}\left[\exp\left[i\int_0^t d\tau\, G(\tau)\right]\int_0^t ds\langle\sigma_x(s)\rangle\exp\left[-i\int_0^s d\tau\, G(\tau)\right]M(t-s)+\text{c.c.}\right]=0. \tag{3.5}$$

If $G(t)$ tends asymptotically to the finite value $G(\infty)$, the limit of the first exponential term in Eq. (3.5) does not exist, so that it is convenient to subtract from $G(t)$ its asymptotic limit and define

$$\tilde{G}(t)=G(t)-G(\infty). \tag{3.6}$$

From the Laplace-transform theory we know that if the limit of $f(t)$ for $t$ going to infinity exists, then the relation

$$\lim_{z\to 0} z\hat{f}(z)=\lim_{t\to+\infty} f(t) \tag{3.7}$$

holds true. Using this theorem and Eq. (3.4), we show that

$$G(\infty)=4g^2\omega_c(1-\langle\sigma_x(\infty)\rangle) \tag{3.8}$$

and

$$\hat{\tilde{G}}(0)=-\frac{\pi}{2}g^2(1-\langle\sigma_x(\infty)\rangle) -4g^2\omega_c\int_0^\infty dt[\langle\sigma_x(t)\rangle-\langle\sigma_x(\infty)\rangle]. \tag{3.9}$$

At this stage let us make the crucial assumption

$$\int_0^\infty dt[\langle\sigma_x(t)\rangle-\langle\sigma_x(\infty)\rangle]<+\infty. \tag{3.10}$$

This means that $\hat{\tilde{G}}(0)$ is finite and makes Eq. (3.5) read as follows:

$$e^{i\hat{\tilde{G}}(0)}\lim_{t\to\infty}\left[\int_0^t ds\, M(t-s)\exp[iG(\infty)(t-s)] \times\langle\sigma_x(s)\rangle\exp\left[-i\int_0^s d\tau\,\tilde{G}(\tau)\right]\right] +\text{c.c.}=0. \tag{3.11}$$

By assuming that the limit of the time convolution exists and again using Eq. (3.7), we obtain

$$\langle\sigma_x(\infty)\rangle\hat{M}_G(0)=0, \tag{3.12}$$

where

$$\hat{M}_G(0)=\int_0^\infty dt\,\mathrm{Re}\left[\left\{(1+i\omega_c t)\prod_{n=1}^{\infty}\left[1+\left[\frac{\omega_c t}{1+n\beta\omega_c}\right]^2\right]\right\}^{-4g^2}\exp[iG(\infty)t]\right]. \tag{3.13}$$

Let us now consider the case of zero temperature, $T=0$, which is the crucial condition for the existence of the symmetry breaking. The infinite product in Eq. (3.13) becomes equal to one and the resulting integral gives [21]

$$\hat{M}_G(0)=\frac{\pi\exp-[G(\infty)/\omega_c][G(\infty)/\omega_c]^{4g^2-1}}{\omega_c\Gamma(4g^2)}. \tag{3.14}$$

Finally, using Eqs. (3.8), (3.12), and (3.14), we obtain

$$\langle\sigma_x(\infty)\rangle\exp\{-4g^2[1-\langle\sigma_x(\infty)\rangle]\}\times[1-\langle\sigma_x(\infty)\rangle]^{4g^2-1}=0\ , \quad (3.15)$$

which is the condition that the solution to Eq. (3.1) must fulfill in the asymptotic-time limit.

From this central result we see that the "delocalized" solution $\langle\sigma_x(\infty)\rangle=0$ is admitted for any value of the coupling strength $g$. From Eq. (3.15) we see that when $g>\frac{1}{2}$ also, a broken-symmetry state, namely, $\langle\sigma_x(\infty)\rangle=1$, would seem to be possible. Nevertheless, we can now show that this additional solution must be disregarded. This can be explained with the following simple arguments. The density matrix of the whole system at the time $t$ can always be expressed in the general form

$$\rho(t)=\sum_{\alpha,\alpha'=+,-}|\alpha\rangle_x\langle\alpha'|_xF^{(\alpha\alpha')}(t)\ , \quad (3.16)$$

where $F^{(\alpha\alpha')}(t)$ is an operator over the oscillator space. The condition $\langle\sigma_x(\infty)\rangle=1$ is equivalent to the condition

$$\rho(\infty)=|+\rangle_x\langle+|_xF^{(++)}\ . \quad (3.17)$$

This would actually imply that $\rho(\infty)$ as given by Eq. (3.17) is an eigenstate of the Liouvillian superoperator associated with the Hamiltonian of Eq. (1.1). A quick inspection of the structure of the Hamiltonian of Eq. (1.1) shows that the finite value of the Larmor frequency $\omega_0$ prevents the state of Eq. (3.17) from being an eigenstate of the Liouvillian superoperator and thus prevents the mean value $\langle\sigma_x(\infty)\rangle$ from being equal to 1. In principle, this would not conflict with either the NBA, Eqs. (1.6), or the KW theory, Eqs. (1.7), since within both theories the precise condition $\langle\sigma_x(\infty)\rangle=1$ is only reached in the limiting case of an infinitely large coupling strength $g$. Equation (3.15), on the contrary, would imply the theoretical prediction $\langle\sigma_x(\infty)\rangle=1$ to hold true also at finite values of the coupling strength $g$, which cannot be correct. In conclusion, the theoretical prediction of the PPT theory is that the depolarized condition $\langle\sigma_x(\infty)\rangle=0$ holds true over the whole range of the coupling strength $g$ and that no localization is admitted.

## IV. NUMERICAL STUDY OF THE EVOLUTION OF $\langle\sigma_x(t)\rangle$

To confirm the analytical prediction of Sec. III we have solved Eq. (1.4) numerically in the Ohmic case [see Eq. (1.5)] at zero temperature. This allows us to describe the early stage of the dynamical transition from the initial state of Eq. (1.3) to the long-time regime. Furthermore we compare the dynamical evolution of the PPT theory to those of the NBA and KW theories. We remind the reader that the equation associated with the NBA can be obtained from Eq. (2.17) by setting the third exponential term equal to one. In the zero-temperature case it reads [see also Eqs. (3.1) and (3.3)]

$$\langle\dot\sigma_x(t)\rangle=-\omega_0^2\int_0^t ds\langle\sigma_x(s)\rangle\times\mathrm{Re}\left[\left[\frac{1}{1+i\omega_c(t-s)}\right]^{4g^2}\right]\ . \quad (4.1)$$

As pointed out in Ref. [6], the KW theory is derived from Eq. (2.17) by neglecting the quantum fluctuations of the oscillators and making the Markovian assumption. These approximations lead to the following set of equations:

$$\begin{aligned}\langle\dot\sigma_x(t)\rangle&=\omega_0\langle\sigma_y(t)\rangle\ ,\\ \langle\dot\sigma_y(t)\rangle&=-\omega_0\langle\sigma_x(t)\rangle+4g^2\omega_c\langle\sigma_x(t)\rangle\langle\sigma_z(t)\rangle\\ &\quad-2\pi g^2\omega_0\langle\sigma_z(t)\rangle\langle\sigma_y(t)\rangle\ ,\\ \langle\dot\sigma_z(t)\rangle&=-4g^2\omega_c\langle\sigma_x(t)\rangle\langle\sigma_y(t)\rangle+2\pi g^2\omega_0\langle\sigma_y(t)\rangle^2\ .\end{aligned} \quad (4.2)$$

Note that under the condition $\omega_c\gg\omega_0$ these equations become equivalent to Eqs. (2.6) and (2.7) of the theory of Kenkre and Wu [11] [see also Eqs. (2.2)–(2.5) of Ref. [22]). For this reason we shall refer to (4.2) as the KW prediction.

The comparison among the three theories is illustrated in Figs. 1 and 2, which refer, respectively, to coupling strengths slightly smaller and larger than that corresponding to the NBA localization [see Eq. (1.6a)].

We see from Fig. 1 that at $g=0.55$ the NBA and the PPT theories are very close to each other at short times and, although at larger times they begin to move apart, both widely depart from the polarized state. This is indeed the case where, according to the analytical prediction of Eq. (1.6a), the NBA theory does not lead to localization.

Figure 2, referring to $g=0.75$, clearly shows that the NBA theory tends towards localization, whereas, in

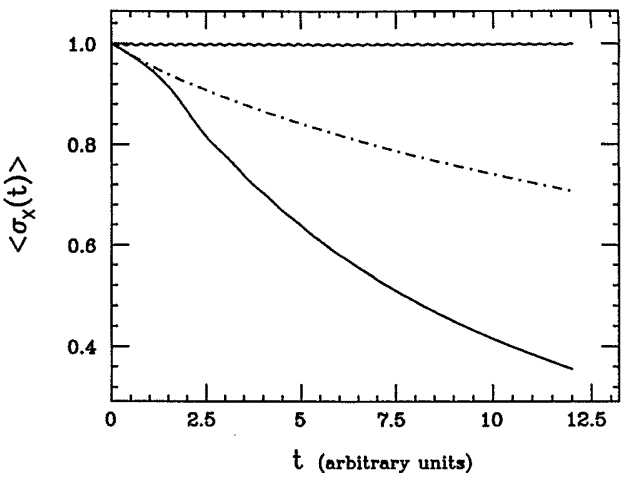


FIG. 1. $\langle\sigma_x\rangle$ vs time at zero temperature. The values of the parameters are $\omega_0=1$, $\omega_c=20$, and $g=0.55$ [below the localization threshold predicted by the NBA theory, see Eq. (1.6a)]. The lower solid line denotes the evolution predicted by the PPT theory [Eq. (2.17)]; the dotted-dashed line denotes the prediction of the NBA theory [Eq. (4.1)] and the upper solid line denotes the prediction of the KW theory [Eq. (4.2)].

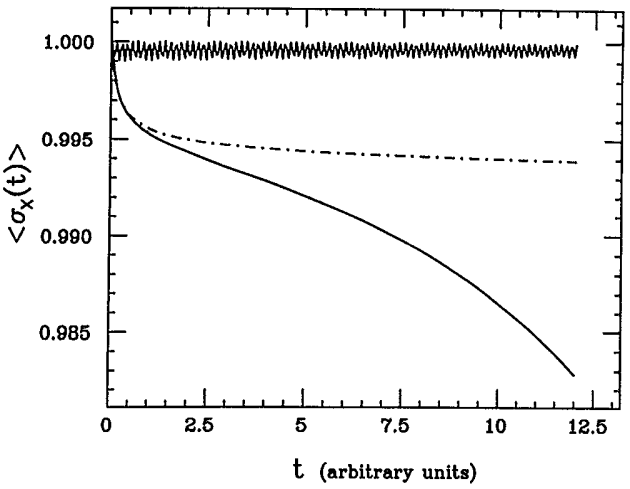


FIG. 2. $\langle\sigma_x\rangle$ vs time at zero temperature. The values of the parameters are $\omega_0=1$, $\omega_c=20$, and $g=0.75$ [above the localization threshold predicted by the NBA theory, see Eq. (1.6a)]. The lower solid line denotes the evolution predicted by the PPT theory [Eq. (2.17)]; the dotted-dashed line denotes the prediction of the NBA theory [Eq. (4.1)] and the upper solid line denotes the prediction of the KW theory [Eq. (4.2)].

agreement with the major result of this paper (see Sec. III), the PPT theory prediction departs from the NBA theory and does not seem to lead to any localization. Actually, to reach an irrefutable confirmation of this theoretical prediction, we should have explored a much more extended time region. However, although there have been no particular technical difficulties in exploring the NBA theory in the long-time limit, the numerical study of the PPT theory within the time region explored in Fig. 2 required the use of special tricks (see Appendix) and the exploration of a more extended time region would have implied a prohibitive amount of central processing unit (CPU) time calculation.

The time behavior predicted by the KW theory is found to be in striking qualitative disagreement with that of the other two theories, and one would be tempted to conclude that this is a sign of theoretical weakness. However, we would like to point out that the KW theory rests on the nonlinearity triggered by the reaction field, and that this is precisely the key ingredient making the PPT depart from the NBA theory on the problem of the asymptotic-time symmetry breaking. The strong discrepancy between the KW predictions and those of the other two theories is largely due to the fact that we are here exploring the case of vanishing temperature, where the quantum-mechanical fluctuations of the oscillators, neglected by the KW theory, play the predominant role. Similar discrepancies between the predictions of the DNSE and a fully quantum-mechanical treatment have already been illustrated in Ref. [23].

## V. CONCLUDING REMARKS

The major result of this paper is that the PPT theory is incompatible with any dynamic symmetry breaking. Since the PPT theory is a sort of combination of two distinct theoretical approaches, the NBA [1] and the KW theory [11], each of them leading to the dynamic symmetric breaking, at first sight this conclusion would seem counterintuitive.

We want here to show that, on the contrary, the major conclusion of this paper is correct precisely because the PPT theory wisely balances the sound physical aspects of the KW theory with those of the NBA theory, and vice versa. The localization predicted by the NBA theory depends on a physical mechanism distinct from that producing localization within the KW theory. Within the NBA approach, localization is produced by a sort of a "critical overdamping" [1], whereas within the KW theory, localization is thought of as a particle settling at the bottom of one well of a double-well potential [11].

When we "put the two theories together," each of them contains the element which destroys the localization mechanism of the other one. The PPT theory can be looked at from two different perspectives, and precisely, (a), as the NBA theory supplemented by the inclusion of the nonlinear effects of the reaction field, and, (b), as the KW theory supplemented by the inclusion of the quantum fluctuations of the oscillators. Both perspectives lead to a localization breakdown. Let us explain this crucial issue in detail.

(a) Within the NBA theory, the oscillators of the bath are initially set in a condition of canonical equilibrium with respect to the spin-$\frac{1}{2}$ dipole polarized along the $x$ direction [see Eq. (1.3)], and are, so to speak, frozen in this initial condition. Correspondingly, the condition of the spin-$\frac{1}{2}$ dipole remaining close to the initial polarization state is favored. The PPT theory supplements the NBA theory with the proper inclusion of the reaction field. This means that the oscillators are allowed to leave their initial state, thereby making it easier for the spin-$\frac{1}{2}$ dipole to depart from the initial polarized state. In other words, the reaction field makes the bath more flexible and consequently leads to the localization breakdown.

(b) From Eq. (2.17) we see that the PPT theory is derived by supplementing the KW theory with the thermal and quantum fluctuations of the bath of oscillators [first exponential term within the time convolution on the right-hand side of Eq. (2.17)]. At zero temperature the thermal fluctuations are quenched, but the quantum fluctuations are not frozen. The classical oscillator of the KW theory rearranges itself within the shifted harmonic potential corresponding to the state of the spin-$\frac{1}{2}$ dipole, and settles at the bottom of this potential. However, the classical assumption on the oscillator fails in reproducing the overlap of oscillator ground-state wave functions based at the minima corresponding to the two polarizations of the spin-$\frac{1}{2}$ dipole along the $x$ axis. As pointed out by Leggett [24], this Franck-Condon effect is an important mechanism for depolarization. As also noticed in Ref. [23], this effect produces the breakdown of the localization predicted by the KW theory. In conclusion, the PPT theory is proved to be incompatible with localization even within this second perspective.

The conclusions of this paper are supported by the recent results of Cápek and Chvosta [25]. These authors

made an asymptotic analysis of the formally exact solution for $\langle \sigma_x(t) \rangle$ in the Ohmic case and proved the absence of any asymptotic-time symmetry breaking. It is remarkable that the PPT theory, affording also a detailed illustration of the intermediate-time region (see the numerical results illustrated in Sec. IV) leads to a long-time limit fitting the predictions of Cápek and Chvosta [25]. This means that the essential physical effects are retained by the PPT theory.

The absence of the asymptotic-time symmetry breaking is not in contradiction with the predictions of current literature. Chakravarty and Bray and Moore [15] studied the *static* properties of the model of Eq. (1.1) and showed that in the Ohmic case at zero temperature there is a symmetry breaking at the critical value of the coupling $g$ given by Eq. (1.6a). This means that the ground state becomes twofold degenerate so that it is possible for the system to stay in a broken-symmetry equilibrium state, i.e., a state with $\langle \sigma_x \rangle \neq 0$. The predictions of this static analysis have been confirmed by the results of the rigorous approach of Spöhn and Dumcke [26]. The present paper shows that this localized state cannot be reached starting from the initial condition of Eq. (1.3) and this prediction, in principle, does not conflict with the phase transition to the localized situation of Refs. [15,26]. This view agrees with that of Cápek and Chvosta [25] but it is more transparent from a physical point of view. We show indeed that the localization breakdown is an effect of the joint action of reaction field and quantum-mechanical fluctuations. Furthermore the PPT theory makes it possible to carry out the calculation of the time evolution of the system (see Sec. IV).

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## APPENDIX: NUMERICAL DETAILS

The algorithm used to solve Eqs. (2.2) and (3.3) is basically an Adams-Bashfort predictor of zeroth order followed by a corrector of Adams and Moulton of first order [27]. The major problem, from a computational point of view, is that the integration time grows like $t^4$ where $t$ is the upper limit in Eq. (3.1), and that any algorithm would be intrinsically scalar. With a typical integration time step of order $3\times10^{-3}$, and an upper limit $t\sim10$, one needs to evaluate the integrand of Eq. (3.2) some $10^{14}$ times. At the very best, a simple estimate of the time necessary to perform $10^{14}$ elementary FORTRAN instructions would still imply about two years of CPU time on a machine that is capable of $4\times10^7$ floating-point operations per second. Apart from the usual stratagems, e.g., to tabulate all nonlinear functions which appear in Eq. (3.1), it is clearly necessary to find a way to possibly reduce the power of $t$ from 4 to something less. The trick we employed consists of replacing $1-\langle \sigma_x(t-\tau) \rangle$ in Eq. (3.2) by its Padé approximant (with three points). Equation (3.2) then can be exactly solved, leading to a CPU-time increase which only goes like $t^3$. In practice, we broke the integral of Eq. (3.2) into two or more integrals, dividing the interval $0-t$ into some smaller intervals $0-t_1,\ldots,t_n-t$ with $0<t_1<\ldots<t_n<t$. Then we evaluated exactly the integral from $t_n$ to $t$ and used the Padé approximant for the other integrals. Extensive checks at short-to-intermediate times done using the Padé approximants or the exact integration showed no difference in the final $\langle \sigma_x(t) \rangle$. This trick dramatically decreased the CPU time necessary for the integration by a factor of order 300.

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