Beyond the semiclassical approximation of the discrete nonlinear Schrödinger equation: Collapses and revivals as a sign of quantum fluctuations

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We study a two-state quantum-mechanical system, equivalent to a $\frac{1}{2}$-spin dipole, with frequency ω_0, linearly interacting with a set of quantum oscillators. The corresponding discrete nonlinear Schrödinger equation (DNSE) has been given an analytical solution by Kenkre and Campbell [Phys. Rev. B **34**, 4959 (1986)]. We show that in the strong-coupling limit their analytical expression is recovered from our microscopic approach when the thermal and quantum fluctuations of the bath of oscillators are neglected. To take into account the influence of thermal and quantum fluctuations on the prediction of the DNSE in the strong-coupling limit, we adopt a straightforward procedure based on the direct evaluation of $\langle \sigma_x(t) \rangle$, under the assumption alone that the frequency ω_0 is very weak. A special initial condition is used, with $\langle \sigma_x(t) \rangle = 1$ and the oscillator at equilibrium in the corresponding effective potential. It is shown that in the strong-coupling limit this expression coincides with the noninteracting-blip approximation of Leggett *et al.* [Rev. Mod. Phys. **59**, 1 (1987)] and the result of the equivalent projection approach of Aslangul, Pottier, and Saint-James [J. Phys. (Paris) **46**, 2031 (1985); **47**, 1657 (1986)]. Then, this expression is used to study the special case where the $\frac{1}{2}$ spin interacts with only one oscillator at zero temperature. It is shown that the fast oscillations predicted by Kenkre and Campbell in the strong-coupling limit are damped by a Gaussian-like relaxation process provoked by the quantum fluctuations of the oscillator, which eventually lead to the destruction of the trapped state. These collapses are followed by periodical revivals reminiscent of those observed in quantum optics.

I. INTRODUCTION

The model of one $\frac{1}{2}$-spin dipole interacting with one or more quantum-mechanical oscillators plays a central role in many different fields of investigation. Relevant examples are quantum-mechanical dissipation,[1] quantum optics,[2–4] and the discrete nonlinear Schrödinger equation (DNSE).[5–11]

The latter field of investigation is currently the subject of a debate[6] concerning the microscopic derivation of the DNSE proposed by Davydov. The DNSE was derived by Davydov by modeling the energy transport in biological macromolecules via the Fröhlich Hamiltonian[7] and making use of an *Ansatz* for the form of the state vector which is assumed to be a product of a normalized one-exciton vector and a many-mode product of phonon coherent states. The essential ideas of Davydov's theory were used by Brown *et al.*[6] to develop a variation of the Zwanzig-Nakajima projection technique[8] that allowed them to recover with a more rigorous statistical approach the same nonlinear structure as that characterizing the DNSE of Davydov. The problem of the microscopic derivation of the DNSE is rather closely connected to that of the microscopic approach to quantum dissipation.[1] This is made evident by considering the two-site version of the Fröhlich Hamiltonian. In this case the microscopic Hamiltonian has precisely the same structure as that used within the field of quantum dissipation, i.e., a $\frac{1}{2}$-spin dipole interacting with a set of quantum-mechanical oscillators. In this special case, termed adiabatic dimer, Kenkre and co-workers[9–11] have been able to predict interesting effects produced by the strong interactions of quasiparticles with the vibrations of a solid. Within the perspective of this paper, more important than that is the fact that they have been able to derive the analytical solution of the DNSE. Since the Hamiltonian behind their analytical results is the same as that used in the field of quantum dissipation, we have available an alternative approach to the microscopic derivation of the DNSE. This is as follows. Instead of discussing the *Ansätze* made by Davydov[5,6] and the problems of the rigorous statistical derivation of his equation, we can proceed to a direct comparison between the analytical solution found by Kenkre and Campbell[9] and the solutions available in the field of quantum dissipation after the investigative work of Leggett and co-workers.[1]

Actually, instead of using the results of Ref. 1, we derive an expression for the time evolution of the mean value of the x component of the spin at second order in the unperturbed precession frequency. At this order our result is proven to coincide with the theory of Leggett and co-workers.[1] This approximation allows us to discuss the effects of quantum fluctuations on the adiabatic dimer of Kenkre and Campbell[9] with a fully analytical expression, but it will oblige us to keep our analysis in the region of high couplings. Another reason for us to "rederive" the result of Leggett and co-workers is that within our approach it is straightforward to make the semiclassical assumption, i.e., that the oscillator is classical. This approximation is proved to result in a simple analytical expression coinciding with the prediction of Kenkre and Campbell[9] in the same limiting condition of small ω_0's.

We are thus in a position to accomplish the proposed plan. We proceed to a direct comparison between the analytical expression of Kenkre and Campbell[9] and a fully quantum-mechanical result that in the semiclassical limits reduces to the expression of Kenkre and Campbell.[9] It is thus correct to interpret the discrepancies between these two different predictions as being an effect of the quantum-mechanical corrections to the DNSE. A crucial issue[12] on the DNSE is whether or not its significant predictions are invalidated by the quantum-mechanical nature of the oscillators, and we believe that our approach serves very well the purpose of answering it.

The outline of the paper is as follows. In Sec. II we show that the adiabatic dimer of Krenkre and Campbell[9] implies the influence of both quantum and thermal fluctuations to be totally neglected. In Sec. III we study the time evolution of the mean value of the observable of interest and we express it by an analytical equation obtained with no approximation but that the spin precession frequency is very small. In Sec. IV we adapt this equation to the special case of an interaction with only one oscillator at temperature $T=0$. We then discuss the effects of quantum fluctuations on the adiabatic dimer of Kenkre and Campbell.[9] Concluding remarks are found in Sec. V.

II. HEISENBERG REPRESENTATION AND HIGH-COUPLING LIMIT

We study the system described by the following Hamiltonian:

$$\mathcal{H}=\mathcal{H}_A+\mathcal{H}_B+\mathcal{H}_I \ , \tag{2.1}$$

where

$$\mathcal{H}_A=-\frac{\omega_0}{2}\sigma_z \ , \tag{2.2a}$$

$$\mathcal{H}_B=\sum_i \omega_i b_i^\dagger b_i \ , \tag{2.2b}$$

$$\mathcal{H}_I=g\sigma_x\sum_i \Gamma_i(b_i+b_i^\dagger) \ , \tag{2.2c}$$

and the operators b_i and $b_i^\dagger$ are the conventional creation and destruction operators satisfying the commutation rules

$$[b_i,b_1^\dagger]=1 \tag{2.3}$$

σ_x, σ_y, and σ_z are the Pauli spin operators. For the sake of concision we define the operator x,

$$x\equiv\sum_i \Gamma_i(b_i+b_i^\dagger) \ . \tag{2.4}$$

Thus the interaction Hamiltonian reads

$$\mathcal{H}_I=g\sigma_x x \ . \tag{2.5}$$

In a recent paper,[13] a theoretical procedure has been adopted aiming at retaining the essence of Davydov's idea, namely, the fact that the phonon system is held away from equilibrium through a constraint supplied by the moving excitation. It has been stressed that if the bath consists of only one damped oscillator, then this oscillator must quickly relax towards an equilibrium distribution with respect to a shifted harmonic potential. This property has been partially taken into account by the theory of Ref. 13, where at $t=0$ the spin is assumed to be polarized along the x direction and the oscillator is forced to stay at equilibrium in the correspondingly shifted potential well. The theoretical approach of Ref. 13 has quite an attracting property: when thermal and quantum-mechanical fluctuations are neglected, this theory recovers the analytical predictions of Kenkre and Campbell[9] in the strong-coupling limit. However, the thermal and quantum-mechanical corrections are introduced with a Markovian assumption, and the resulting theoretical predictions are then supported by comparison with the results of a numerical method. In this paper we plan to retain from this approach only the assumption on the special initial condition. As far as the evaluation of quantum and thermal fluctuations is concerned, this will be carried out with no approximation but that the oscillation frequency ω_0 is very small. This is the reason why the comparison with the adiabatic dimer of Kenkre and Campbell can only be carried out in their strong-coupling limit.

To be more specific, let us assume that at $t=0$ the spin is in the state $|+\rangle_x$, the eigenstate of σ_x with positive eigenvalue, therefore satisfying the condition

$$\sigma_x|+\rangle_x=|+\rangle_x \ . \tag{2.6}$$

Then the bath oscillators are subject to harmonic potentials with unperturbed frequencies but with a minimum shifted by the quantity

$$\Delta x_i=-\frac{2g\Gamma_i^2}{\omega_i} \ , \tag{2.7}$$

the unperturbed equilibrium position being assumed to be placed at $x=0$. We choose an initial condition with the oscillators of the bath placed in an equilibrium state with respect to this shifted potential and we study the ensuing evolution of the system.

In accordance with the above remarks it is convenient to adopt the following change of variables:

$$b_i=\tilde{b}_i-\frac{g\Gamma_i}{\omega_i}\ ,\qquad b_i^\dagger=\tilde{b}_i^\dagger-\frac{g\Gamma_i}{\omega_i}\ . \tag{2.8}$$

This means that we are using the new coordinates

$$\tilde{x}_i=\Gamma_i(\tilde{b}_i+\tilde{b}_i^\dagger)\ , \tag{2.9}$$

which correspond indeed to shifting the reference frame by the quantity of Eq. (2.7). In this new system of reference the Hamiltonian of Eq. (2.1) reads

$$\mathcal{H}=-\frac{\omega_0}{2}\sigma_z-2P_-g\sum_i\Gamma_i(\tilde{b}_i+\tilde{b}_i^\dagger)+\sum_i\omega_i\tilde{b}_i^\dagger\tilde{b}_i-2\sigma_x\sum_i\frac{g^2\Gamma_i^2}{\omega_i}+\sum_i\frac{g^2\Gamma_i^2}{\omega_i}\ , \tag{2.10}$$

where

$$P_-\equiv\tfrac{1}{2}(1-\sigma_x)\ . \tag{2.10$'$}$$

Starting from the initial condition of Eq. (2.6), we are tempted to assume the interaction between spin and system, [second term on the right-hand side of (2.10)], to be negligible. We then immediately obtain

$$\dot{\sigma}_x(t)=\omega_0\sigma_y(t)\ ,\quad \dot{\sigma}_y(t)=-\omega_0\sigma_x(t)+4\Delta\sigma_z(t)\ ,\quad \dot{\sigma}_z(t)=-4\Delta\sigma_y(t)\ , \tag{2.11}$$

where

$$\Delta\equiv g^2\sum_i\frac{\Gamma_i^2}{\omega_i}\ . \tag{2.11$'$}$$

This is formally identical to the dynamics of a linear nondegenerate dimer, where the localized state appears to be an effect of the disparity in the energy levels. However, the microscopic Hamiltonian is the same as that behind the degenerate dimer of Kenkre and Campbell[9] and the self-trapping is a consequence of the strong coupling with the phonon bath. In other words, a degenerate dimer strongly coupled to the phonon bath appears to be equivalent to a nondegenerate dimer decoupled by its bath. The solution of this set of differential equations is

$$\langle\sigma_x(t)\rangle=\frac{\omega_0^2\cos[(16\Delta^2+\omega_0^2t)^{1/2}]+16\Delta^2}{16\Delta^2+\omega_0^2}\ , \tag{2.12}$$

$$\langle\sigma_y(t)\rangle=-\frac{\omega_0\sin[(16\Delta^2+\omega_0^2t)^{1/2}]}{(16\Delta^2+\omega_0^2)^{1/2}}\ , \tag{2.13}$$

$$\langle\sigma_z(t)\rangle=\frac{4\omega_0\Delta}{16\Delta^2+\omega_0^2}\{1-\cos[(16\Delta^2+\omega_0^2t)^{1/2}]\}\ . \tag{2.14}$$

This coincides with the strong-coupling limit of the degenerate dimer of Kenkre and Campbell.[9] Thus we can regard Eqs. (2.12)–(2.14) as the prediction of the DNSE in the strong-coupling limit. This is equivalent to *disregarding completely both thermal and quantum-mechanical fluctuations.* This can be made clearer by noticing that if the second term on the right-hand side of (2.10) is not disregarded, the set of Eq. (2.11) must be replaced by

$$\dot{\sigma}_x(t)=\omega_0\sigma_y(t)\ ,\quad \dot{\sigma}_y(t)=-\omega_0\sigma_x(t)+4\Delta\sigma_z(t)-2g\tilde{x}(t)\sigma_z(t)\ ,\quad \dot{\sigma}_z(t)=-4\Delta\sigma_y(t)+2g\tilde{x}(t)\sigma_y(t)\ . \tag{2.15}$$

If we think of $\tilde{x}(t)$ as being a fluctuation, either classical or quantum mechanical, then we see that the deterministic dynamics of the set of Eq. (2.11) is perturbed by a sort of multiplicative stochastic process which is reminiscent of the well-known stochastic oscillator of Kubo.[14] In the present paper we shall focus our attention on the effect of quantum-mechanical fluctuations. The thermal fluctuations will be ruled out by reducing the bath of oscillators to a single oscillator at the temperature $T=0$. We want to remark in advance that if the quantum-mechanical fluctuations are conceived as erratic motions of $\tilde{x}(t)$ surviving also at $T=0$, then it is not surprising that the motion of the $\frac{1}{2}$-spin dipole is characterized by collapses, i.e., a sort of relaxation process triggered by the multiplicative nature of the "noise" appearing in Eq. (2.15). The Kubo stochastic oscillator[14,15] sheds light on this important aspect.

Note that the DNSE was derived by Davydov[5] by assuming the oscillators to be in coherent states, and thus very close to the classical condition. Thus it is reasonable that the exact equations of (2.15) lead to the same prediction as the DNSE when the quantum fluctuations of $\tilde{x}(t)$ are disregarded. The major purpose of the present paper is precisely determining the physical effects of quantum fluctuations in the strong-coupling limit.

III. EFFECTS OF QUANTUM-MECHANICAL FLUCTUATIONS

Instead of adopting the procedure of Ref. 13, we approach the problem of determining the influence of quantum-mechanical fluctuations on the predictions of the DNSE in quite a different way. This consists of determining the time evolution of $\langle\sigma_x(t)\rangle$ under the assumption alone that the transition frequency ω_0 is very small, while retaining the initial condition of the preceding section. The resulting expression for a generic bath of oscillators is virtually equivalent to that of Leggett and coworkers.[1] However, our procedure makes the connection with the DNSE of Davydov clearer. For this reason, we think it worthy of a fairly detailed illustration. We proceed as follows.

In principle, the exact expression for the time evolution of $\langle\sigma_x(t)\rangle$, ensuing from the special initial condition of the preceding section, is given by

$$\langle\sigma_x(t)\rangle\equiv\mathrm{Tr}[P_+\rho_B\sigma_x(t)]\equiv\mathrm{Tr}\{P_+\rho_B[\exp(\mathcal{L}t)\sigma_x]\}\ , \tag{3.1}$$

where

$$P_+ \equiv \tfrac{1}{2}(1+\sigma_x) = |+\rangle_x\langle +|_x \; . \tag{3.1'}$$

The superoperator $-i\mathcal{L}$ is the commutator associated with the Hamiltonian of Eq. (2.1). It can be divided into two parts as follows:

$$\mathcal{L} = \mathcal{L}_A + \mathcal{L}_0 \; , \tag{3.2}$$

where

$$\mathcal{L}_0 \equiv \mathcal{L}_I + \mathcal{L}_B \tag{3.3}$$

and $\mathcal{L}_A$, $\mathcal{L}_B$, and $\mathcal{L}_I$ denote the commutators associated to $\mathcal{H}_A$, $\mathcal{H}_B$, and $\mathcal{H}_I$ of Eqs. (2.2a)–(2.2c). As mentioned above, we make the assumption alone that the transition frequency ω_0 is very small. This is equivalent to assuming $\mathcal{L}_A$ to be small compared to $\mathcal{L}_I + \mathcal{L}_B$. For this reason it is convenient to write Eq. (3.1) under the following form:

$$\langle \sigma_x(t)\rangle = \mathrm{Tr}\left[P_+\rho_B \exp(\mathcal{L}_0 t)\exp_T \times \left[\int_0^t ds\, \exp(-\mathcal{L}_0 s) \times \mathcal{L}_A \exp(\mathcal{L}_0 s)\sigma_x\right]\right] . \tag{3.4}$$

The symbol $\exp_T$ denotes the time-ordered exponential. Let us expand this time-ordered exponential at second order in $\mathcal{L}_A$, or at second order in the tunneling frequency ω_0. We obtain

$$\langle \sigma_x(t)\rangle = \mathrm{Tr}[P_+\rho_B\exp(\mathcal{L}_0 t)\sigma_x] + \mathrm{Tr}\left[P_+\rho_B\exp(\mathcal{L}_0 t)\int_0^t ds\,\exp(-\mathcal{L}_0 s)\mathcal{L}_A\exp(\mathcal{L}_0 s)\sigma_x\right]$$
$$+\mathrm{Tr}\left[P_+\rho_B\exp(\mathcal{L}_0 t)\int_0^t ds\int_0^s ds'\exp(-\mathcal{L}_0 s)\mathcal{L}_A\exp[\mathcal{L}_0(s-s')]\mathcal{L}_A\exp(\mathcal{L}_0 s')\sigma_x\right] . \tag{3.5}$$

We note that the definition of Eq. (3.3) implies

$$\mathcal{L}_0\sigma_x = 0 \; , \tag{3.6}$$

Thereby resulting in

$$\exp(\mathcal{L}_0 t)\sigma_x = \sigma_x \; . \tag{3.7}$$

Thus Eq. (3.5) becomes

$$\langle \sigma_x(t)\rangle = \mathrm{Tr}(P_+\rho_B\sigma_x) + \int_0^t ds\,\mathrm{Tr}\{P_+\rho_B\exp[\mathcal{L}_0(t-s)]\mathcal{L}_A\sigma_x\}$$
$$+\int_0^t ds\int_0^s ds'\mathrm{Tr}\{P_+\rho_B\exp[\mathcal{L}_0(t-s)]\mathcal{L}_A\exp[\mathcal{L}_0(s-s')]\mathcal{L}_A\sigma_x\} . \tag{3.8}$$

Using the properties

$$\exp[\mathcal{L}_0(t-s)]\sigma_x = \exp[i\mathcal{H}_0(t-s)]\sigma_x\exp[-i\mathcal{H}_0(t-s)] \; , \tag{3.9}$$

$$\mathcal{L}_A\sigma_x = \omega_0\sigma_y \; , \tag{3.10}$$

$$[P_+,\mathcal{H}_0] = 0 \; , \tag{3.11}$$

and

$$P_+\sigma_y P_+ = 0 \; , \tag{3.12}$$

we see that the second term on the right-hand side of Eq. (3.8) vanishes and this equation reads

$$\langle \sigma_x(t)\rangle = 1 + \omega_0\int_0^t ds\int_0^s ds'\mathrm{Tr}_B\{\rho_B\langle +|_x\exp(i\mathcal{H}_0 s)\mathcal{L}_A[\exp(\mathcal{L}_0 s')\sigma_y]\exp(-i\mathcal{H}_0 s)|+\rangle_x\} . \tag{3.13}$$

Applying the commutators $\mathcal{L}_A$ and $\mathcal{L}_0$ to σ_y and averaging over the spin variables, we obtain

$$\langle \sigma_x(t)\rangle = 1 - \frac{\omega_0^2}{2}\int_0^t ds\int_0^s ds'\left[\mathrm{Tr}_B\{\rho_B\exp[i(\mathcal{H}_B+gx)s]\exp[i(\mathcal{H}_B-gx)s']\exp[-i(\mathcal{H}_B+gx)(s+s')]\} + \mathrm{c.c.}\right] . \tag{3.14}$$

Let us now express the operators appearing in Eq. (3.14) in terms of the reference system of the preceding section. We obtain

$$\mathcal{H}_B + gx = \tilde{\mathcal{H}}_B - \Delta \tag{3.15}$$

and

$$\mathcal{H}_B - gx = \tilde{\mathcal{H}}_B + 3\Delta - 2g\tilde{x} \; . \tag{3.16}$$

Using Eqs. (3.15) and (3.16) we can write Eq. (3.14) as follows:

$$\langle \sigma_x(t)\rangle = 1-\frac{\omega_0^2}{2}\int_0^t ds\int_0^s ds'[\mathrm{Tr}_B(\rho_B \exp\{i[\tilde{\mathcal{H}}_B-2g\tilde{x}(s)]s'\}\exp(-i\tilde{\mathcal{H}}_B s')\exp(4i\Delta s'))+\mathrm{c.c.}] . \quad (3.17)$$

The time evolution of $\tilde{x}(t)$ is defined by

$$\tilde{x}(t)\equiv \exp(i\tilde{\mathcal{H}}_B t)\tilde{x}\exp(-i\tilde{\mathcal{H}}_B t) = \sum_i \Gamma_i[\tilde{b}_i^\dagger \exp(i\omega_i t)+\tilde{b}_i\exp(-i\omega_i t)] . \quad (3.18)$$

With this definition, Eq. (3.17) can be rewritten under the following form:

$$\langle \sigma_x(t)\rangle = 1-\frac{\omega_0^2}{2}\int_0^t ds\int_0^s ds'[\exp(4i\Delta s')\mathrm{Tr}_B(\rho_B \exp(-i\tilde{\mathcal{H}}_B s')\exp\{i[\tilde{\mathcal{H}}_B-2g\tilde{x}(s+s')]s'\})+\mathrm{c.c.}] . \quad (3.19)$$

Adopting the new integration variables

$$z\equiv s+s' \quad (3.20a)$$

and

$$q\equiv s' , \quad (3.20b)$$

we obtain

$$\langle \sigma_x(t)\rangle = 1-\frac{\omega_0^2}{2}\int_0^t dq\int_{2q}^{q+t} dz[\exp(4i\Delta q)\mathrm{Tr}_B(\rho_B \exp(-i\tilde{\mathcal{H}}_B q)\exp\{i[\tilde{\mathcal{H}}_B-2g\tilde{x}(z)]q\})+\mathrm{c.c.}] . \quad (3.21)$$

Note that

$$\exp\{i[\tilde{\mathcal{H}}_B-2g\tilde{x}(z)]q\} = \exp\left[i\left(\sum_i \omega_i \tilde{b}_i^\dagger \tilde{b}_i - 2g\sum_i \Gamma_i(\tilde{b}_i^\dagger e^{i\omega_i z}+\tilde{b}_i e^{-i\omega_i z})\right)q\right] . \quad (3.22)$$

This means that we have to deal with a product of terms, the form of each of which, omitting the index i, is of the following kind:

$$\exp[i(\omega\tilde{b}^\dagger\tilde{b}+\delta^*\tilde{b}^\dagger+\delta\tilde{b})q] , \quad (3.23)$$

where

$$\delta = -2g\Gamma e^{-i\omega z} . \quad (3.24)$$

Using Eq. (A9) of Appendix A, derived from a result of Weiss and Maradudin,[16] and Eq. (3.24), we get

$$\exp\{i[\tilde{\mathcal{H}}_B-2g\tilde{x}(z)]q\} = \exp(i\tilde{\mathcal{H}}_B q)\prod_i \exp\left[\frac{2g\Gamma_i}{\omega_i}e^{i\omega_i z}(e^{-i\omega_i q}-1)\tilde{b}_i^\dagger - \frac{2g\Gamma_i}{\omega_i}e^{-i\omega_i z}(e^{i\omega_i q}-1)\tilde{b}_i\right] \times \exp\left[-\frac{i4g^2\Gamma_i^2}{\omega_i^2}[\omega_i q-\sin(\omega_i q)]\right] . \quad (3.25)$$

Note that the exponential $\exp(4i\Delta q)$ appearing in Eq. (3.21) can be expressed as follows:

$$\exp(4i\Delta q) = \prod_i \exp\left[\frac{4ig^2\Gamma_i^2}{\omega_i}q\right] . \quad (3.26)$$

Using Eqs. (3.25) and (3.26), from Eq. (3.21) we derive

$$\langle \sigma_x(t)\rangle = 1-\frac{\omega_0^2}{2}\int_0^t dq\int_{2q}^{q+t} dz\left\{\mathrm{Tr}_B\left[\rho_B\left\{\prod_i \exp[\alpha_i(z,q)\tilde{b}_i^\dagger-\alpha_i^*(z,q)\tilde{b}_i]\exp\left[i\frac{4g^2\Gamma_i^2}{\omega_i^2}\sin(\omega_i q)\right]\right\}\right]+\mathrm{c.c.}\right\} , \quad (3.27)$$

with

$$\alpha_i(z,q) = \frac{2g\Gamma_i}{\omega_i}e^{i\omega_i z}(e^{-i\omega_i q}-1) . \quad (3.28)$$

We study the case where

$$\rho_B = \prod_i \rho_i \,, \tag{3.29}$$

$$\rho_i = \frac{\exp(-\beta\omega_i \tilde{b}_i^\dagger \tilde{b}_i)}{\mathrm{Tr}(\exp|-\beta\omega_i \tilde{b}_i^\dagger \tilde{b}_i|)} \,. \tag{3.29'}$$

Using Eq. (3.29) and the well-known relation for generic operators A and B, only fulfilling the condition that $[A,B]$ is a c number,

$$\exp(A+B) = \exp(A)\exp(B)\exp(-\tfrac{1}{2}[A,B]) \,, \tag{3.30}$$

from Eq. (3.27) we obtain

$$\langle \sigma_x(t)\rangle = 1 - \frac{\omega_0^2}{2}\prod_i \int_0^t dq \int_{2q}^{q+t} dz \left[\mathrm{Tr}\{\rho_i \exp[\alpha_i(z,q)\tilde{b}_i^\dagger]\exp[-\alpha_i^*(z,q)\tilde{b}_i]\}\exp\left[\frac{4g^2\Gamma_i^2}{\omega_i^2}(e^{i\omega_i q}-1)\right] + \mathrm{c.c.}\right] . \tag{3.31}$$

The calculations leading to the evaluation of the trace on the right-hand side of Eq. (3.31) are illustrated in Appendix B. Using Eqs. (B6) and evaluating by means of Eq. (3.28) the square modulus of α_i, involved by Eq. (B6), we obtain

$$\mathrm{Tr}[\rho_i \exp(\alpha_i \tilde{b}_i^\dagger)\exp(-\alpha_i^* b_i)] = \exp\left[\frac{8g^2\Gamma_i^2[1-\cos(\omega_i q)]}{\omega_i^2(1-e^{\beta\omega_i})}\right] . \tag{3.32}$$

Inserting Eq. (3.32) into Eq. (3.27) and evaluating the inner time integral, we finally derive

$$\langle \sigma_x(t)\rangle = 1 - \omega_0^2 \int_0^t dq(t-q)\mathrm{Re}\left\{\exp\left[\sum_i \frac{4g^2\Gamma_i^2}{\omega_i^2}\left[e^{i\omega_i q} - 1 + 2\frac{\cos(\omega_i q)-1}{e^{\beta\omega_i}-1}\right]\right]\right\} . \tag{3.33}$$

To discuss the relation between this result and that of Leggett and co-workers,[1] let us rewrite Eq. (3.33) as follows:

$$\langle \sigma_x(t)\rangle = 1 - \omega_0^2 \int_0^t dq \int_q^t dz\, \mathrm{Re}[\exp(e^{\psi(q)})] \,, \tag{3.34}$$

where

$$\psi(q) = \sum_i \frac{4g^2\Gamma_i^2}{\omega_i}\left[e^{i\omega_i q} - 1 + 2\frac{\cos(\omega_i q)-1}{e^{\beta\omega_i}-1}\right] . \tag{3.35}$$

The Laplace transform of $\rho(t) \equiv \langle \sigma_x(t)\rangle$, $\hat{\rho}(z)$, reads

$$\hat{p}(z) = \frac{1}{z} - \omega_0^2 \frac{\hat{\Phi}(z)}{z^2} \,, \tag{3.36}$$

where $\hat{\Phi}(z)$ is the Laplace transform of $\mathrm{Re}\{\exp[\psi(t)]\}$. On the other hand, in the limiting condition of a very small ω_0, Eq. (3.36) can be considered as a second-order Taylor expansion in ω_0 of

$$\hat{p}(z) = \frac{1}{z + \omega_0^2 \hat{\Phi}(z)} \,. \tag{3.37}$$

If we replace the approximant of Eq. (3.36) with Eq. (3.37), then we recover the result of Aslangul *et al.*,[17] which, in turn, coincides with the well-known noninteracting-blip approximation of Leggett and co-workers.[1] Since we limit the investigation of the present paper to the case of very small ω_0, we can conclude by saying that the comparison, carried out in the next section, between the prediction of the DNSE and Eq. (3.34), is equivalent to comparing the prediction of the DNSE (Refs. 5 and 9–11) to the theory of Leggett and co-workers.[1] This is certainly true in the time region defined by $t \le 1/\omega_0$. Actually, as shown at the end of this section and in the next section, the region of validity of Eq. (3.33) is much more extended. Equation (3.33) is basically exact provided that $\langle \sigma_x(t)\rangle$ does not significantly depart from the initial condition $\langle \sigma_x(0)\rangle = 1$.

In Sec. II we saw that if both thermal and quantum-mechanical fluctuations are suppressed, Eq. (2.15) becomes identical to Eq. (2.11) and the result of Eq. (2.12) is recovered. In the strong-coupling limit, Eq. (2.12) coincides with the prediction of Kenkre and Campbell,[9] which is merely the analytical solution of the DNSE in the same regime. Thus we expect that in the absence of both quantum and thermal fluctuations, Eq. (3.33) also results in the analytical expression of Kenkre and Campbell. To prove that the central theoretical result of this section fulfills this crucial property, let us rewrite Eq. (3.19) under the following form:

$$\langle \sigma_x(t)\rangle = 1 - \omega_0^2 \int_0^t ds \int_0^s ds' \mathrm{Re}(\exp(4i\Delta s')\langle \exp(-i\tilde{\mathcal{H}}_B s')\exp\{i[\tilde{\mathcal{H}}_B - 2g\tilde{x}(s+s')]s'\}\rangle) \,. \tag{3.38}$$

With the symbol $\langle\ \rangle$ we denote an average which must be evaluated over the equilibrium distributions of the bath oscillators regarded as being classical. At temperature $T=0$ the coordinate $\tilde{x}$, thought of as a classical variable, is obliged by the classical equilibrium distribution to keep the value $\tilde{x}=0$. The classical equilibrium distribution at zero temperature behaves indeed as the delta of Dirac, $\delta(\tilde{x})$. In conclusion we have

$$\langle \exp(-i\tilde{\mathcal{H}}_B s')\exp\{i[\tilde{\mathcal{H}}_B - 2g\tilde{x}(s+s')]s'\}\rangle = 1 \ . \quad (3.39)$$

In the genuinely quantum-mechanical case, on the contrary, we have to take into account the ground-state fluctuations which are equivalent to a background noise making $\tilde{x}$ fluctuate around $\tilde{x}=0$. In other words, the approximation of Eq. (3.39) corresponds to neglecting both thermal and quantum fluctuations. Using Eq. (3.39) we get from Eq. (3.38) the following result:

$$\langle \sigma_x(t)\rangle = 1-\omega_0^2 \int_0^t ds \int_0^s ds' \cos(4\Delta s') \ , \quad (3.40)$$

which can be rewritten as follows:

$$\langle \sigma_x(t)\rangle = 1+\frac{\omega_0^2}{16\Delta^2}[\cos(4\Delta t)-1] \ . \quad (3.41)$$

On the other hand, the prediction of the DNSE, Eq. (2.12), can be rewritten under the following form:

$$\langle \sigma_x(t)\rangle = 1+\frac{\omega_0^2}{(\omega_0^2+16\Delta^2)}\{\cos[(\omega_0^2+16\Delta^2)^{1/2}t]-1\} \ . \quad (3.42)$$

We thus find that in the strong-coupling limit $\omega_0 \ll \Delta$, and when both quantum and thermal fluctuations are neglected, Eq. (3.38) coincides with Eq. (2.12) and consequently with the predictions of Kenkre and Campbell.[9] In the same limiting condition, the theory of Leggett and co-workers[1] would have led us precisely to Eq. (3.42). This supports the view that the result of Eq. (3.38) coincides with the prediction of Ref. 1 beyond the time region $t \le 1/\omega_0$, provided that $\langle \sigma_x(t)\rangle$ does not significantly depart from the trapped condition $\langle \sigma_x(t)\rangle = 1$. Within our approach, the breakdown of the localized state would be signaled by the presence of secular terms, which in the large time region would conflict with the constraint $|\langle \sigma_x(t)\rangle| \le 1$. The renormalization approach of Leggett and co-workers[1] serves indeed the purpose of amending Eq. (3.38) from this fault, by replacing the secular terms with harmonic functions of time. Our secular terms are derived from these harmonic functions of time via an expansion up to second order in ω_0. However, it is much easier to handle Eq. (3.38) than the resulting differential equation of Leggett and co-workers.[1] This is the key reason why the comparison with the prediction of the DNSE will be made (see the next section) using Eq. (3.38) rather than the renormalized version of it.

IV. INTERACTION WITH ONE OSCILLATOR

By using the result of the preceding section, we can easily evaluate the effect of quantum fluctuations on the adiabatic dimer of Kenkre and co-workers.[9–11] In the special case of a single oscillator, with frequency Ω at zero temperature, we obtain from our general result of Eq. (3.33) the following simple expression:

$$\langle \sigma_x(t)\rangle = 1-\omega_0^2 \int_0^t dq\,(t-q) \times \mathrm{Re}\left[\exp\left[\frac{4\Gamma^2 g^2}{\Omega^2}(e^{i\Omega q}-1)\right]\right] . \quad (4.1)$$

From the analysis of the preceding section, it is now clear that the discrepancies between the prediction of this simple formula and the DNSE must be attributed to the influence of quantum-mechanical fluctuations. We have seen that the dimer of Kenkre and Campbell[9] disregards the Kubo-like multiplicative fluctuations. At zero temperature these fluctuations are of merely quantum-mechanical origin and, due to their multiplicative structure, can produce dissipation.[14] This is fully taken into account by Eq. (4.1). To make clearer why quantum-mechanical fluctuations imply that dissipation comes into play, let us now make the assumption that the coupling $g\Gamma$ is very large compared to the frequency Ω. At times much smaller than $1/\Omega$ we should see many of the oscillations predicted by the adiabatic dimer.[9] On the other hand, this short-time region can be safely explored by expanding the exponential $\exp(i\Omega q)$ into a Taylor series truncated at the second order. We thus obtain

$$\langle \sigma_x(t)\rangle \cong 1-\omega_0^2 \int_0^t dq\,(t-q) \times \mathrm{Re}\left[\exp\left[\frac{4ig^2\Gamma^2}{\Omega}q-4g^2\Gamma^2 q^2\right]\right] . \quad (4.2)$$

Equation (4.2) shows that in this time region the effect of quantum fluctuations is perceived as a sort of Gaussian-like dissipation process, eroding the harmonic oscillations of the adiabatic dimer. Of course, the mere fact that Ω is finite, and not infinitely small, implies that collapses are followed by revivals. Thus we are in a position to predict a physical property quite similar to that discovered by Eberly *et al.*[4] At finite values of Ω we expect indeed revivals to take place with the time period $T=2\pi/\Omega$.

To make this aspect clearer, let us rewrite Eq. (4.1) in the completely equivalent form

$$\langle \sigma_x(t)\rangle = 1-\frac{(\omega_0 t)^2}{2}\exp\left[-\frac{4g^2\Gamma^2}{\Omega^2}\right] -\omega_0^2\exp\left[-\frac{4g^2\Gamma^2}{\Omega^2}\right] \times \sum_{n=1}^{\infty}\left[\frac{4g^2\Gamma^2}{\Omega^2}\right]^n \frac{1}{n!}\,\frac{1-\cos(n\Omega t)}{n^2\Omega^2} \ . \quad (4.3)$$

If we neglect the second term on the right-hand side of this equation, we see indeed that revivals are predicted to take place with the time period $T=2\pi/\Omega$.

In Figs 1 and 2 we explicitly compare the prediction of Eq. (4.1) [or (4.3)] to that of the adiabatic dimer of Kenkre and Campbell.[9] We see that the effect of the quantum-mechanical fluctuations is that of damping out the fast oscillations of Kenkre and Campbell.[9] This relaxation process is followed by periodical revivals with the time period $T=2\pi/\Omega$. In Fig. 1, the occurrence of periodical revivals is clearly illustrated. Figure 2 shows the early decay process in an enlarged scale. It is evident from this figure that due to the relaxation process associated to the quantum-mechanical fluctuations, the original oscillation survives approximately for only one half of its

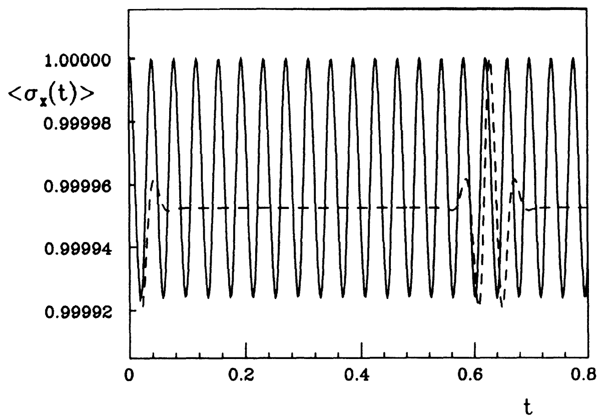

FIG. 1. $\langle \sigma_x(t) \rangle$ as a function of time. The solid line denotes the prediction of the theory of Kenkre and Campbell [Eq. (2.12)]. The dashed line denotes the prediction of Eq. (4.1). The parameters used area $g=90$, $\omega_0=1$, $\Omega=10$, and $\Gamma=1/\sqrt{20}$.

time period.

The results illustrated in Figs. 1 and 2 refer to cases where $2g\Gamma \gg \Omega$. This has the effect of making negligible the second term on the right-hand side of Eq. (4.3). The effect of this term is that of producing a breakdown of the localized state in a time T_B, whose order of magnitude is given by this Arrhenius-like expression

$$T_B = \frac{1}{\omega_0} \exp\left[\frac{2\Delta}{\Omega}\right] . \tag{4.4}$$

This expression suggests this appealing physical interpretation. The strong coupling between spin and oscillator is perceived by the spin as a barrier of intensity Δ. The classical approximation on the oscillator means an equilibrium state with vanishing energy, thereby resulting in a trapped state with an infinite lifetime, in complete agreement with the prediction of the DNSE. When the classical assumption is rejected and a completely quantum-mechanical picture is adopted, we have to take into account the fluctuations accompanying the motion of the oscillator, even at zero temperature, i.e., the zero-point energy of a quantum oscillator. The fluctuations associated with this zero-point energy have the capability of making the system overcome the strong-coupling barrier.

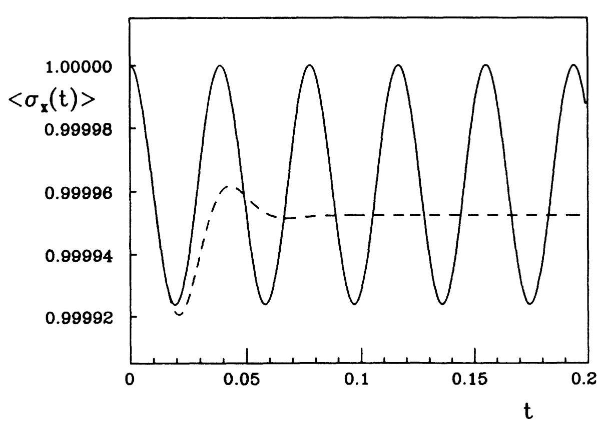

FIG. 2. $\langle \sigma_x(t) \rangle$ as a function of time. This figure refers to the same condition as Fig. 1, but in an enlarged time scale.

Note that the time T_B of Eq. (4.4) coincides with the period of oscillation corresponding to the renormalized tunneling frequency of Ref. 18. This is in line with our preceding remarks that the secular terms stemming from our approximation at the second order in ω_0 correspond to the oscillation frequencies of the renormalized approaches.

V. CONCLUDING REMARKS

The major result of the present paper concerns the microscopic derivation of the DNSE. The fully quantum-mechanical treatment of Sec. III is based on the key assumption that the frequency ω_0 is very weak or, equivalently, the coupling between system and oscillator is very large. In this condition the DNSE predicts that the initial condition $\langle \sigma_x(t) \rangle = 1$ results in a localized state. This is the self-trapping state, first found by Eilbeck, Lomdahl, and Scott.[19] The dimer of Kenkre and co-workers[9-11] affords an attractive picture of this localization process. They show indeed[9-11] that the variable $\langle \sigma_x(t) \rangle$ can be regarded as the space coordinate of a particle moving in a double-well potential. Then the strong-coupling limit corresponds to the weak oscillations of this particle at the bottom of one of the two wells. This means that in spite of the anharmonic nature of their double-well potential, the resulting oscillations are harmonic. This paper proves that the coherent oscillations sustained by these wells are destroyed by the quantum fluctuations of the bath oscillator. These coherent oscillations are replaced by collapses and revivals, reminiscent of those taking place in quantum optics.[4] In addition to this, the effect of quantum-mechanical fluctuations is that of making unstable the trapped state. The lifetime T_B of the trapped state is given by the Arrhenius-like expression of Eq. (4.4) and this does not conflict with Fig. 2. The time scale of Fig. 2 is indeed very small compared to T_B and it is rendered necessary to illustrate collapses and revivals. In a time scale comparable to T_B one would see $\langle \sigma_x(t) \rangle$ oscillate around 0. It is interesting to notice that according to Eq. (4.4) the lifetime of the trapped state decreases upon increasing the frequency of the quantum oscillator. This results in an apparent contrast with the spirit of the adiabatic approximation,[9] according to which the validity of the DNSE rests on the assumption that the time scale of the oscillator is much shorter than that of the system. We believe this to imply a strong dissipation process to drive the oscillator dynamics, whereas the oscillator of the model under discussion here is totally undamped. Note that we make the basic assumption that at $t=0$ the spin is polarized along the x direction and the oscillator is at equilibrium in the corresponding shifted potential. For this special condition to be naturally reached by the system, the oscillator must be driven by a fast relaxation process. On the basis of the results of this paper, we can predict that a fast relaxation is actually necessary for this special condition to be reached, and that, at zero temperature, the lower the frequency of the quantum-mechanical oscillator, the more stable the ensuing trapped state is.

A further limitation of our approach is the fact that it is limited to the second order in ω_0. As we have seen, this obliges us to keep our analysis in close proximity with the trapped condition. The direct use of the theory of Leggett and co-workers[1] would have prevented us from carrying out the discussion in terms of simple analytical results. Furthermore, there are still doubts as to the reliability of the noninteracting-blip approximation in the regions of intermediate couplings.[1,20] We believe that the feedback of the system on the bath is properly taken into account by this theory only in the proximity of the condition $\langle \sigma_x(t) \rangle = 1$. Our view is based in part on our independent rederivation of the results of Ref. 1 in the strong-coupling limit (Sec. III). For these reasons we are not yet in a position to discuss the interesting discovery of Tsironis and Kenkre,[21] who found that initial conditions play a very important role in the self-trapped regime and can enhance the role of nonlinearity. Thus we plan to study this aspect along completely different lines in a forthcoming publication.

APPENDIX A

We plan to write the expression (3.23) under the following form:

$$\exp[i(\omega\tilde{b}^{\dagger}\tilde{b}+\delta^{*}\tilde{b}^{\dagger}+\delta\tilde{b})q] = \exp(i\omega\tilde{b}^{\dagger}\tilde{b}q)\exp(\alpha\tilde{b}^{+}+\beta\tilde{b})\exp(i\varphi)\ , \quad (A1)$$

where α, β, and φ are complex numbers to be determined. This will allow us to make the factor $\exp(-i\tilde{\mathcal{H}}_B q)$ disappear, thereby simplifying the evaluation of the Trace in Eq. (3.21).

Let us consider the operator $f(q)$, function of the time q, defined by

$$f(q) \equiv \exp(-i\omega\tilde{b}^{\dagger}\tilde{b}q)\exp[i(\omega\tilde{b}^{\dagger}\tilde{b}+\delta^{*}\tilde{b}^{\dagger}+\delta\tilde{b})q]\ . \quad (A2)$$

Through differentiation with respect to q we obtain the differential equation

$$f'(q)=A(q)f(q) \quad (A3)$$

with, in our case,

$$A(q) \equiv i(\delta^{*}e^{-i\omega q}\tilde{b}^{\dagger}+\delta e^{i\omega q}\tilde{b}) \quad (A4)$$

and the initial condition

$$f(0)=1\ . \quad (A5)$$

According to Weiss and Maradudin,[16] the solution of Eq. (A3) with the initial condition of Eq. (A5) and A as a general operator is given by

$$f(q)=\exp[\Omega(q)] \quad (A6)$$

with

$$\begin{aligned}\Omega(q)=&\int_0^q A(\tau)d\tau+\tfrac{1}{2}\int_0^q d\tau\left[A(\tau),\int_0^{\tau}A(\sigma)d\sigma\right]\\&+\tfrac{1}{4}\int_0^q d\tau\left[A(\tau),\left[\int_0^{\tau}A(\sigma),\int_0^{\sigma}d\rho\,A(\rho)\right]d\sigma\right]\\&+\tfrac{1}{12}\int_0^q d\tau\left[\left[A(\tau),\int_0^{\tau}d\sigma\,A(\sigma)\right],\int_0^{\tau}d\rho\,A(\rho)\right]\\&+\cdots\ .\end{aligned} \quad (A7)$$

In our case this series is truncated at the second order, since the nested commutator is in our case a c number. Thus we have

$$\Omega(q)=-\frac{\delta^{*}}{\omega}(e^{-i\omega q}-q)\tilde{b}^{\dagger}+\frac{\delta}{\omega}(e^{i\omega q}-1)\tilde{b} - i\frac{|\delta|^2}{\omega}\left[q-\frac{\sin(\omega q)}{\omega}\right]. \quad (A8)$$

From Eqs. (A2), (A6), and (A8) we get

$$\begin{aligned}\exp[i(\omega\tilde{b}^{\dagger}\tilde{b}+\delta^{*}\tilde{b}^{\dagger}+\delta\tilde{b})q] &= \exp(i\omega\tilde{b}^{\dagger}\tilde{b}q)\exp\left[-\frac{\delta^{*}}{\omega}(e^{-i\omega q}-q)\tilde{b}^{\dagger}+\frac{\delta}{\omega}(e^{i\omega q}-1)\tilde{b}\right]\\&\quad\times\exp\left[-\frac{i|\delta|^2}{\omega^2}[\omega q-\sin(\omega q)]\right].\end{aligned} \quad (A9)$$

APPENDIX B

In this Appendix we plan to evaluate the trace appearing on the right-hand side of Eq. (3.31). From the definition of trace, we have, omitting the index i,

$$\mathrm{Tr}[\exp(-\beta\omega\tilde{b}^{\dagger}\tilde{b})\exp(\alpha\tilde{b}^{\dagger})\exp(-\alpha^{*}\tilde{b})] = \sum_{n=0}^{\infty}\exp(-\beta\omega n)\langle n|\exp(\alpha\tilde{b}^{\dagger})\exp(-\alpha^{*}\tilde{b})|n\rangle\ . \quad (B1)$$

Via expansion of the exponentials in a Taylor series and using the properties of the destruction and creation operators, we obtain

$$\exp(-\alpha^{*}\tilde{b})|n\rangle=\sum_{p=0}^{\infty}\frac{(-\alpha^{*}b)^p}{p!}|n\rangle = \sum_{p=0}^{n}\frac{(-\alpha^{*})^p}{p!}\left[\frac{n!}{(n-p)!}\right]^{1/2}|n-p\rangle\ . \quad (B2)$$

Then, using Eqs. (B2) and (B1), it is shown that

$$\mathrm{Tr}[\exp(-\beta\omega\tilde{b}^{\dagger}\tilde{b})\exp(\alpha\tilde{b}^{\dagger})\exp(-\alpha^{*}\tilde{b})] = \sum_{p=0}^{\infty}\frac{(-|\alpha|^2)^p}{(p!)^2}\sum_{n=p}^{\infty}\frac{n!}{(n-p)!}\exp(-\beta\omega n)\ . \quad (B3)$$

Let us define

$$x \equiv e^{-\beta\omega}\ . \quad (B4)$$

Using this definition, we show that

$$\begin{aligned}\sum_{n=p}^{\infty}\frac{n!}{(n-p)!}\exp(-\beta\omega n)&=\sum_{n=p}^{\infty}x^{n}\frac{n!}{(n-p)!}\\&=x^{p}\frac{\partial^{p}}{x^{p}}\sum_{n=p}^{\infty}x^{n}\\&=x^{p}\frac{\partial^{p}}{x^{p}}\left[\sum_{n=0}^{\infty}x^{n}-\sum_{n=0}^{p-1}x^{n}\right]\\&=\frac{1}{(1-e^{-\beta\omega})}p!\frac{e^{-\beta\omega p}}{(1-e^{-\beta\omega})^{p}}\ .\end{aligned}\qquad \text{(B5)}$$

Inserting Eq. (B5) in Eq. (B3) and taking the normalization factor of the density matrix into account, we finally get the following result:

$$\mathrm{Tr}[\rho_i\exp(\alpha\tilde{b}_i^{\dagger})\exp(-\alpha^{*}\tilde{b}_i)]=\exp\left[\frac{|\alpha|^2}{(1-e^{\beta\omega_i})}\right].$$

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