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Quantum ohmic dissipation: coherence vs. incoherence and symmetry-breaking. A simple dynamical approach

C. Aslangul (1), N. Pottier (1) and D. Saint-James (2)

(1) Groupe de Physique des Solides de l'Ecole Normale Supérieure (*), Université Paris VII, 2 place Jussieu, 75251 Paris Cedex 05, France
(2) Laboratoire de Physique Statistique, Collège de France, 11 place Marcelin Berthelot, 75231 Paris Cedex 05, France

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Résumé. — La dynamique d'une particule située dans un double puits de potentiel et couplée à un bain de phonons suivant une loi de dissipation « ohmique » est étudiée à l'aide de méthodes usuelles de mécanique statistique quantique.

Nous complétons les résultats déjà connus sur la brisure de symétrie à T = 0 de la manière suivante :

(i) en déterminant le comportement critique du paramètre d'ordre, on montre que la brisure de symétrie n'est complète que pour un couplage infini ;
(ii) la dynamique suit une loi de Kohlrausch généralisée de la forme exp(- atb), où les deux paramètres a et b sont calculés exactement; un ralentissement critique est très clairement mis en évidence.

A température finie, la brisure de symétrie ne se produit plus, bien qu'un comportement précurseur de la transition se manifeste lorsque T ~ 0+.

Ces résultats sont généralisés à une particule dans un potentiel à puits multiples : en présence de dissipation ohmique, un phénomène de localisation peut se produire à T = 0.

En dernier lieu, nous examinons d'autres lois de dissipation (non ohmiques) et nous montrons que seul le modèle ohmique est capable de produire une telle transition, bien que, là encore, un comportement précurseur existe pour des lois de dissipation quasi ohmiques.

Abstract. — By using standard quantum-statistical methods, we study the dynamics of a particle in a double-well potential, coupled dissipatively, in an « ohmic » way, to a bath of phonons.

We refine previous results about the T = 0 symmetry breaking :

(i) the critical behaviour of the order parameter is exhibited and the symmetry is shown to be only fully broken for infinite coupling ;
(ii) the dynamics follows a generalized Kohlrausch law of the type exp(- atb), where both parameters a and b are exactly calculated; a critical slowing down is very clearly displayed.

At finite temperature, the symmetry breaking does disappear, although a precursor behaviour of the transition exists when T ~ 0+.

These results are extended to a particle in a multiple-well potential for which a localization phenomenon is seen to occur at T = 0.

Finally, we investigate other dissipation laws (i.e. non ohmic) and we show that the ohmic model is unique by its ability to produce such a transition, although a precursor behaviour can be obtained for near-ohmic dissipation laws.

1. Introduction.

The question which we intend to discuss in the present paper is that of the influence of dissipation on the fundamental quantum mechanism of quantum coherence. The underlying idea is to decide whether dissipation destroys phase coherence.

This question is evidently related to the general problem of relaxation in quantum systems, for which, as it is well known, the lines of attack fall into two
main categories [1] : either people have tried new schemes of quantization or they have used standard quantum mechanics, considering the evolution of the (small) system and of the reservoir as a whole.

As underlined in reference [1], the first type of approach contains either controversial results or obscurities. In the second type of approach, known as the system-plus-reservoir approach, and pioneered by Senitzky [2], the interaction of the system of interest with the reservoir is explicitly taken into account. Irreversible behaviour of the small system arises when the reservoir is considered as a continuum of modes, thus rejecting Poincaré times to infinity.

The new aspect of dissipation which we would like to study here is the following : since 1982, it has been shown by several authors [3, 4] that, for a certain type of dissipation (the so-called « ohmic » dissipation), a spontaneous symmetry breaking may appear in some dissipative quantum systems when the dissipation becomes greater than a critical value.

This is all the more interesting as, in these « ohmic » dissipative quantum systems, the Heisenberg representation of a certain coordinate \( q \) follows a classical equation of motion

\[
M \ddot{q} + \gamma \dot{q} + \frac{\partial V}{\partial q} = F(t)
\]

which is generally believed to be obeyed by macroscopic quantum variables [5] \((M)\) is the mass of the particle submitted to a potential \( V(q) \); \( \gamma \) is a phenomenological damping constant or friction coefficient and \( F(t) \) is a fluctuating force). These systems have been the centre of recent interest in the testing of the applicability of quantum mechanics to macroscopic variables [6].

Following references [3, 4], we shall mainly study here a particle in a double-well potential, coupled dissipatively (in an « ohmic » way) to its environment. This problem can be very clearly settled down, but it cannot be given an exact solution. Thus approximate treatments have been proposed in the literature. Most of them use either path-integral Feynman formulation in imaginary time and instanton techniques, or renormalization group approaches [3, 4, 7]. Two other approaches must equally be quoted : that of reference [8], in which a variational method of displaying the transition is proposed, and that of reference [9] in which a linear response calculation is handled. As for the real-time dynamics, it has not been investigated in detail, except for references [9, 10] outside the critical region.

Our purpose in this paper is thus to refine and to supplement previous treatments of this problem, and that will be attained by using standard quantum-mechanical theory. Indeed, by using standard methods, we recover qualitatively and quantitatively nearly all previous results, and in particular the spontaneous symmetry breaking which occurs at zero temperature [11]. The improvements over previous treatments are the following : we are able to give a description of the real-time dynamics of the particle, for zero as well as for finite temperature ; in the vicinity of the transition point, we find a critical slowing down. Another advantage of our methods is that the approximations involved are more transparent from a physical point of view. Moreover it will be shown that the order parameter is continuous and reaches its maximum value only for infinite coupling; the particle is then fully localized.

The paper is organized as follows. In section 2, we describe the model under study; in section 3, we present an approximate method, based on a master equation formalism, which yields the real-time dynamics in the case of intermediate or strong coupling. In section 4, we present another approximation scheme, based on a one-boson assumption, which yields the real-time dynamics in the weak coupling case. Section 5 contains a comparison between our results and previous results on the real-time dynamics [9, 10]. Then, in section 6, we discuss the specificity of the ohmic dissipation model. In section 7, we show how the results on the particle in a double-well potential can be extended to a particle in a multiple well. Finally, in section 8, we present our conclusions.

2. The model.

2.1 THE DAMPED PARTICLE IN THE SYMMETRIC DOUBLE-WELL. — As indicated in the Introduction, following references [3, 4], we consider a particle of mass \( M \) moving in a symmetric double-well potential \( V(q) = V(-q) \) with its minima located at \( q = \pm q_0/2 \) and separated by a local maximum at \( q = 0 \).

This particle is in contact with a dissipative medium, which is generally modelled by a phonon reservoir of bandwidth \( \hbar \omega_0 \) [5]. As previously indicated, we shall mostly be interested here in the case of « ohmic » dissipation, in which the coordinate of the particle evolves with time according to the classical equation of motion (1).

The problem is the following : at time \( t = t_0 \), a particle is located in one of the two wells; the temperature is supposed to be low enough so that thermal activation over the potential barrier can be neglected. The question arises : how does its average position evolve with time ? Evidently, a purely classical particles, initially located in one of the two wells, remains localized on the same side for an infinite time. On the contrary, a purely quantum-mechanical particle (without bath), initially located in one of the two wells, can tunnel through the potential barrier, and thus oscillates back and forth between the two wells. This is the phenomenon of « quantum coherence ». Such a particle can be said to be delocalized : its average position is equal to zero. Let us now consider a quan-
tum-mechanical particle coupled to a bath, in such a way so that its position operator in the Heisenberg picture obeys the equation of motion (1). In this situation, Chakravarty [3] and Bray and Moore [4] have found a transition: for a weak coupling with the bath, the regime is akin to the pure quantum regime and the particle undergoes a damped oscillation between the two wells; for higher values of the coupling, the mean coordinate of the particle relaxes towards zero without oscillating, but when the coupling to the bath becomes greater than a critical value, a spontaneous symmetry breaking occurs, which here signifies that the mean coordinate of the particle eventually relaxes towards a non-zero value, indicating a localization in one of the two wells. This regime thus bears a resemblance to the classical regime and corresponds to a complete loss of phase coherence [12, 13].

In the system-plus-reservoir approach, one begins by writing down the total Hamiltonian for this problem. Following Caldeira and Leggett [5], the dissipative interaction of the system with its environment is modelled by a linear coupling with a bath of harmonic oscillators. In obvious notations:

\[ H = \frac{p^2}{2M} + V(q) + \sum_n M\Omega_n^2 q_n + \]

\[ \sum_n \hbar \omega_n b_n^\dagger b_n + \sum_n \frac{1}{2} \frac{M^2}{m_n \omega_n^2} q^2. \] (2)

The last term has been added in order to cancel spurious unphysical divergences; it ensures that there is not shift in the potential due to the coupling [5].

It is easy to derive from equation (2) the equations of motion for the coordinate \( q(t) \) and the momentum \( p(t) \) of the particle in the Heisenberg picture. As we already shown in a previous paper about the damped free particle [14], once \( p(t) \) is eliminated, the dynamical equation for \( q(t) \) reads as follows:

\[ \ddot{q}(t) + \int_{t_0}^t dt' K(t - t') \dot{q}(t') + \frac{1}{M} \frac{\partial V}{\partial q} = \frac{1}{M} F(t). \] (3)

where the interaction with the bath manifests itself, as it is well-known, by a dissipative retarded term and by a fluctuating force term, both being related by the fluctuation-dissipation theorem. Note that equation (3), which has been established without any approximation, contains the exact dynamics of the particle. Let us now discuss the conditions under which it can be given the form of the classical equation of motion (1).

2.2 THE OHMIC DISSIPATION MODEL. — As usual, the bath is described in the continuous limit by its density of modes \( \rho(\omega) \). Following the same line of reasoning as in reference [14] in the case of the damped free particle, a classical equation of motion of the type of equation (1) for \( q(t) \) is obtained by setting down

\[ \rho(\omega) \frac{\Omega^4(\omega)}{\omega^3} \frac{M}{m(\omega)} = \frac{2}{M\pi} f_\omega(\omega/\omega_c) \] (4)

where \( f_\omega(\omega/\omega_c) \) is some cut-off function such that \( f_\omega(0) = 1 \), and decreasing on a frequency range of order \( \omega_c \). When the choice (4) is made, it can be shown [14] that \( K(t) \) is a memory kernel essentially given by the Fourier transform of the cut-off function \( f_\omega(\omega/\omega_c) \) and that, for temperatures such that \( \hbar k_B T > \hbar \omega_c \), \( F(t) \) is a rapidly fluctuating force of correlation time of order \( \sim \omega_c^{-1} \). The constraint (4) imposed on the bath density of modes and on the coupling constant in order to obtain a classical-like equation of motion will from now on be referred to as the ohmic dissipation model. Let us emphasize that, in accordance with the fluctuation-dissipation theorem, not only the friction, but also the fluctuating force term have a determined form.

2.3 REDUCTION TO A SPIN-BOSON HAMILTONIAN [4]. —

Let us consider the particle in the double-well and let \( \Omega_0 \) denote the frequency of small oscillations around one of the minima, and \( V_0 \) the barrier height. We shall limit the study to the low-temperature situation \( k_B T < V_0 \), in which thermal activation over the potential barrier can be neglected. Moreover, we shall suppose that this barrier is sufficiently high and large \( (V_0 \gg \hbar /M\Omega_0^2) \) for the splitting \( \omega_0 \) between the symmetric and antisymmetric states (tunnelling frequency) to be much lower than \( \Omega_0 \). Finally, we shall suppose that the temperature is such that \( k_B T < \hbar \Omega_0 \): the system can then be safely truncated to only one level in each well.

After this truncation, we are left with an effectively two-level system coupled to a bath of phonons; this ensemble can be described by the spin-boson Hamiltonian \( (\sigma_x, \sigma_y, \sigma_z) \) are the standard Pauli matrices):

\[ H_{sb} = -\frac{1}{2} \hbar \omega_0 \sigma_x + \sum_n \hbar G_n (b_n + b_n^\dagger) + \]

\[ \sum_n \hbar \omega_n b_n^\dagger b_n + \sigma_z^2 \sum_n \frac{\hbar G_n^2}{\omega_n}. \] (5)

where the operator \( \frac{1}{2} q_0 \sigma_x \) corresponds to the position \( q_0 \) of the particle; in order to be complete, we have now to identify the coupling term of the spin-boson Hamiltonian \( H_{sb} \) (5) with the coupling term of the Hamiltonian (2). This can be done by identifying

\[ \frac{2 \hbar G_n}{q_0} \text{ with } M\Omega_0^2 \left( \frac{\hbar}{2 m_n \omega_n} \right)^{1/2}. \] (6)

The ohmic constraint (4) then takes the form

\[ \rho(\omega) \left| G(\omega) \right|^2 = \frac{2}{\omega_c} f_\omega(\omega/\omega_c). \] (7)
where the dimensionless parameter \( \alpha \) is related to the friction coefficient \( \eta \) by

\[
\alpha = \frac{\eta q_0^2}{2 \hbar}.
\]  

(8)

The cut-off frequency \( \omega_c \) has to be chosen such that \( \omega_c \gg \omega_0 \) and \( \omega_c \gg kT/h \). Clearly, with these assumptions, one expects that the precise form of \( J \) has no bearing on the dynamics of the system in the time domain \( \omega_c t \gg 1 \) and may be chosen at convenience.

To conclude this section, let us now comment briefly on the reduction of the Hamiltonian (2) to the spin-boson Hamiltonian (5). Clearly, the operator \( 1/2 q_0 \sigma_z \) possesses only two discrete eigenvalues \( \pm q_0^2/2 \) whereas the genuine position operator \( q \) has a continuous spectrum. The kinetic and potential energy have been contracted into the \( \sigma_z \) term, and since, as well-known, the Pauli matrices algebra is completely different from the algebra of the position and momentum operators (in particular it is impossible to find an operator having the same commutation relation with \( \sigma_z \) than \( p \) with \( q \)), this amounts to carry out a kind of coarse-graining in which some information has been lost; one may loosely speak of a reduction of the Hamiltonian. Conversely, the results obtained on the dynamics of \( \sigma_z \) can be cast in terms of \( q \) as well, but one cannot expect \( \sigma_z(t) \) to obey any classical-like equation of motion of type (1), which, as explained above, is obtained for a quantum system coupled to a bath when writing down the equations of motion for both \( q(t) \) and \( p(t) \).

In the following two sections, we shall successively analyse the cases of weak and moderate or strong coupling.

3. Intermediate or strong coupling case.

3.1 PARTIAL DIAGONALIZATION OF THE HAMILTONIAN. — As pointed out by Silbey and Harris [8] and by Zwerger [9], the unitary transformation

\[
S = \exp \left\{ \sigma_z \sum_n \frac{G_n}{\omega_n} (b_n^\dagger - b_n) \right\}
\]  

(9)

diagonalizes the Hamiltonian \( H_{sb}(5) \) when \( \omega_0 = 0 \). The transformed Hamiltonian \( \hat{H} = SH_{sb}S^{-1} \) reads:

\[
\hat{H} = -\frac{1}{2} \hbar \omega_0 (B_+ \sigma_+ + B_- \sigma_-) + \sum_n \hbar \omega_n b_n^\dagger b_n.
\]  

(10)

The operators \( B_\pm \) are defined as

\[
B_\pm = \exp \left\{ \pm 2 \sum_n \frac{G_n}{\omega_n} (b_n^\dagger - b_n) \right\}.
\]  

(11)

Formally, \( \hat{H} \) divides into an interaction term

\[
H_{\text{int}} = -\frac{1}{2} \hbar \omega_0 (B_+ \sigma_+ + B_- \sigma_-)
\]  

(12)

and a bath term.

In what follows, we shall be interested in the time evolution of the average value of \( \sigma_z \), defined in the Schrödinger picture as

\[
\langle \sigma_z(t) \rangle = \text{Tr} \{ \rho(t) \sigma_z \}
\]  

(13)

(\( \rho(t) \) is the full (i.e. system plus bath) density matrix and the trace operator acts in the whole space).

The basic remark is the following: the unitary transformation \( S \) leaves \( \sigma_z \) invariant, and, consequently, one gets

\[
\langle \sigma_z(t) \rangle = \text{Tr} \{ \rho(t) \sigma_z \} = \text{Tr} \{ \bar{\rho}(t) \sigma_z \}
\]  

with

\[
\bar{\rho}(t) = S\rho(t)S^{-1}.
\]  

(14)

Since \( \sigma_z \) is a pure spin operator, equation (14) takes the form

\[
\langle \sigma_z(t) \rangle = \text{Tr}_s \{ \sigma_z \rho_s(t) \}
\]  

(15)

where the trace operator acts in the spin space and \( \rho_s(t) \) is the reduced spin density matrix

\[
\rho_s(t) = \text{Tr}_b \bar{\rho}(t)
\]  

(16)

(the trace operator acts in the bath space).

Similarly, the time derivative \( \langle \dot{\sigma}_z(t) \rangle \) is given by

\[
\langle \dot{\sigma}_z(t) \rangle = \text{Tr} \left\{ \frac{\partial \rho}{\partial t} \sigma_z \right\} = \text{Tr} \left\{ S \frac{\partial \bar{\rho}}{\partial t} S^{-1} \sigma_z \right\} = \frac{1}{\hbar} \text{Tr} \left\{ [\bar{\rho}, \hat{H}] \sigma_z \right\}.
\]  

(17)

By setting

\[
\langle \frac{\partial \bar{\rho}}{\partial t} \rangle = \frac{1}{\hbar} [\bar{\rho}, \hat{H}]
\]  

(18)

one gets

\[
\langle \dot{\sigma}_z(t) \rangle = \text{Tr} \left\{ \left\langle \frac{\partial \rho_s}{\partial t} \right\rangle \sigma_z \right\} = \text{Tr}_s \left\{ \left\langle \frac{\partial \rho_s}{\partial t} \right\rangle \sigma_z \right\}.
\]  

(19)

The time evolution of \( \bar{\rho} \) has thus been calculated by using \( \hat{H} \) instead of \( \hat{H} \), this being legitimate as long as one is interested in quantities such as \( \sigma_z \) which are invariant under the unitary transformation \( S \).

3.2 MASTER EQUATION FOR THE REDUCED SPIN DENSITY MATRIX \( \rho_s(t) \). — According to the general damping theory [15], an evolution equation for the reduced
spin density matrix $\rho_s(t)$ can be deduced from the Liouville equation for $\rho(t)$ by using for instance standard projection operators techniques. One assumes, as usual, that the initial density matrix $\rho(t_0 = 0)$ is factorized, i.e., that

$$\rho(0) = \rho_b \rho_s(0)$$

(20)

where $\rho_b$ is the equilibrium bath density matrix. The time rate of change $\langle \partial \rho_s/\partial t \rangle$ then comprises only two terms: one is a proper evolution term, and the other one is a relaxation term, due to the interaction with the bath. As pointed out by several authors [16-19], this relaxation term can be given two forms, either the usual time-convolution or retarded form, or a « time-convolutionless » (i.e., non retarded) one. Clearly both forms are exact as long as no supplementary approximations are made; however, in what follows, we would like to consider the interaction between the system and the bath in $\hat{H}$ (the $H_{int}$ term) as a perturbation. The calculation will be restricted to the Born approximation (1). It has been argued [16-19] that, from the point of view of a systematic expansion, the time-convolutionless formalism prevails over the usual convolution one, since in the latter formalism, a certain amount of rearrangement of the terms is necessary to obtain a coherent expansion to a given order. This is the fundamental reason why, besides its greater practical simplicity, we preferred the time-convolutionless formalism.

Following van Kampen [16] and Hashitsume et al. [18], as long as two time scales can clearly be delineated, in other words, as long as there is a short time scale $\tau_s$, characteristic of the relaxation kernel, and a long time scale $\tau_o$, characteristic of the operator of interest (here the density matrix $\rho_s(t)$), one can write, for times $t \gg \tau_o$, a time-convolutionless evolution equation for $\rho_s(t)$ which takes the form of a systematic expansion with respect to the perturbation

$$H'_{int} = H_{int} - \langle \rho_{int} \rangle_b$$

(21)

where $\langle \cdots \rangle_b$ stands for $\text{Tr}_b \rho_s \cdots$. The time-convolutionless equation for $\rho_s(t)$ takes the form, in the Born approximation

$$\langle \partial \rho_s/\partial t \rangle = -\frac{i}{\hbar} \langle \rho_{int} \rangle_b \rho_s + \frac{1}{\hbar^2} \int_0^t \text{d}t' \text{Tr}_b \{[H'_{int}, \rho_s(t)] \rho_b \rho_{int}(-t')\} + \text{h.c.}$$

(22)

where $H'_{int}(-t')$ is written in the interaction representation. It is easy to give equation (22) a more explicit form by detailing $H_{int}$ and $H'_{int}(-t')$. One obtains

$$\langle \partial \rho_s/\partial t \rangle = \frac{i\omega_0}{2} \langle B_+ \rho_b [\sigma_+, \rho_s] + \text{h.c.} \rangle + (\phi_{++}(t) [\sigma_+, \rho_s \sigma_+] + \phi_{+-}(t) [\sigma_+, \rho_s \sigma_-] + \phi_{-+}(t) [\sigma_-, \rho_s \sigma_+] + \phi_{--}(t) [\sigma_-, \rho_s \sigma_-] + \text{h.c.})$$

(23)

where the relaxation functions $\phi_{++}(t)$, $\phi_{+-}(t)$, $\phi_{-+}(t)$ and $\phi_{--}(t)$ are defined as

$$\phi_{++}(t) = \left(\frac{i\omega_0}{2}\right)^2 \int_0^t \text{d}t' \langle (B_+(-t') - \langle B_+ \rangle_b)(B_+ - \langle B_+ \rangle_b) \rangle_b$$

$$\phi_{+-}(t) = \left(\frac{i\omega_0}{2}\right)^2 \int_0^t \text{d}t' \langle (B_-(-t') - \langle B_- \rangle_b)(B_+ - \langle B_+ \rangle_b) \rangle_b$$

$$\phi_{-+}(t) = \left(\frac{i\omega_0}{2}\right)^2 \int_0^t \text{d}t' \langle (B_+(-t') - \langle B_+ \rangle_b)(B_- - \langle B_- \rangle_b) \rangle_b$$

$$\phi_{--}(t) = \left(\frac{i\omega_0}{2}\right)^2 \int_0^t \text{d}t' \langle (B_-(-t') - \langle B_- \rangle_b)(B_- - \langle B_- \rangle_b) \rangle_b$$

(24)

Remember that the operators $B_{\pm}(t)$ are computed in the non-interacting scheme for the bath. Equations (22) to (24) constitute general relaxation equations; note that they are valid whatever the precise form of the dissipation, ohmic or non ohmic. Let us now examine the consequences of the ohmic constraint (7) on the relaxation equation of the reduced spin density matrix $\rho_s(t)$.

### 3.3 Time Evolution of the Reduced Spin Density Matrix $\rho_s(t)$ in the Ohmic Model

At first, let
us calculate the average value
\[ \langle B_\pm \rangle_b = \left\langle \exp \left\{ \pm 2 \sum_n \frac{G_n^2}{\omega_n^2} (b_n^\dagger - b_n) \right\} \right\rangle. \] (25)

Since \( b_n^\dagger \) and \( b_n \) are boson operators, one gets
\[ \langle B_\pm \rangle_b = \exp \left( -2 \sum_n \frac{G_n^2}{\omega_n^2} \coth \frac{\beta \hbar \omega_n}{2} \right); \quad \beta = 1/k_B T. \] (26)

When the ohmic constraint (7) is imposed, the exponent in equation (26) is seen to diverge, for \( T = 0 \), as well as for finite temperature, so that \( \langle B_\pm \rangle_b \) is equal to zero in this model. Let us however emphasize here that the ohmic model is not the only one in which \( \langle B_\pm \rangle_b = 0 \). Any model of dissipation in which \( \rho(\omega) \propto G(\omega)^2 \propto \omega^\delta \) with \( \delta \leq 1 \) at zero temperature or \( \delta \leq 2 \) at finite temperature will share this property. This point, and, more generally, the question of the specificity of the ohmic dissipation model, will be discussed later on in detail (see Sect. 6).

Thus, in the ohmic model, the relaxation equation (23) of the reduced spin density matrix \( \rho_s(t) \) considerably simplifies. It is then straightforward to deduce from equation (19) the equation of motion of \( \langle \sigma_z(t) \rangle \). This will be achieved in the following paragraph.

3.4 Spin Dynamics. — In order to obtain a detailed expression, it is necessary to calculate the relaxation function \( \phi(\tau) \), which, in the ohmic model, are just time-integrals of the correlation functions of the operators \( B_\pm(t) \), expressed in the non-interacting scheme. By using the commutation relations between the Pauli matrices and the symmetry properties of the \( \phi(\tau) \), one gets a closed equation for \( \langle \sigma_z(t) \rangle \):
\[ \frac{d\langle \sigma_z(t) \rangle}{dt} = -A(t) \langle \sigma_z(t) \rangle \] (27)

where \( A(t) \) is defined as
\[ A(t) = \omega_0^2 \int_0^t dt' \cos \left( A_1(t') \right) \exp(-A_2(t')). \] (28)

with
\[ A_1(t) = 4 \sum_n \frac{G_n^2}{\omega_n^2} \sin \omega_n t \] (29)

and
\[ A_2(t) = 4 \sum_n \frac{G_n^2}{\omega_n^2} \left( 1 - \cos \omega_n t \right) \coth \frac{\beta \hbar \omega_n}{2}. \] (30)

Equations (27) to (30) constitute our basic equations; they contain explicitly all the dynamics of the spin. Note that the exponential time behaviour found by Chakravarty and Leggett ([10a]) is simply obtained from equations (27) and (28) by rejecting \( t \) to infinity in the integral (28); in our context, this corresponds to a short memory approximation. Using the exponential cut-off introduced by the same authors:
\[ f_c(\alpha/\omega_s) = \exp(-\alpha/\omega_s) \] (31)
in the ohmic constraint (7), one can calculate simply the functions \( A_1(t) \) and \( A_2(t) \):
\[ A_1(t) = 2 \alpha \tan^{-1} (\omega_s t) \] (32a)
\[ A_2(t) = \alpha \ln(1 + \omega_s^2 t^2) + 2 \alpha \ln \prod_{n=1}^{\infty} \left( 1 + \frac{\omega_s^2 t^2}{1 + n \beta \hbar \omega_s} \right)^2. \] (32b)

For \( k_B T \ll \hbar \omega_s \), expression (32b) for \( A_2(t) \) reduces to:
\[ A_2(t) = \alpha \ln(1 + \omega_s^2 t^2) + 2 \alpha \ln \left( \frac{\sinh(t/\tau)}{t/\tau} \right) \] (33)
\( \tau \) is the « temperature time », as defined by
\[ \tau = \pi^{-1} \hbar \beta. \] (34)

Equation (28) then yields
\[ A(t) = \omega_0^2 \Re \int_0^\infty dr' \left( 1 - \omega_s t' \right)^{-2x} \left( \frac{t'/\tau}{\sinh(t'/\tau)} \right)^{2x}. \] (35)

The explicit dynamics of \( \langle \sigma_z(t) \rangle \) can now be found by integrating equation (27). Let us present and physically discuss the results we obtain for \( \langle \sigma_z(t) \rangle \). This will be done successively for zero and for finite temperature.

3.4.1 Zero-temperature case. — When the temperature is equal to zero, expression (35) for \( A(t) \) reduces to
\[ A(t) = \omega_0^2 \Re \int_0^\infty dr' \left( 1 - \omega_s t' \right)^{-2x} \] (36)

and the solution of equation (27) is easily obtained in a closed form:
\[ \Sigma(t) \equiv \langle \sigma_z(t) \rangle = \exp \left\{ \frac{\omega_0^2}{4 x} \frac{1}{(a-1/2)(1-a)} \times \right. \]
\[ \times \left( 1 - \cos \left( \frac{2(1-a) \tan^{-1} (\omega_s t)}{1 + \omega_s^2 t^2} \right) \right). \] (37)

(Note that for the particular values \( a = 1/2 \) and \( x = 1 \) the preceding expression of \( \Sigma(t) \) is still valid provided the limits are correctly taken.)

In the meaningful time domain \( \omega_s t \gg 1 \), \( \Sigma(t) \) takes
the simpler form:

\[
\Sigma(t) \approx \exp \left\{ \frac{\omega_0^2}{4 \omega_c^2} \frac{1}{(\alpha - 1/2)(1 - \alpha)} \left(1 + (\cos \alpha \pi) (\omega_c t)^{2(1 - \alpha)} \right) \right\}
\]

\[
\approx (\omega_c t)^{-a_0^2/\omega_c^2} \exp \left(- \pi \frac{\omega_0^2}{\omega_c^2} \omega_c t \right) \quad (\alpha = 1)
\]

\[
\approx (\omega_c t)^{a_0^2/\omega_c^2} \exp \left(- \frac{\pi}{2} \frac{\omega_0^2}{\omega_c^2} \omega_c t \right) \quad (\alpha = 1/2)
\]

(i) As long as \( \alpha \leq 1, \Sigma(+\infty) \) is equal to zero. In terms of the particle evolving in the double-well potential, this means that its average position at infinite time is equal to zero. Therefore, in this regime, the particle can be said to be delocalized, albeit no oscillation does appear. However, since for \( \alpha = 0 \), the situation evidently reduces to the pure quantum situation in which the particle oscillates back and forth between the two wells, it is likely that the present calculation is no more valid for too low values of the coupling; this will be discussed later.

(ii) When \( \alpha \) becomes greater than 1, \( \Sigma(+\infty) \) takes a finite value, given by

\[
\Sigma(+\infty) = \exp \left\{ - \frac{\omega_0^2}{4 \omega_c^2} \left( (\alpha - 1/2)(\alpha - 1) \right) \right\}.
\]

The average position at infinite time of the particle evolving in the double-well potential is then different from zero. The particle is thus partly localized on the side where it was at time \( t = 0 \).

The degree of localization, which can be characterized by the value of \( \Sigma(+\infty) \), is a continuous function of \( \alpha \), which grows very rapidly (i.e. on a region of width \( \sim (\omega_0/\omega_c)^2 \)) towards 1 as soon as \( \alpha \) exceeds 1. Therefore, this system does display a continuous symmetry breaking at the value \( \alpha = 1 \) of the coupling; however, the symmetry is fully broken (i.e. \( \Sigma(+\infty) = 1 \)) only for infinite coupling, which seems a physically sensible result (see Fig. 1).

The symmetry breaking can be described in the phase transition language, the inverse coupling parameter \( \alpha^{-1} \) playing the rôle of the temperature, and \( \Sigma(+\infty) \) acting as the order parameter. This phase transition is of infinite order (see Eq. (39)), and the width of the critical region is of order \( (\omega_0/\omega_c)^2 \), i.e. very narrow. This is to be compared with the result of references [3, 4] in which a discontinuous transition at \( \alpha = 1 \) is found. Note however that, for \( \omega_c \to \infty \), \( \Sigma(+\infty) \) in our calculation will also present a jump at \( \alpha = 1 \).

The time-dependence of \( \Sigma(t) \) reveals very interesting features. The full time-dependence of \( \Sigma(t) \) is given by equation (37); however, it is sufficient to analyse formula (38) which corresponds to the meaningful domain \( \omega_c t \gg 1 \). The following characteristics appear:

(i) As long as \( \alpha < 1/2 \), \( \Sigma(t) \) relaxes towards zero more rapidly than a pure exponential, i.e. \( \Sigma(t) \sim \exp(-at^b), \ b > 1 \).

(ii) For \( \alpha = 1/2 \), \( \Sigma(t) \) has a purely exponential behaviour.

(iii) When \( 1/2 < \alpha < 1 \), \( \Sigma(t) \) has a stretched exponential form; in other words, it evolves according to the so-called Kohlrausch law \( \Sigma(t) \sim \exp(-at^b), \ 0 < b < 1 \). Such laws are believed to occur in a wide range of phenomena and materials, and to contain the essential physics of relaxation in complex, strongly interacting materials [20, 21]. This law appears here as a consequence of the ohmic dissipation model, and manifests itself in a certain range of values of the coupling constant.

(iv) As \( \alpha \) approaches 1 from below, the relaxation of \( \Sigma(t) \) towards zero is slower and slower. At \( \alpha = 1 \), the relaxation is seen to take the power law form \( (1 + \omega_c^2 t^2)^{-a_0^2/\omega_c^2} \); since \( \omega_0/\omega_c \ll 1 \), it is extremely slow; this can be viewed as a critical slowing down.

(v) For \( \alpha > 1 \), \( \Sigma(t) \) starts from 1 and goes uniformly very slowly to its final value \( \leq 1 \); \( \Sigma(t) \) behaves as \( \exp(-at^b), \ b < 0 \).

So in all cases, one can say that the relaxation of \( \Sigma(t) \) follows for \( \omega_c t \gg 1 \) a « generalized » Kohlrausch law; the corresponding curves are plotted on figure 2. To give an idea of the extremely slow character of the evolution of \( \Sigma(t) \) when \( \alpha > 1 \), let us indicate some orders of magnitude. For instance, when \( \alpha = 1.02 \), \( \Sigma(+\infty) = 0.786 \) and \( \Sigma(\omega_c t = 10^{19}) = 0.865 \). If \( \omega_c \sim 10^{13} \text{s}^{-1} \), which is a typical phonon
frequency, this corresponds to a macroscopic time \( t \sim 10^{-3} \text{s} \), for which \( \Sigma(t) \) is still relatively far from its final value. This behaviour is clearly apparent on figure 3, which displays the variations of \( \Sigma(t) \) for \( \alpha = 1.02 \) and \( \alpha = 0.9 \).

3.4.2 Finite temperature case. — In this case, \( \Lambda(t) \) is given by equation (35) and then it is not easy to derive from equation (27) a closed form expression for \( \Sigma(t) \). Thus one must in general resort to a numerical integration.

However, an asymptotic formula, valid for times \( t > \tau/2 \alpha \), can be obtained. Indeed, provided that \( \tau \) is finite, the upper bound of the integral in equation (35) can be extended to infinity when \( t > \tau/2 \alpha \). One thus gets in this time domain

\[
\langle \sigma_1(t) \rangle \approx -\Lambda(\infty) \langle \sigma_0(t) \rangle
\]

or

\[
\langle \sigma_2(t) \rangle = \text{Const.} \cdot e^{-\Lambda(\infty) t}.
\]

The rate \( \Lambda(\infty) \) can easily be calculated:

\[
\Lambda(\infty) = \Re \omega_0^2 \int_0^\infty dt' (1 - i \omega_c t')^{-2a} \left( \frac{t'}{(t'/\tau)^{1/2}} \right)^{2a}
\]

or

\[
\frac{\omega_0^2}{\omega_c^2} \frac{\Gamma(\alpha)}{2 \Gamma(\alpha + 1/2)} (\omega_c \tau)^{1-2a} \left( 1 + 0(1/\omega_c \tau) \right)
\]

where \( \Gamma \) denotes the standard Euler's gamma function. Besides, one can verify, by directly expanding the integral expression for \( \langle \sigma_2(t) \rangle \) which can be deduced from equation (35), that the constant in equation (41) is indeed equal to \( \langle \sigma_2(0) \rangle \). This calculation thus shows that, at finite temperature, \( \langle \sigma_2(t) \rangle \) relaxes towards zero in an exponential manner as soon as \( t \gg \tau/2 \alpha \).

Moreover, equation (35) also proves that the effect of temperature on the time evolution of \( \langle \sigma_2(t) \rangle \) is negligible as long as \( t \ll \tau/2 \alpha \); in other words, on this time range, the behaviour of \( \langle \sigma_2(t) \rangle \) is the same as at zero temperature.

Stricto sensu, the symmetry breaking disappears at finite temperature: whatever the value of \( \alpha \) (greater or lower than 1, provided our calculation should be valid, a condition which only excludes low values of \( \alpha \), as it will be seen later, and perhaps the vicinity of 1), \( \Sigma(t) \) goes to zero as \( t \to \infty \). The particle in the double-well potential is always delocalized. However, the « relaxation time », as defined by

\[
T_R = 1/\Lambda(\infty) \sim \tau^{-1-2a}
\]

has for limit value as \( T \to 0 \), either 0 (when \( \alpha < 1/2 \)), or \( \infty \) (when \( \alpha > 1/2 \)). This is related to the corresponding zero-temperature behaviour of \( \langle \sigma_1(t) \rangle \) as mentioned above in 3.4.1. For \( T > 0 \), one could naively expect that the decay time of \( \langle \sigma_1(t) \rangle \) should be of the order of \( \tau \). However, equations (41) and (43) show that this time is renormalized by a factor

\[
\left( \frac{\sqrt{\pi}}{2} \frac{\Gamma(\alpha)}{\Gamma(\alpha + 1/2)} \left( \frac{\omega_0}{\omega_c} \right)^{1-2a} \right)^{-1}
\]

which, for \( \alpha > 1 \), becomes extremely large when \( T \to 0 \). The spin thus displays a behaviour which is a precursor of the zero-temperature transition at \( \alpha = 1 \). It can be seen that, at finite temperature, the relaxation of \( \Sigma(t) \) takes place on a microscopic time even when \( \alpha > 1 \). Let us consider for instance the case \( \alpha \gtrsim 1 \). When \( \omega_c \tau = 10 \), which for \( \omega_c \sim 10^{13} \text{s}^{-1} \) corresponds to a temperature \( T \sim 2.4 \text{K} \), one gets \( \omega_c T_R = 10^3 \) or \( T_R \sim 10^{-10} \text{s} \). Thus it is only for extremely low values of the temperature that \( T_R \) would take macroscopic values; for instance, for \( T \sim 2.4 \times 10^{-7} \text{K} \), one would get \( T_R = 10^{-3} \text{s} \).

The curves representing \( \langle \sigma_2(t) \rangle \) as a function of \( t \) for different values of \( \alpha \) are plotted on figure 4. These curves have been obtained by numerical integration of equation (27), with \( \Lambda(t) \) given by equation (35). By comparison with the corresponding \( T = 0 \) curves (Fig. 2), two trends are observed: for relatively high values of the coupling, \( \langle \sigma_1(t) \rangle \) closely follows the exponential law as given by equation (41), but for relatively small \( \alpha \) values, the dynamics appears to be quite similar to the dynamics at \( T = 0 \). These two trends will be confirmed by a
more detailed quantitative analysis, which will be done in the following paragraph.

3.5 Conditions of validity of the treatment. — Let us now precise the conditions under which the convolutionless equation (27) and the results which were derived from it in the two preceding paragraphs are valid. Our discussion will follow the arguments developed by van Kampen [16] and by Hashitsume et al. [18], and will be carried out successively for zero and for finite temperature.

3.5.1 Zero-temperature case. — When \( T = 0 \), an exact analytical solution of equation (27) can be found (Eqs. (37) and (38)). Thus it is sufficient to discuss the conditions of validity of the convolutionless equation itself. As already indicated, this equation is valid as long as two time scales can be clearly delineated: the short one, \( \tau_c \), which characterizes the relaxation kernel, and the long one, \( \tau_m \), which characterizes the operator of interest (here \( \langle \sigma_z(t) \rangle \)).

Since the two functions to be considered are not just exponential functions, it is not so simple to assign to them well-defined time scales, all the more as they possess different time dependences. However, one can roughly define \( \tau_c \) as the time after which the relaxation kernel \((1 + \omega_c^2 t^2)^{-\alpha}\) (see Eq. (36)) has decreased by a factor \( 1/e \), which yields:

\[
\tau_c \sim \omega_c^{-1} (e^{1/\alpha} - 1)^{1/2}.
\]  

(45)

One must have \( \tau_c \ll \tau_m \), where \( \tau_m \) is linked to \( \langle \sigma_z(t) \rangle \). For \( \alpha > 1 \), this condition is automatically satisfied, since the time scale of \( \langle \sigma_z(t) \rangle \) is extremely long, as indicated above. For \( \alpha < 1 \), equation (38) approximately yields:

\[
\tau_m \sim \omega_0^{-1} (\omega_0/\omega_c)^{-\mu(1-\alpha)}.
\]

(46)

Note that \( \tau_m^{-1} \) is the so-called renormalized tunnelling frequency appearing in equation (15) of reference [10a]. The separation of time scales implies that:

\[
(e^{1/\alpha} - 1)^{1/2} \ll (\omega_0/\omega_c)^{1/(1-\alpha)}
\]

and, for \( \omega_0/\omega_c \gg 1 \), this can be rewritten as:

\[
1/\alpha \ll 2 \ln (\omega_0/\omega_c).
\]

(47)

The separation of the two time scales also means that the renormalized tunnelling frequency has to be small as compared to the bare one; in other words, the effective tunnelling time \( \tau_m \) must be great in comparison with the relaxation time of the bath as measured by \( \tau_c \).

Our calculation thus has a wide range of applicability since, according to equation (47), only values of \( \alpha \) near zero are excluded. When the condition (47) is satisfied, the convolutionless equation (27) and its solution are valid for times \( t \gg \tau_c \), as long as the expansion parameter \( \omega_0/\omega_c \) is small, i.e.:

\[
(\omega_0/\omega_c)(e^{1/\alpha} - 1)^{1/2} \ll 1.
\]

(48)

Note that, for high \( \alpha \) values, the expansion parameter reduces to \( \omega_0/\sqrt{\alpha} \omega_c \) (an effectively small quantity in the model), whereas, for small \( \alpha \) values, it is approximately equal to \( (\omega_0/\omega_c) e^{1/2\alpha} \), this latter quantity being indeed small as long as the separation of time scales, as given by equation (47), is achieved.

3.5.2 Finite temperature case. — The discussion of the validity of the convolutionless equation (27) at finite temperature is more involved; indeed, the solution of equation (27) has been obtained through a numerical integration, which renders uneasy the discussion of the separation of time scales. However, as shown above, in certain cases, analytical approximations of the solution can be given, which then simplifies the discussion.

Let us first define the short time scale at finite temperature. The relaxation kernel (see Eq. (35)) is the product of two functions, one of which being the relaxation kernel at \( T = 0 \), \((1 + \omega_c^2 t^2)^{-\alpha}\), of time scale \( \tau_c \) (Eq. (45)), and the other one, \((t/\tau_c)^2 / \sinh (t/\tau_c)^2\), decreasing approximately on a time scale of the order \( \tau/2 \alpha \). One can thus roughly define the short time scale at finite temperature as \( \min(\tau_c, \tau/2 \alpha) \).

Since for times \( t \gg \tau/2 \alpha \), \( \langle \sigma_z(t) \rangle \) approximately relaxes according to an exponential law of time constant \( T_R \) (see Eq. (41)), this approximation would be meaningful for nearly the whole time domain provided that:

\[
\tau/2 \alpha \ll T_R.
\]

(49)

Condition (49) is fulfilled in the region above the solid curve 1 of the \((\alpha, T)\) plane (see Fig. 5). In this region, the condition of separation of time scales is automatically realized, which in turn insures the validity of the convolutionless equation itself.

As explained in paragraph 4, the \( \alpha \) behaviour of \( \langle \sigma_z(t) \rangle \) in the time range \( t \leq \tau_c/2 \alpha \) is the same as at zero temperature. Therefore, as long as:

\[
\tau_m \ll \tau_c/2 \alpha
\]

(50)

\( \langle \sigma_z(t) \rangle \) is well represented by its zero-temperature expression, of time scale \( \tau_m \). Condition (50) is fulfilled in the region below the solid curve 2 of the \((\alpha, T)\) plane (see Fig. 5). In contradistinction to the preced-
ing case, the condition of separation of time scales is not automatically realized. In particular, when \( \min(\tau_c, \tau/2) / \tau/2 \alpha \), the calculation is inconsistent, which excludes the region of the \((\alpha, T)\) plane below the dotted curve 3. Once this region has been excluded, the condition of separation of time scales reduces to the zero-temperature condition \( \tau_c \approx T \) discussed above, which excludes the region of the \((\alpha, T)\) plane below the horizontal broken line 4 (see Fig. 5).

Combining all these results delineates the validity domain (non hatched region of Fig. 5).

4. Weak coupling case.

As previously explained, the weak-coupling case \( \alpha \ll 1 \) cannot be treated by the method outlined above and a different approximation scheme has to be followed. When \( \alpha \) is very small, it can safely be assumed that, at any time, the bath can at most deviate by one excitation from its equilibrium state; this single boson assumption, discarding multiple scattering processes, should be valid when the lifetime of any created phonon is quite small as compared to all other pertinent times. Moreover, we only consider the zero-temperature case where the quantum coherence is best displayed; the \( T \approx 0 \) situation could be treated along the same line.

The central quantity to be calculated is the effective time evolution operator \( U \) for the spin dressed with the phonons; then, \( \Sigma(t) = \langle \sigma_x(t) \rangle \langle \sigma_x(0) \rangle \) can be written as:

\[
\Sigma(t) = \text{Re} \ U^*_+ U_-(t) \tag{51}
\]

where \( U_{\pm} \) are the matrix elements of \( U \) on the \(| \pm \rangle \) eigenstates of \( \sigma_x \).

A convenient way to obtain these matrix elements is to first calculate as usual the Fourier transform \( G(z) = 1/(z - H) \) [22] such that

\[
U(t > 0) = (2\pi t)^{-1} \int_{C_+} \, dz \, e^{-izt/H} G(z) \tag{52}
\]

where \( C_+ \) is a contour extending from \(+\infty\) to \(-\infty\) just above the real axis. From the spin-boson Hamiltonian (5), it is seen that, within the single boson approximation, the renormalized propagators have the form:

\[
G_{++}(z) = (z - \hbar\omega_0 - R(z))^{-1} \tag{53}
\]

\[
G_{--}(z) = (z - \hbar\omega_0) R(z) \tag{54}
\]

where \( R(z) = \sum_n (\hbar G_n)^2/(z - \hbar\omega_n) \) is a function depending, \textit{inter alia}, on the cut-off function \( f_\alpha \) (see Eq. (7)); as explained above, for times such that \( \omega_0 t \gg 1 \), the precise form of \( f_\alpha \) has no bearing on the dynamics of the system. We here choose a Lorentzian cut-off function \( \left( 1 + \left( \omega_0 / \omega_0^* \right)^2 \right)^{-1} \); then, \( R(z) \) can be given an explicit expression (2):

\[
R(z) = \frac{1}{\pi} \int f_\alpha(\omega/\omega_0) \left( \ln \frac{z}{\hbar\omega_0} - \text{Im} \right) - \frac{\pi}{2} \hbar\omega_0 \right) \tag{55}
\]

In this expression, \( \text{Im} \) denotes the logarithm branch such that \( 0 \leq \text{Im} \ln < 2\pi \). So, as usual, \( G_{++} \) has a cut extending from \( 0 \) to \( +\infty \) on the real axis but no other singularity in the first Riemann sheet. On the other hand, its analytical continuation into the second sheet does have a pole, \( z_+ \), with a negative imaginary part. When \( \alpha \) increases from zero, \( z_+ \) starts from \( \hbar\omega_0 \) and follows a curve merging with the real axis at the origin for \( \alpha = \alpha_0 \approx 4/\omega_0/\omega_0^* \). \( G_{--} \) is easily seen to have a cut from \( \hbar\omega_0 \) to \( +\infty \) and a real negative pole \( z^- \) starting from zero \( \alpha = 0 \), with an ever increasing magnitude when \( \alpha \) increases.

The inverse relation (52) is now used to obtain \( U_{++} \) and \( U_{--} \). The integral can be calculated via the residue theorem but, because of the cuts of \( G_{++} \) and \( G_{--} \), two additional contributions (denoted by \( \Sigma_{\pm}(t) \)) arise besides the residues [22]. Thus one has:

\[
\Sigma(t) = \text{Re} \left\{ \left( A_+ e^{-i\omega t} + C_+ \right) \times \left( A_- e^{-i\omega t} + C_+ \right) \right\} \tag{56}
\]

In the limit \( \alpha \ll 1 \), approximate closed expressions can be easily obtained for the various quantities appearing in equation (56). In particular the poles \( z_{\pm} \) are such that

\[
z_+ = \hbar\omega_0 \frac{1 - \pi \omega_0 \omega / 4 \omega_0^*}{1 + \pi \omega_0 \omega / 2 (\omega_0 / \omega_0^*) + \pi \omega_0 \omega / 2} + 0(\alpha \ln \alpha) \tag{57}
\]

(2) Had we chosen an exponential cut-off function, \( R(z) \) would have contained an exponential integral function, which in the meaningful frequency domain would imply the same type of behaviour of \( R(z) \) as given by equation (55).
In the same limit, the coefficients $A_\pm$ (quite close to 1) are given by

$$z_- = -\hbar \omega_0 \frac{\alpha (\pi \omega_\epsilon/2 \omega_0 - \ln (\omega_\epsilon/\omega_0))}{1 + \frac{\alpha}{2} (\ln (\omega_\epsilon/\omega_0) - 1)} + 0(\alpha \ln \alpha)$$

(58)

In the same limit, the coefficients $A_\pm$ (quite close to 1) are given by

$$A_+ = \left(1 + \frac{\alpha}{2} (\ln (\omega_\epsilon/\omega_0) + i \pi - 1)\right)^{-1} + 0(\alpha \ln \alpha)$$

(59)

$$A_- = \left(1 + \frac{\alpha}{2} (\ln (\omega_\epsilon/\omega_0) - 1)\right)^{-1} + 0(\alpha \ln \alpha).$$

(60)

In the limit $\omega_\epsilon |t| \gg 1$, the contributions $\zeta_\pm(t)$ can be analysed and both have an asymptotic expansion starting with a $t^{-2}$ term:

$$\zeta_+(t) = -\frac{\alpha}{2} \frac{1}{(\pi \omega_\epsilon) (\omega_\epsilon t)^{-2} + 0(\omega_\epsilon t)^{-4}}$$

(61)

$$\zeta_-(t) = -\frac{\alpha}{2} \frac{\omega_0 \omega_\epsilon}{(\pi \omega_\epsilon)^2} (\omega_\epsilon t)^{-2} + 0(\omega_\epsilon t)^{-4}.$$  

(62)

Combining all these expressions, $\Sigma(t)$ can be written as:

$$\Sigma(t) = e^{-\gamma t} \left\{ (1 - \alpha (\ln (\omega_\epsilon/\omega_0) - 1)) \cos \omega_\epsilon t - \frac{\pi \omega_\epsilon}{2} \sin \omega_\epsilon t \right\} - \frac{\alpha}{2} (\omega_\epsilon t)^{-2} + \ldots$$

(63)

where the dots stand for small corrections of higher order in $\alpha$ and/or $(\omega_\epsilon t)^{-2}$. In equation (69), the decay rate $\gamma$ and the renormalized frequency $\omega_\sigma$ are

$$\gamma = \frac{\pi \omega_\epsilon}{2} + 0(\alpha \ln \alpha)$$

(64)

$$\omega_\sigma = \omega_0 (1 - \alpha (\ln (\omega_\epsilon/\omega_0)) + 0(\alpha \ln \alpha).$$

(65)

Finally, note that, were $\alpha$ greater than $\omega_\epsilon$, no imaginary part would appear in the time-dependent exponentials in equation (56); the only (small) imaginary contributions come from $\zeta_+$ and $\zeta_-$. Physically, this means that, if the coupling is strong enough, the dressed spin appears to be a quasi-stable entity somehow analogous to a polaron. However, since we are concerned with the $\alpha \to 0$ limit, we will not further consider this polaron-like effect (all the more as the validity of the single-boson approximation could even be dubious in such a case).

5. Comparison with previous results on the dynamics.

Many authors have discussed the spontaneous symmetry breaking which occurs at $T = 0$ for the particle in the double-well potential. However, as indicated in the introduction, in most papers, the dynamics has not been investigated in detail. Therefore, we shall restrict the discussion to a comparison with the results of Zwerger [9] and of Chakravarty and Leggett [10a] about the dynamics.

5.1 Zero-temperature results.

Let us now briefly recall the results of references [9] and [10a]. In reference [9], Zwerger carries out a linear response calculation, which leads him to conclude that, for any coupling strength $\alpha \geq \omega_\epsilon/\omega_\sigma$, the coherence is almost completely destroyed; beyond this value of the coupling, he finds an essentially incoherent relaxation, following an exponential law of time constant $\omega_\epsilon^{-1}$, where $\omega_\epsilon$ is the so-called renormalized tunnelling frequency, as given by $\omega_\epsilon = \omega_0 (\omega_\epsilon/\omega_0)^{1/2}$. As far as they are concerned, Chakravarty and Leggett [10a] find that for $0 < \alpha < 1/2$ the coherent oscillations of the uncoupled system do persist, while for $1/2 < \alpha < 1$ they assess that the essentially incoherent relaxation follows an exponential law with a rate $\sim \omega_\epsilon$.

Our results, presented in sections 3 and 4, show, in agreement with Zwerger's ones, that the coherent oscillations persist only for very low values of the coupling (i.e. $\alpha \leq \omega_\epsilon/\omega_\sigma$); in this region, the behaviour we find for the mean value $\langle \sigma_\epsilon(t) \rangle$ is very similar to that found by Chakravarty and Leggett, i.e. a damped oscillating part plus a negative power-law time tail. When $1/2 \ln (\omega_\epsilon/\omega_0) \ll \alpha < 1$, — the former being a small number in the problem —, we find that $\langle \sigma_\epsilon(t) \rangle$ decays according to a generalized Kohlrausch law (i.e. $\sim \exp(-\omega_\epsilon t)$), more rapidly or more slowly than a pure exponential, depending on whether $\alpha < 1/2$ or $\alpha > 1/2$. It is worthwhile to note that the inverse time scale $\tau_\epsilon^{-1}$ of $\langle \sigma_\epsilon(t) \rangle$ in our calculation (see formula (46)) is precisely identical to the renormalized tunnelling frequency $\omega_\epsilon$, appearing in references [9] and [10a]. In other words, once the coupling strength is sufficient in order for the oscillating behaviour of $\langle \sigma_\epsilon(t) \rangle$ to have disappeared, we predict, instead of the exponential relaxation of $\langle \sigma_\epsilon(t) \rangle$ mentioned in references [9] and [10a] a generalized Kohlrausch law decay of $\langle \sigma_\epsilon(t) \rangle$, becoming slower and
slower as the coupling constant approaches from below the value $\alpha = 1$ at which the transition towards a localized regime takes place. For $\alpha > 1$, $\langle \sigma_z(t) \rangle$ decreases towards a finite value, showing that the particle is on the average partly localized on the side where it was at time $t = 0$. In addition, we also give the dynamics above the transition point. When $\alpha > 1$, we find an «infinite» time scale $\tau_m$ for $\langle \sigma_z(t) \rangle$, in accordance with $\tau_m = \omega_0^{-1}$ where $\omega_0 = 0$ for $\alpha > 1$ as indicated in reference [10a].

5.2 Finite temperature results. — In the finite temperature case, Chakravarty and Leggett [10a] find an exponential relaxation of $\langle \sigma_z(t) \rangle$ with a time constant which is identical to our «relaxation time» $T_R$ as defined by formula (44). Essentially similar results are given by Zwerger [9]. Moreover, the calculation by Chakravarty and Leggett is shown to be valid under a condition of separation of time scales which is precisely identical to the condition (49) under which we find an asymptotic exponential relaxation of $\langle \sigma_z(t) \rangle$. However, one must emphasize that it is only in an asymptotic regime, i.e. for times $t \gg 1/\alpha$ that $\langle \sigma_z(t) \rangle$ in our calculation displays this exponential behaviour, its full time-dependence, as yielded by equations (27) and (35), being more complicated.

To conclude this section, we shall say that our methods thus allow for a more detailed description of the real-time dynamics, and this for any value of the coupling, including the vicinity of the transition point, where a critical slowing down is very clearly displayed and appears as a limiting case of a stretched Kohlrausch law. As for the coherent behaviour, it is seen in a simple way to persist only for very low values of the coupling.

6. Specificity of the ohmic dissipation model.

In the preceding sections, we used the ohmic dissipation model, as defined by equation (7). In such a framework, a symmetry breaking takes place at zero temperature for $\alpha > 1$. Now the following natural question arises: is this «phase transition» specific to the ohmic dissipation model, or can it happen in other types of dissipative situations?

In order to answer this question, we shall use, instead of equation (7), the relation

$$\rho(\omega) = \frac{\alpha}{2} \frac{\omega^\delta}{\omega_0^{\delta-1}} f_\xi(\omega/\omega_0)$$

where the exponent $\delta$ reduces to 1 in the ohmic dissipation case.

As already indicated, when the ohmic constraint (7) is imposed, the averages values $\langle B_z \rangle$ are equal to zero, and $\langle \sigma_z(t) \rangle$ obeys the closed equation of motion (27). However, when $\delta \leq 1$ (at zero temperature) or when $\delta \leq 2$ (at finite temperature), this property still holds and equation (27) for $\langle \sigma_z(t) \rangle$ remains appropriate, provided nonetheless that the functions $A_1(t)$ and $A_2(t)$ are finite; this clearly imposes a lower limit on the exponent $\delta$. One readily sees indeed that $A_1(t)$, which is temperature-independent, is finite for $\delta > 0$, and that $A_2(t)$, which depends on the temperature, is finite for $\delta > -1$ (at zero temperature) or for $\delta > 0$ (at finite temperature). In short, the closed equation of motion (27) for $\langle \sigma_z(t) \rangle$ is valid in the range $0 < \delta \leq 1$ (at zero temperature) or in the range $0 < \delta < 1$ (at finite temperature). Since however the symmetry breaking is a zero-temperature property of the ohmic model and disappears at any finite temperature, it is sufficient for our purpose to analyse the zero-temperature case with the hypothesis (66).

When $T = 0$, with the assumption (66), the expression of $A(t)$ takes the form

$$A(t) = \omega_0^\delta \text{Re} \left\{ \int_0^t \text{d}t' \exp \left\{ -2 \alpha t' (\delta - 1) \times \left( 1 - (1 - \text{i}\omega_0 t')^{1-\delta} \right) \right\} \right\}$$

valid for all $\delta > 0$, $\delta \neq 1$; note however that equation (67) reduces to the corresponding expression of the ohmic case (Eq. (36)) when the limit $\delta \to 1$ is correctly taken.

We shall separately study the «under-ohmic» case $0 < \delta < 1$ and the «over-ohmic» case $\delta > 1$. Finally, we shall conclude by analysing the «near-ohmic» region, $\delta \approx 1$, which displays some interesting features.

6.1 Under-ohmic case: $0 < \delta < 1$. — In this case, since $\langle B_z \rangle = 0$, equation (27) is valid. By expanding the exponential in equation (67) and integrating the series term by term, one can write $A(t)$ as

$$A(t) = \omega_0^\delta \text{Re} \left\{ e^{-2\alpha t (\delta - 1)} (F(t, \delta) - F(0, \delta)) \right\}$$

where $F(t, \delta)$ is given by

$$F(t, \delta) = (-\text{i}\omega_0)^{-1} \sum_{n=0}^\infty \frac{(2\alpha t (\delta - 1))^n}{n!} \times \left( 1 - (1 - \text{i}\omega_0 t)^{(\delta - 1) + 1} \right) \frac{1}{n}(1 - \delta + 1).$$

When $t \to \infty$, $F(t, \delta)$ tends to infinity; so does $A(t)$, which in turn implies (see Eq. (27)) that $\langle \sigma_z(t) \rangle$ goes to zero when $t \to \infty$, independently of the coupling strength $\alpha$. Thus, in the under-ohmic case $0 < \delta < 1$, no symmetry breaking can occur at zero temperature for any value of the coupling with the bath. It would be interesting to check this result by other techniques such as renormalization group methods.

6.2 Over-ohmic case: $\delta > 1$. — At zero temperature, $\langle B_z \rangle$ is then no longer equal to zero. One must therefore resort to the full relaxation equation (23) of the reduced spin density matrix. As a result, $\langle \sigma_z(t) \rangle$, $\langle \sigma_\xi(t) \rangle$ and $\langle \sigma_\eta(t) \rangle$ obey then a system of three coupled equations of motion, and it is im-
possible to write down any simple closed equation for \( \langle \sigma(t) \rangle \).

However, equation (27), though invalid when the temperature is strictly equal to zero, can still be used when the temperature is very close to zero (\( T \rightarrow 0^+ \)) in the range \( 0 < \delta \leq 2 \). If we set \( T = 0^+ \), \( A(t) \) is, to a good approximation, still given by equation (67), provided that \( t \) is smaller than a nearly infinite time of order \( \tau \), as defined by equation (34). From equation (68) it is seen that now \( F(t, \delta) \) is equivalent to \( t \) in the meaningful time domain \( \omega_c t \gg 1 \). So, within the large interval \( \omega_c^{-1} \ll t \leq \tau \), \( A(t) \) is essentially given by

\[
A(t) \approx \omega_c^3 e^{-2a\Gamma(\delta-1) t}.
\]

One gets then

\[
\Sigma(t) \equiv \frac{\langle \sigma_x(t) \rangle}{\langle \sigma_x(0) \rangle} \approx \exp\left( -\frac{1}{2} \frac{1}{\omega_c^2} \frac{2a\Gamma(\delta-1) \omega_c^3 t^2}{2} \right)
\]

\( \Sigma(t) \) thus tends to zero for large time for any \( \alpha \), showing that no symmetry breaking occurs in this case.

Note that the case \( \delta > 2 \) cannot be considered so simply, since the condition \( \langle B^+ \rangle_b = 0 \) is never satisfied, even for finite temperature. It therefore would need a separate analysis, based on the full relaxation equation (23).

### 6.3 NEAR-Ohmic Region: \( \delta \approx 1 \)

As previously indicated, equation (67) for \( A(t) \) reduces to the corresponding equation of the ohmic case (36) when the limit \( \delta \rightarrow 1 \) is correctly taken. However, expression (71) for \( \Sigma(t) \) shows that, since \( \Gamma(\delta-1) \rightarrow \infty \) when \( \delta \rightarrow 1 \), the coefficient of \( t^2 \) goes to zero in this limit; this indicates a slowing down of the decay of \( \Sigma(t) \) towards its limit value zero.

More precisely, when \( |\delta - 1| \ll 1 \), one can, in the large time domain \( 1 \ll \omega_c t \ll \exp(1/|\delta - 1|) \), use the development

\[
\omega_c t \approx 1 + (1 - \delta) \ln \omega_c t.
\]

The functions \( A_1(t) \) and \( A_2(t) \) involved in the expression of \( A(t) \) (see Eq. (28)) are then approximately given by

\[
A_1(t) \approx \pi a\Gamma(\delta) \quad \text{(73a)}
\]

\[
A_2(t) \approx 2 a\Gamma(\delta) \ln \omega_c t. \quad \text{(73b)}
\]

One thus gets, in this time domain

\[
A'(t) = dA(t)/dt \approx \omega_c^3 \cos (\pi a\Gamma(\delta)) (\omega_c t)^{-2a\Gamma(\delta)} \quad \text{(74)}
\]

This expression is quite analogous to the corresponding (i.e. when \( \omega_c t \gg 1 \)) development of \( A'(t) \) in the ohmic case (see Eq. (36)).

One therefore can conclude that, in the near-ohmic region, an apparent symmetry breaking does take place for a value of \( \alpha \) such that

\[
x\Gamma(\delta) = 1
\]

and thus lower or higher than 1 depending on whether \( \delta < 1 \) or \( \delta > 1 \). By apparent symmetry breaking, we mean that it exists only in the large, but finite time interval \( 1 \ll \omega_c t \ll \exp(1/|\delta - 1|) \). When \( t \) grows outside this interval, \( \Sigma(t) \) decays towards zero. It is worthwhile to note that the width of the time interval of interest becomes larger and larger as \( \delta \) approaches 1; this fact can be viewed as a precursor of the transition which takes place at \( \delta = 1 \).

As a matter of conclusion, let us say that, when \( \delta \) is restricted to the range \( 0 < \delta \leq 2 \), the symmetry breaking can only occur when \( \delta \) is exactly equal to 1. Thus, among all the models satisfying equation (66) and \( 0 < \delta \leq 2 \), the ohmic model is unique by its ability to give such a transition, although a precursor behaviour does exist near the value \( \delta = 1 \).

### 7. Generalization to a multiple well.

It is interesting to observe that an Hamiltonian of the form (2) describing a particle in a succession of wells in ohmic interaction with a bath of harmonic oscillators can be treated along the same line as in section 3. Indeed, one can reduce this Hamiltonian to a spin-boson Hamiltonian of the type (5) in which \( \sigma \equiv (x, y, z) \) is replaced by \( 2S_\alpha \) and where \( 2S + 1 \) is the number of wells.

The coordinate is as before pictured by the operator \( q_0 S_\alpha \). The interaction term is proportional to \( S_\alpha \). Clearly, the \( S_\alpha \) term corresponds to an hopping term from the site \( M \) to the site \( M + 1 \), proportional to \( \sqrt{S(S + 1) - M(M + 1)} \); it increases when one moves from one end to the middle of the chain of wells. Note that this could correspond to a physical situation in an open chain.

The calculation proceeds along the same line as in section 3 and one obtains a relaxation equation equivalent to equation (23), with obvious modifications of notations. The relaxation functions \( \phi^{+}_+(t) \) and \( \phi^{+}-(t) \) which are irrelevant in the spin 1/2 calculation are expected to play a role for \( S \neq 1/2 \); however, they vanish under the ohmic dissipation assumption. Thus the time differential equation obeyed by \( \langle S_y(t) \rangle \) (for any value of \( S \)) is exactly the same as equation (27) with \( \langle \sigma_x(t) \rangle = 2 \langle S_y(t) \rangle \).

Therefore, all the results obtained in section 3 can be applied here; in particular, for \( \alpha > 1 \), the particle will tend to stay in the same site, while for \( \alpha < 1 \), its average position goes to zero.

Yet another interesting quantity now has a non trivial time dependence: as opposed to the \( S = 1/2 \) situation, the mean-square value \( \langle S_x^2(t) \rangle \), which gives a measure of the extent of the particle, is no more a constant when \( S \neq 1/2 \).

The evolution equation for \( \langle S_x^2(t) \rangle \) is readily found to be:

\[
\frac{d}{dt} \langle S_x^2(t) \rangle = 4 \Re \phi^{+}-(t) \langle S^2 - 3 S_x^2(t) \rangle \quad \text{(76)}
\]
where \( A(t) \) is given by equation (28). Equation (77) can be rewritten as
\[
\langle S_x^2(t) \rangle = \frac{1}{3} S(S + 1) + \langle S_x^2(0) \rangle - \frac{1}{3} S(S + 1) e^{-3 \int_0^t dt' A(t')} \qquad (77)
\]
where \( \Lambda(t) \) is given by equation (28). Equation (77) can be rewritten as
\[
\langle S_x^2(t) \rangle = \frac{1}{3} S(S + 1) + \langle S_x^2(0) \rangle - \frac{1}{3} S(S + 1) \Sigma^2(t) \qquad (78)
\]
where \( \Sigma(t) = \langle S_x(t) \rangle / \langle S_x(0) \rangle \).

Let us now calculate the relative mean-square fluctuations
\[
\Delta^2 S_x(t) \equiv \langle (S_x^2(t)) - \langle S_x(t) \rangle^2 \rangle / S(S + 1). \quad (79)
\]
Assuming that, at \( t = 0 \), the particle is fully localized on the site \( M \) (i.e. the spin is in the state \( |S, M\rangle \) at \( t = 0 \)), one obtains:
\[
\Delta^2 S_x(t) = \frac{1}{3} - \frac{M^2}{S(S + 1)} \Sigma^2(t) - \left( \frac{1}{3} - \frac{M^2}{S(S + 1)} \right) \Sigma^3(t). \quad (80)
\]

The results derived in section 3 about \( \Sigma(t) \) can be used in order to get an explicit expression for \( \Delta^2 S_x(t) \).

Let us discuss the zero-temperature situation. It appears that:

(i) When \( \alpha < 1 \), \( \Delta^2 S_x(t) \) tends to \( 1/3 \) when \( t \) goes to infinity; in other words, the average position of the particle relaxes towards the middle of the chain and its extent is of the same order of magnitude as the length of the chain: the particle is delocalized.

(ii) When \( \alpha > 1 \), \( \Delta^2 S_x(t) \) tends to a value lower than \( 1/3 \); indeed, for \( \alpha \) large enough, \( \Sigma(+\infty) \) is quite close to \( 1 \) (see Fig. 1) so that \( \Delta^2 S_x(+\infty) \approx (1 - M^2/S(S + 1)) (1 - \Sigma(+\infty)) \) is very small. Thus, when the symmetry is nearly fully broken, the particle hardly moves and displays a very small spatial extent, the initial location being of little importance. So, clearly, the picture of a localized non mobile particle comes out. Despite the rather special variation of the hopping term explicitly used here, this localization process is expected to be a characteristic feature of the ohmic model, as it can be deduced from calculations on an infinite one-dimensional lattice with a constant site-to-site hopping [23-26].

8. Conclusion.

In this paper, we investigated a model, in which a quantal particle in a potential is coupled with a phonon bath in an « ohmic » way. This kind of model has raised considerable interest in the literature, especially in the context of testing the applicability of quantum mechanics to macroscopic variables, which are inherently dissipative. A spontaneous symmetry breaking takes place in these particular systems when the strength \( \alpha \) of the coupling with the bath goes past some critical value (\( \alpha = 1 \) in suitable units).

Our aim was to thoroughly investigate the dynamics: that revealed to be possible in the framework of standard quantum-statistical mechanics. We mainly studied a particle in a double-well potential, a particularly interesting system indeed, since it is concerned with the question of the persistence of quantum coherence in the presence of ohmic dissipation. For this system, a reduced description in terms of a particular version of the spin 1/2-boson model is available.

We used two types of methods, depending on the coupling strength. In the intermediate or strong coupling region (i.e. \( \alpha \) not too small), we used a master equation formalism for the reduced spin density matrix, written in a convolutionless form, which allowed to get a closed equation for the average value of the operator \( \sigma_z(t) \) (which is associated with the position of the particle in the reduced description).

The calculation takes the form of a perturbation expansion with respect to a parameter linked roughly to the ratio of the tunnelling frequency \( \omega_0 \) to some cut-off frequency \( \omega_c \) characteristic of the phonon bath. In the Born approximation, the results are the following:

(i) At \( T = 0 \), the system does display a spontaneous (continuous, but sharp) symmetry breaking at \( \alpha = 1 \). In other words, below this value of the coupling, the average position at infinite time of the particle evolving the double-well potential is equal to zero. In this regime, the particle is said to be delocalized, albeit no oscillation does appear. When \( \alpha \) becomes greater than \( 1 \), the average position at infinite time of the particle is different from zero; the particle eventually localizes itself more on one side. This symmetry breaking is formally analogous to a phase transition of infinite order; nevertheless, the width of the critical region is extremely narrow, so that our result is in fact very similar to the result of references [3, 4], in which a discontinuity of the order parameter is displayed.

As for the dynamics of \( \langle \sigma_z(t) \rangle \), it is shown to follow a generalized Kohlrausch law of the type \( \exp(-at^b) \), the exponent \( b \) being positive or negative depending on whether \( \alpha < 1 \) or \( \alpha > 1 \). The parameters \( a \) and \( b \) have been exactly calculated, and it is seen that, below the value \( \alpha = 1 \), the Kohlrausch law becomes slower and slower as one approaches the transition; this can be viewed as a critical slowing down.

(ii) At finite temperature, the symmetry breaking \emph{stricto sensu} disappears, and the particle in the double-well is always delocalized. However, the relaxation time increases exponentially with \( \alpha \) and becomes extremely large when \( \alpha \) is greater than \( 1 \); this property can be viewed as a precursor of the transition found at zero temperature.
Numerical estimates show that at $T = 0$ and $\alpha \gtrsim 1$ the time scale is macroscopic ($\sim 10^{-3}$ s), but is very sensitive to the temperature and recovers quickly microscopic values when $T > 0$ even extremely small. If these conclusions are correct, this would render very difficult a direct experimental observation of such a symmetry breaking.

The conditions of validity of the convolutionless master equation have been analysed in detail and the domain of validity delineated in the $(\alpha, T)$ plane. The treatment fails for $\alpha$ small, in which case, at $T = 0$, we have used a standard single boson calculation. As a result, for $\alpha \lesssim \omega_0/\omega_e$, the quantal coherence is preserved. The average position exhibits a damped oscillation plus a power-law negative tail term $\sim -t^{-2}$. Such a power-law is well known in the theory of decaying states, the $-2$ exponent being characteristic of the ohmic model.

These results have been extended (at $T = 0$) to a particle in a multiple well. We have calculated both the mean position and its quadratic dispersion in this situation. One obtains here again a genuine localization for $\alpha > 1$.

For the sake of completeness, we also investigated other dissipation laws. We have shown that the ohmic model is unique by its ability to produce such a transition, although a precursor behaviour can be obtained in the close vicinity of the ohmic dissipation.

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References