How to calculate a decoherence matrices numerically and the microscopic mechanism for decoherence in the Caldeira-Leggett model

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January 1994

Abstract

A central object in the interpretation of quantum mechanics of closed systems with decoherent histories is the decoherence matrix. But only for a very small number of models one is able to give explicit expressions for its elements. So numerical methods are required. Unfortunately the dimensions of this matrices are usually very high, which makes also a direct numerical calculation impossible. A solution of this problem would be given by a method which only calculates the dominant matrix elements. This includes to make a decision about the dominance of an element before it will be calculated. In this paper I will develop an algorithm that combines the numerical calculation of the elements of the decoherence matrix with a permanent estimation, so that finally the dominant elements will be calculated only. As an example I apply this procedure to the Caldeira-Leggett-modell.

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1 Introduction

The Copenhagen interpretation of quantum mechanics rests on the artificial division of reality in quantum systems and measuring devices. The result of a measurement is produced by a collapsing wave function, which is induced by interaction with a measuring device. This is inadequate for a quantum cosmology, where the universe is to be considered as a quantum system. By definition, there is nothing else outside the universe dealing as a measuring device. An interpretation of a quantum theory of closed systems is needed. Such an interpretation has been developed by Griffiths [1], Omns [2], Gell-Mann, Hartle [3], Joos, Zeh [4] and others. It makes no reference to external observers, classical apparatus or the collapse of the wave function.

The main feature of this formulation is to consider a time sequence of possible outcomes of measuring processes. They are called histories. Fine-grained or elementary histories are the basic set of histories, from which all other coarse-grained histories can be obtained by unification in the sense of set theory. The way, the coarse-graining is done depends on the physical properties of the system one is interested in.

To connect the coarse-grained histories with observables, one has to assign each of these coarse-grained histories a probability. The problem is that some of these histories may have a quantum interference, which violates the sum rules of the probability theory. These interference’s are expressed by means of a decoherence matrix. If all the non-diagonal elements of this matrix are vanishing, the histories will be decoherent. Only in this case one is able to assign a probability to each history.

To find the coarse grained sets of decoherent histories is a central problem of this quantum theory of closed systems. One can define a decoherence matrix. Its elements describe the quantum interference between two histories.

Given the histories, the decoherence matrix can be calculated easily in principle. The usual type of calculations is simple, but their number is very large, because the number of possible histories that is related to the numbers of elements of the decoherence matrix is usually very huge. This makes it impossible, to calculate the decoherence matrix even numerically. For example: Consider a particle in one-dimensional space divided in m intervals. A coarse-grained history should correspond to the situation, in which the particle has been detected in one of these intervals at the times \((t_1, t_2, \ldots, t_n)\). The number of possible histories would be \(m^n\) and the number of elements of the decoherence matrix would be \(m^{(2n-1)}\).

Not all is lost, we are not interested in the decoherence matrix for any coarse-graining. We are usually interested in such coarse-grainings, that provide decoherent histories. So if we combine the process of constructing such coarse-grainings together with the calculation of the decoherence matrix, we might be more successful. In this case for instance we already know, that the non-diagonal elements are vanishing.
So we can try to calculate the decoherence matrix in two steps. In the first step we have to find qualitative features of the decoherence process to get the orders of magnitude for a coarse-graining that guaranties the dominance of the diagonal elements of the decoherence matrix. In a second step we can use these data for a numerical calculation.

In this paper we want to show how to do these two steps, especially how to design the numerical calculation for the Caldeira-Leggett model, which gives us some deeper insight in the mechanism of decoherence.

2 Qualitative features of the Caldeira-Leggett model

This model has been developed by Caldeira and Leggett [3], to explain the Brownian motion. It consists of one distinguished harmonic oscillator in an interaction with a huge number of other harmonic oscillators, which we will call the environment. The action of the distinguish oscillator is

$$S_A[x] = \frac{M}{2} \int_0^t dt (\dot{x}^2 - \omega^2 x^2) \quad (2.1)$$

and the action of the oscillators of the environment are given by

$$S_E[R] = \sum_k \frac{m}{2} \int_0^t dt (\dot{R}_k^2 - \omega^2 R_k^2). \quad (2.2)$$

The meaning of the variables is obvious. The interaction between the environment and the distinguished oscillator is given by

$$S_I[x, R] = -\sum_k \int_0^t dt C_k R_k x. \quad (2.3)$$

The $C_k$'s are coupling constants. At an initial time $t_1$ the density matrix of the whole system should be

$$\rho(x_1, R_1, y_1, Q_1; t_1) = \rho_A(x_1, y_1; t_1) \rho_E(R_1, Q_1) \quad (2.4)$$

and we assume that the density matrix of the environment is in thermal equilibrium.

$$\rho_E(R_0, Q_0) = \prod_k \exp \left[ -\frac{m\omega_k}{2 \sinh(\omega_k/kT)} \left( (R_k^2 + Q_k^2) \cosh(\omega_k/kT) - 2R_kQ_k \right) \right] \times \frac{m\omega_k}{2\pi \sinh(\omega_k/kT)} \quad (2.5)$$

The space of all possible results of a measuring process is the phase space $(x, R; p, P)$ with positions $x$ and momenta $p$ of the distinguished oscillator and
$R, P$ are the coordinates and momenta of the environment. An elementary history corresponds to the classical situation, that at the times ($t_1, t_2, ..., t_n$) the system can be found at \((x_1, R_1; p_1, P_1), (x_2, R_2; p_2, P_2), ..., (x_n, R_n; p_n, P_n)\).

We are only interested in the position of the distinguished oscillator, neither in its momenta nor in the phase space coordinates of the environment. In this sense we collect all elementary histories with equal position coordinates $x_1, x_2, ..., x_n$ together in one family. The most general description of the above defined families of histories is given by the reduced density matrix

$$\rho(x, y; t) = \int dRdQ \delta(R - Q) \rho(x, R, y, Q; t) \quad (2.6)$$

Now we want to investigate the time development of the reduced density matrix. Following the papers by Caldeira and Leggett [5], and Halliwell and Dowker [6] we can represent the evolution of this density matrix with the help of a propagator $J$

$$\rho(x_f, y_f; t) = \int dx_0 dy_0 J(x_f, y_f; t|x_0, y_0; 0) \rho(x_0, y_0; 0). \quad (2.7)$$

By replacing the huge number of oscillators of the environment by a continuum with the distribution

$$\rho_D(\omega) C^2(\omega) = \begin{cases} 4M m \gamma \omega^2/\pi & , \omega < \Omega \\ 0 & , \omega > \Omega \end{cases} \quad (2.8)$$

the authors could give an explicit formula for the propagator in the high temperature limit:

$$J(x_f, y_f; t|x_0, y_0; 0) = F^2(t) \exp(iS_{cl} - \Phi) \quad (2.9)$$

where the functions in the exponent are as follows:

$$S_{cl} = K_1(t)(x^2_f - y^2_f) + K_2(t)(x^2_0 + y^2_0) - L(t)(x_0 + y_0)(x_f - y_f) - N(t)(x_f + y_f)(x_0 - y_0) \quad (2.10)$$

and

$$\Phi = A(t)(x_f - y_f)^2 + B(t)(x_f - y_f)(x_0 - y_0) + C(t)(x_0 - y_0)^2 \quad (2.11)$$

The explicit expressions for the time dependent functions $K_1, K_2, L, N$ and $A, B, C$ will be given in the appendix, they consist mainly of the exponential function $\exp(-\gamma t)$ and trigonometric functions in $t$. This propagator has the remarkable property, that its time dependence includes only the difference between the initial and final time. Originally one should have expected, that the propagator is not time-like translational symmetric, caused by a time dependence of the environment. But by replacing the discrete oscillators by a...
continuum, the environment became infinitely large and so the influence of the distinguished oscillator on it can be neglected.

With the explicit formula (2.10) we have all information about the evolution of the density matrix. But the structure of these formulae is very complex and the high number of parameters makes it difficult to analyze the evolution in detail. So I decided, to study the decoherence matrix numerically. The result was, that for a sufficiently large final time we got asymptotically always the same density matrix. This reflects the fact, that the oscillator comes to a thermal equilibrium with the environment. Now we want to confirm this result analytically.

For the moment we assume, the initial state of the distinguished oscillator at the time \( t_1 \) can be described by the Gaussian density matrix

\[
\rho_A(x_1, y_1; t_1) = V \exp\left(-\frac{(x_1 - \xi_1)^2}{\sigma_x} - \frac{(y_1 - \eta_1)^2}{\sigma_y} - \frac{(x_1 - \xi_1)(y_1 - \eta_1)}{\sigma_{xy}}\right). \tag{2.12}
\]

with arbitrary parameters \( \sigma_x, \sigma_y \) and \( \sigma_{xy} \). This density matrix is normalized by the function \( V \). The function \( \rho_A \) represents a Gaussian wave packet in the "squared" configuration space of the distinguished oscillator. The variables \( \xi_0 \) and \( \eta_0 \) denote complex numbers, which give an information about the position and "momentum" of this packet. Using the formula (2.7) it is easy to get the density matrix at a later time. One has simply to perform a Gaussian integration. The result is again a Gaussian concerning the new position variables \( x_f \) and \( y_f \). The coefficients are rational functions of the functions \( A, B, C, \ldots, N \) and thus rational functions of exponential and trigonometric functions. So one should assume, that these coefficients can be expanded in a power series with respect to \( \exp(-\gamma t) \) for large \( t \). These calculations are very tedious, but can be carried out by means of computers. The result is:

\[
\rho_S(x_f, y_f; t) = V' \exp\left[-\frac{(\gamma^2 + \omega^2)M}{2kT}\left(x_f + y_f\right)^2 - \frac{kTM}{2}(x_f - y_f)^2
+ \exp(-\gamma t)(a(t) x_f + b(t) y_f)
+ O(\exp(-2\gamma t))\right]\tag{2.13}
\]

The functions \( a(t) \) and \( b(t) \) describe a harmonic oscillation with the frequency \( \omega \). The evolution of the density matrix in the squared configuration space can be splitted in three phases: In the first phase, which has a characteristic period of \( \tau = \gamma t/2 \), the shape of the wave packet relaxes to a certain form, that does not depend on the initial parameters of the packet at \( t_1 \). In the squared configuration space this form represents a two dimensional Gaussian bell which is located over an ellipsis \( S \). It corresponds to a certain "equi-density" line. This can be seen from our formula (2.13) by the fact, that all terms with the coefficient \( \exp(-\gamma t) \) become of smaller order compared to others. In this sense they can be neglected and thus the coefficients of the terms quadratic in \( x_f \) and
become independent of time and also independent of the initial parameters of the packet. From formula (2.13) we can see also, that the main axes of the corresponding ellipsis $S$ have a length of

$$d_B^{-2} = \frac{(\gamma^2 + \omega^2)M}{2kT} \quad (2.14)$$

and

$$d_S^{-2} = \frac{kTM}{2}. \quad (2.15)$$

They are oriented at an angle of 45 degrees against the coordinate axes.

While the shape of the packet becomes fixed after the first phase, its motion, corresponding to a damped oscillation of its position in squared configuration space is still present. This can be considered as to be the second phase. Its characteristic time is also $\tau$. After that time the system rests on the origin of our coordinate system in the squared configuration space. This can be considered as the beginning of the third phase. In that phase the distinguished oscillator is in thermal equilibrium with the environment. If we would remove the coupling, e.g. set $\gamma = 0$, then this oscillator will be on equal footing with the oscillators of the environment. The thermal equilibrium can then be recognized from our asymptotic formula (2.13) by the fact, that it is just the high temperature expansion of one of the factors in (2.13), but of course with the specific parameters of the distinguished oscillator. For $\gamma \neq 0$ the whole calculation can be understood as the quantum analog of the damped harmonic oscillator.

By considering, that all initial functions for the density matrix can be composed by a linear superposition of Gaussian waves (This system is even over complete), we see, that the asymptotic behavior, described above, is very general.

Now we want to use these results, to construct a physically interesting set of decoherent histories and to make statements about the corresponding decoherence matrix. At first we have to enlarge our coarse-graining. From the Heisenberg uncertainty relation we know that it makes no sense, to measure exact positions of the distinguished oscillator at the times $t_1, t_2, \ldots, t_n$. We have to ask questions with a higher degree of coarse-graining. So we ask only, if the oscillator goes through definite intervals at these given times. Our coarse-graining is now, that we collect in one family all histories, in which the position of the distinguished oscillator goes through a sequence of intervals $\Delta_{i_1}, \Delta_{i_2}, \ldots, \Delta_{i_n}$ at the times $t_1, t_2, \ldots, t_n$. In our notation for the intervals, the upper index means, that we may use different sets $\Delta^k$ of intervals for different times $t_k$ and the lower index denotes which interval of a set we selected. Sometimes we use also the notation

$$\Delta_{i_1, i_2, \ldots, i_n} = \Delta^1_{i_1}, \Delta^2_{i_2}, \ldots, \Delta^n_{i_n}. \quad (2.16)$$

One family is now understood as one of the new coarse-grained histories. If the sets of intervals for one particular time are disjunct and their union covers
the whole space of positions, the corresponding histories will be complete and alternative.

The decoherence matrix corresponding to the coarse-graining defined above is given by

\[
D(\Delta_{i_1, \ldots, i_n}, \Delta_{j_1, \ldots, j_n}) = \int_{\Delta_{i_n} = \Delta_{j_n}} dx_n dy_n \delta(x_n - y_n) \\
\int_{\Delta_{i_{n-1}} = \Delta_{j_{n-1}}} dx_{n-1} dy_{n-1} J(x_n, y_n; t_n|x_{n-1}, y_{n-1}; t_{n-1}) \\
\int_{\Delta_{i_{n-2}} = \Delta_{j_{n-2}}} dx_{n-2} dy_{n-2} J(x_{n-1}, y_{n-1}; t_{n-1}|x_{n-2}, y_{n-2}; t_{n-2}) \\
\vdots \\
\int_{\Delta_{i_2} = \Delta_{j_2}} dx_2 dy_2 J(x_3, y_3; t_3|x_2, y_2; t_2) \\
\int_{\Delta_{i_1} = \Delta_{j_1}} dx_1 dy_1 J(x_2, y_2; t_2|x_1, y_1; t_1) \rho_A(x_1, y_1; t_1)
\]

(2.17)

This describes a sequence of evolution’s between two subsequent moments of time and following projections. The symbol \(\Delta_{i_1, \ldots, i_n}|j_1, \ldots, j_n\) denotes the set of intervals \(\Delta_{i_1}^1, ..., \Delta_{i_n}^n, \Delta_{j_1}^1, ..., \Delta_{j_n}^n\). We introduce two additional terms: The first is the incomplete decoherent matrix at time \(t_k\). Its elements are defined by the expression

\[
\rho_{-\epsilon}(\Delta_{i_1, \ldots, i_{k-1}}|j_1, \ldots, j_{k-1}; x_k, y_k, t_k) = \\
\int_{\Delta_{i_{k-1}} = \Delta_{j_{k-1}}} dx_{k-1} dy_{k-1} J(x_k, y_k; t_k|x_{k-1}, y_{k-1}; t_{k-1}) \\
\int_{\Delta_{i_{k-2}} = \Delta_{j_{k-2}}} dx_{k-2} dy_{k-2} J(x_{k-1}, y_{k-1}; t_{k-1}|x_{k-2}, y_{k-2}; t_{k-2}) \\
\vdots \\
\int_{\Delta_{i_2} = \Delta_{j_2}} dx_2 dy_2 J(x_3, y_3; t_3|x_2, y_2; t_2) \\
\int_{\Delta_{i_1} = \Delta_{j_1}} dx_1 dy_1 J(x_2, y_2; t_2|x_1, y_1; t_1) \rho_A(x_1, y_1; t_1)
\]

(2.18)

A second term is the projected incomplete decoherent matrix at time \(t_k\). The
elements are given by the expression
\[
\rho_{+\epsilon}(\Delta_{i_1 \ldots i_k}, \Delta_{j_1 \ldots j_k}, |x_k, y_k; t_k) = \\
\begin{cases}
\rho_{-\epsilon}(\Delta_{i_1 \ldots i_{k-1}}, \Delta_{j_1 \ldots j_{k-1}}, |x_k, y_k, t_k), & x_k \epsilon \Delta_{i_k}, y_k \epsilon \Delta_{j_k}^k \\
0, & \text{otherwise}
\end{cases}
\] (2.19)

The physically interesting question is, for which sets of intervals are the corresponding histories decoherent? In all what follow, we assume the timelike distance between two "measurements" is larger than the characteristic time \(\tau\).

The decoherence of the histories is equivalent to vanishing non-diagonal elements of the decoherence matrix. Any of these elements corresponds to a pair of histories which have different intervals at least at one moment of time. Let this time to be \(t_k\). The incomplete decoherence matrix \(\rho_{-\epsilon}(t_k)\) can be written as
\[
\rho_{-\epsilon}(\Delta_{i_1 \ldots i_{k-1}, j_1 \ldots j_{k-1}}, |x_k, y_k; t_k) = \\
\int_\infty dx_{k-1} dy_{k-1} J(x_k, y_k; t_k | x_{k-1}, y_{k-1}; t_{k-1}) \\
\times \rho_{+\epsilon}(\Delta_{i_1 \ldots i_{k-1}, j_1 \ldots j_{k-1}}, |x_{k-1}, y_{k-1}; t_{k-1})
\] (2.20)

This is an evolution of \(\rho_{+\epsilon}(t_{k-1})\) from \(t_{k-1}\) to \(t_k\). If this time interval is larger than the characteristic time \(\tau\), we can assume that \(\rho_{-\epsilon}(t_k)\) is equal to the asymptotic matrix \(\rho_S\). The subsequent projection of the incomplete decoherence matrix on the intervals \(\Delta_{i_k}^k\) and \(\Delta_{j_k}^k\) vanishes approximately, when these intervals do not catch the ellipses. This is guaranteed when the distance of the centers of the intervals will be larger than the width \(d_S\) and because these two intervals must be different and disjunct this is given, when their own width is larger than that of \(d_S\).

If the incomplete decoherence matrix \(\rho_{+\epsilon}(t_k)\) vanishes, then the chain of evolution’s and projections in formula (2.17) is cut off and the corresponding matrix element vanishes also. Because of the criterion, that the intervals for projections should be larger than \(d_S\) does not depend on any other special property of the histories we considered, it guarantees decoherence of all histories with that property. So we will call \(d_S\) the decoherence width from now on. A remarkable fact is, that this width does not depend on \(\gamma\), measuring the strength of the coupling. But the timescale for the decoherence does.

In what follows we will always assume, that the widths of the projections are larger than the decoherence width. So our histories will decohere and we ask now for their probability. For calculating the probabilities the projection intervals \(\Delta_{i_k}^k\) and \(\Delta_{j_k}^k\) have to be identical. We work in the configuration space of the distinguished oscillator.

Again we start with the incomplete decoherence matrix \(\rho_{-\epsilon}(t_k)\), which comes from a projection at \(t_{k-1}\) and has the asymptotic form of a wave packet \(\rho_S\).
Independent on which interval we project at $t_k$, the asymptotic form, at $t_{k+1}$ will be the same. Only the prefactors will become different. Are the intervals for projection at $t_k$ outside the wave packet of $\rho_{-\epsilon}(t_k)$, the prefactor at $t_{k+1}$ will be zero. Otherwise it will always have approximately the same order of magnitude if it goes through the packet. This means that we get approximately the same probability for all histories, whose $k$-th interval is completely within a region, which is the projection of the main axis with $d_B^{-2}$ of the ellipsis $S$ to the coordinate axis $x$. The width of that projection is

$$d_B^{-2} = \frac{(\gamma^2 + \omega^2)M}{kT} \quad (2.21)$$

If we apply the same argument for all other times, we see that all histories having intervals only inside a strip of width $d_B$ in the configuration space of the distinguished oscillator, have the same probability. Is the with $d_B$ larger than the asymptotic decoherence width $d_S$, then the oscillator shows a Brownian motion within an interval of $d_B$.

By analyzing the decoherence width $d_S$ and the width of the Brownian motion we find the familiar result, that with increasing temperature $T$ the decoherence length becomes smaller, while the Brownian motion becomes more intense. A stronger coupling makes the Brownian motion weaker, but has no influence on the decoherence length. A bigger mass makes the decoherence length and the Brownian motion smaller.

This calculation was for the Caldeira-Leggett model. But the fact, that in the process of evolution the distinguished oscillator comes into thermal equilibrium with its environment in general, makes it very likely that in all similar calculations we will find a specific asymptotic behavior of the observed subsystem. This might give the possibility, to set up a quite similar calculation to get the decoherent histories for other more general systems.

It is also interesting to investigate the evolution of the density matrix for short times. For our initial density matrix (2.12) the width for decoherence is:

$$d_0^{-2} = \left( \frac{1}{\sigma_x} + \frac{1}{\sigma_y} - \frac{1}{\sigma_{xy}} \right)/4 \quad (2.22)$$
An expansion of the density matrix for small \( t \) gives the following result:

\[
\rho_S(x_f, y_f; t) = V' \exp \left[ -\left( x_f - y_f \right)^2 \left( \frac{1}{d_0^2} + \left( 2kTM - \frac{4}{d_0^2} \right) \gamma t + \frac{i}{2M} (\sigma_x - \sigma_y)(\sigma_x \sigma_{xy} + \sigma_y \sigma_{xy} - \sigma_x \sigma_y) t \right) - \left( \frac{x_f + y_f}{2} \right)^2 \left( \frac{1}{M\sigma_x^2\sigma_y^2\sigma_{xy}} \right) + C_x x_f + C_y y_f + C_0 \right]
\]

(2.23)

The variables \( C_x, C_y \) and \( C_0 \) represent some time dependent function in which we are not further interested. We focus our attention on the real part of the coefficient of \((x_f - y_f)^2\). It describes the evolution of the decoherence width \( D \).

If we replace the temperature by means of the asymptotic decoherence width \( d_S \), see (2.15), we get

\[
\frac{1}{D^2} = \frac{1}{d_0^2} + 4\left( \frac{1}{d_S^2} - \frac{1}{d_0^2} \right) \gamma t
\]

(2.24)

We see, is the initial decoherence width smaller or larger then the asymptotic one, the width will be immediately increased or decreased respectively. So we can say that the relaxation starts immediately. Suppose the initial width \( d_0 \) is much larger then the asymptotic width \( d_s \). How long does it take, till the decoherence width of the oscillator is smaller than a given value of \( d \). By assuming that this width is also much larger than the asymptotic value, we get from (2.24)

\[
t_D = \frac{1}{4\gamma} \left( \frac{d_s}{d} \right)^2
\]

(2.25)

Depending on the ratio \( d_s/d \) this time might be much shorter, than the relaxation time \( \tau \). From formula (2.23) we see, that the time dependent part of the width of the Brownian motion is imaginary. So the range of the Brownian motion is not influenced by the time dependence in first order. This provides another scenario than described above. If we consider coarse-grainings with intervals much larger than the asymptotic decoherence width, then in a first phase of the scenario the desired decoherence happens in a very short time compared to the relaxation time. After that the damped oscillation and Brownian motion, known from the asymptotic scenario, takes place.

If we choose a coarse-graining with intervals in the order of magnitude of \( d_S \) and the time between measurements in the order of \( \tau \), the diagonal and "near-to-diagonal" elements of the decoherence matrix should be dominant. So we can neglect the others and the number of elements we have to calculate is numerically manageable.

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3 How to calculate the decoherence matrix numerically

In the case of Hamiltonian quantum mechanics the decoherence matrix can be calculated by a sequence of integration’s (2.17). These integration’s might be carried out numerically. But the number of matrix elements is very large in practical cases. So, to get reliable numerical results one has to find out the dominant matrix elements, without spending too much time for non dominant terms. Therefore we want to elaborate some inequalities, to give upper bounds to the matrix elements.

From (2.20) we get

\[
D(\Delta_{i_1}, \ldots, i_n | j_1, \ldots, j_n) = \int_{\Delta_{n-1}} \int_{\Delta_{n-1}} dx_{n-1} dy_{n-1} \left[ \int_{\Delta_n} dx_n J(x_n, x_n; t_n | x_{n-1}, y_{n-1}; t_{n-1}) \times \rho_{-\epsilon}(\Delta_{i_1}, \ldots, i_n | j_1, \ldots, j_n | x_{n-1}, y_{n-1}; t_{n-1}) \right]
\] (3.26)

By Cauchy’s inequality with respect to the integration’s over \( dx_{n-1} dy_{n-1} \) and with the following definitions:

\[
A(\Delta_n | \Delta_{n-1}, \Delta_{n-1})^2 = \int_{\Delta_{n-1}} \int_{\Delta_{n-1}} dx_{n-1} dy_{n-1} \left[ \int_{\Delta_n} dx_n J(x_n, x_n; t_n | x_{n-1}, y_{n-1}; t_{n-1}) \right]^2
\] (3.27)

and

\[
P^2_{i_k, \ldots, i_k | j_k, \ldots, j_k} = \int \int \rho_{-\epsilon}(\Delta_{i_k}, \ldots, i_k | j_k, \ldots, j_k | x_k, y_k; t_k)^2
\] (3.28)

we obtain from (3.26) the inequality

\[
|D(\Delta_{i_1}, \ldots, i_n | j_1, \ldots, j_n)| \leq A(\Delta_n | \Delta_{n-1}, \Delta_{n-1}) P_{i_1, \ldots, i_n | j_1, \ldots, j_n} (3.29)
\]

Now, we want to find an upper bound for \( P_{i_k, \ldots, i_k | j_k, \ldots, j_k} \). With the help of formula

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we can rewrite equation (3.28) and after rearranging the integrals we get
\[ P_{i_k,\ldots,i_1 | j_k,\ldots,j_1} \leq \]
\[ P_{i_k-1,\ldots,i_1 | j_k,\ldots,j_1} \times \int_{\Delta_{i_{k-1}j_{k-1}}} dx_{k-1} dy_{k-1} \int_{\Delta_{i_{k-1}j_{k-1}}} dx'_{k-1} dy'_{k-1} \]
\[ \left| \int dx_k dy_k J(x_k, y_k; t_k | x_{k-1}, y_{k-1}; t_{k-1}) J(x_k, y_k; t_k | x'_{k-1}, y'_{k-1}; t_{k-1}) \right|^2 \]
\[ (3.30) \]
Again by using Cauchy’s inequality and with the definition
\[ B^4(\Delta_{ik}^k, \Delta_{jk}^k | \Delta_{ik-1}^k, \Delta_{jk-1}^k) = \int_{\Delta_{ik-1}^k j_{k-1}} dx_{k-1} dy_{k-1} \int_{\Delta_{ik-1}^k j_{k-1}} dx'_{k-1} dy'_{k-1} \]
\[ \left| \int dx_k dy_k J(x_k, y_k; t_k | x_{k-1}, y_{k-1}; t_{k-1}) J(x_k, y_k; t_k | x'_{k-1}, y'_{k-1}; t_{k-1}) \right|^2 \]
\[ (3.31) \]
we can write
\[ P_{i_k,\ldots,i_1 | j_k,\ldots,j_1} \leq B(\Delta_{ik}^k, \Delta_{jk}^k | \Delta_{ik-1}^k, \Delta_{jk-1}^k) P_{i_{k-1},\ldots,i_1 | j_{k-1},\ldots,j_1}. \]  \[ (3.32) \]
If we know the incomplete density matrix at a time slice \( t_k \), we can calculate \( P_{i_k,\ldots,i_1 | j_k,\ldots,j_1} \) and an iterated use of formula (3.32) together with (3.29) gives the possibility to give an upper bound for the elements of the decoherence matrix at any later time. This is not yet very useful for a numerical calculation, because we can not test the upper bound for all possible path, caused by their large number. So we have to ask: suppose we know an incomplete density matrix at a time \( t_k \), what is the upper bound for all decoherence matrix elements independent of subsequent projections? To answer this question we introduce the quantities
\[ A_{n,n-1}(\Delta_{mn}^{n-1}, \Delta_{jn}^{n-1}) = \max_{\Delta_{mn}^{n-1}} \left[ A(\Delta_{mn}^{n-1}, \Delta_{jn}^{n-1}) \right] \]
\[ A_{n,n-1} = \max_{\Delta_{mn}^{n-1}} \left[ \Delta_{mn}^{n-1} \right] \left[ A(\Delta_{mn}^{n-1}, \Delta_{jn}^{n-1}) \right] \]
\[ B_{k,k-1}(\Delta_{ik}^{k-1}, \Delta_{jk}^{k-1}) = \max_{\Delta_{ik}^{k-1}} \left[ \Delta_{ik}^{k-1} \right] \left[ B(\Delta_{ik}^{k-1}, \Delta_{jk}^{k-1}) \right] \]
\[ B_{k,k-1} = \max_{\Delta_{ik}^{k-1} \Delta_{jk}^{k-1}} \left[ \Delta_{ik}^{k-1} \Delta_{jk}^{k-1} \right] \left[ B(\Delta_{ik}^{k-1}, \Delta_{jk}^{k-1}) \right] \]
\[ (3.33) \]
With these maxima we construct the quantity
\[ K_{i_k,\ldots,i_1 | j_k,\ldots,j_1}^{(k)} = A_{n,n-1} B_{n-1,n-2} \cdots B_{k+1,k} (\Delta_{ik}^{k}, \Delta_{jk}^{k}) P_{i_k,\ldots,i_1 | j_k,\ldots,j_1}. \]  \[ (3.34) \]
The main point is, that the elements of the decoherence matrix satisfy the inequality

\[ D(\Delta_{i_1, \ldots, i_n|j_1, \ldots, j_n}) \leq K_{k_1, \ldots, i_1|j_1, \ldots, j_1}^{(k)} \]  

(3.35)

It says that all matrix elements containing the intervals \( \Delta_{i_1, \ldots, i_n|j_1, \ldots, j_n} \) are smaller than the corresponding value of \( K^{(k)} \), independent of subsequent projections.

Now we can use a computer in the following way: We start with the initial density matrix \( \rho_A(x_1, y_1) \) and calculate the quantities

\[ P^2_{i_1|j_1} = \int_{\Delta_{i_1}^{1}, \Delta_{j_1}^{1}} dx_1 dy_2 \left| \rho_A(x_1, y_1) \right|^2 \]  

(3.36)

and \( K^{(1)}_{i_1|j_1} \). We denote with \( M \) the set of all \( K^{(1)}_{i_1|j_1} \)'s and consider the maximum of its elements to be the norm of \( M \)

\[ M = \bigcup_{i_1, j_1} \{ K^{(1)}_{i_1|j_1} \} \]  

(3.37)

\[ \| M \| = \max(K^{(1)}_{i_1|j_1}) \]  

(3.38)

Now we take the largest element of \( M \), the attached intervals should be \( \Delta_{i_1}^{1}, \Delta_{j_1}^{1} \) and propagate the corresponding incomplete density matrix. This allows us to calculate the quantities

\[ P^2_{i_2, i_1|j_2, j_1} = \int_{\Delta_{i_1}^{2}, \Delta_{j_2}^{1}} dx_2 dy_2 \left| \rho_A(x_2, y_2) \right|^2 \]  

(3.39)

and \( K^{(2)}_{i_2, i_1|j_2, j_1} \). We enlarge our set \( M \) by the quantities \( K^{(2)} \) and reduce it by the element \( K^{(1)}_{i_1|j_1} \). These steps will be repeated: We select the largest element of \( M \), propagate the corresponding incomplete density matrix and replace this largest element of \( M \) by the new obtained \( K \)'s. So for instance, we could have after two steps one of the \( K^{(2)} \)'s as the largest element or one of the \( K^{(1)} \)'s.

By repetition of these steps one of our propagation’s reach the final timeslice \( t_n \) and we can calculate the corresponding element of the decoherence matrix. It is not guarantied that this element is the largest, but we know that all elements we have not yet calculated are smaller than the norm of \( M \). By going on with our procedure we get more and more matrix elements while the norm of \( M \) is decreasing. If this norm becomes smaller than some desired order of magnitude of the already calculated matrix elements, we can neglect the not jet calculated elements and the problem is solved. The only bad thing that can happen is, that the histories are not decoherent enough. So the program will produce more and more matrix elements, but the norm of \( M \) will drop down very slowly. If this happens one can find from the calculated data, which histories are not decoherent and one can combine some of the intervals to increase the coarse-graining.
To demonstrate the efficiency of the algorithm we consider the Caldeira-Leggett model. The decoherence matrix should correspond to the situation where we have 5 intervals at 6 time slices. The parameters of the model and the intervals are chosen in such a way, that the widths of the intervals are one asymptotic decoherence width $d_s$ and the distance of the time slices is half of the relaxation time. With these parameters the decoherence matrix has $5 \times 5 \times 5 \approx 4.8 \times 10^7$ elements and for each element we have to calculate 5 propagation’s of the incomplete density matrices. The time to calculate the decoherence matrix is proportional to the number of projections

$$P \approx 2.4 \times 10^8.$$  \hfill (3.40)

Let us assume, that we are not interested in matrix elements that are smaller than $10^{-1}$ times the largest element.

Furthermore, for the numerical calculation we arrange the parameters of the model such, that the mass of the oscillator corresponds to that of a proton, the asymptotic decoherence width should be equal to one atomic length scale $L = 10^{-10}m$ and the asymptotic width of the Brownian motion will be $3L$.

I made the additional assumption, that the oscillator is in a pure state at the initial time and that the wave function is a Gaussian function with a width of $2L$, located at the origin of the coordinate system.

The program started to calculate 8478 elements of the decoherence matrix. Whenever the program found that the corresponding matrix element will become smaller than one tenth of the largest element, it terminated that calculation, so that finally only 1536 relevant elements had been determined. The number of propagation’s, which had to be performed was 6025. The ratio between the number of executed propagation’s and the total number $P$ is a measure for the efficiency of the algorithm and has a value of $2 \times 10^{-5}$. This numerical calculation, should simply be considered as a demonstration.

4 Discussion

The purpose of this paper has been to provide a guide line for calculating the elements of the decoherence matrix. I developed an algorithm which combines the numerical calculation of the elements of the decoherence matrix with a permanent estimation, so that finally the dominant elements will be calculated only. The algorithm can not be used straight forward to calculate other models. Because other models require different inequalities to estimate the matrix elements. To find these inequalities may require many analytical calculations - better estimations provide a more efficient algorithm because nondominant matrix elements will be ruled out earlier. This has two advantages: the number of steps to be performed is smaller and the amount of data to be saved temporarily. But despite these model-dependent inequalities the main features of
the algorithm remain the same, so that paper may help to study more complex models.

A Appendix

The explicit formulae for the time-dependent Coefficients in the exponent of the propagator $J$ (2.10) and (2.11) are as follows:

\[ a = \frac{kTM}{2} \csc(\omega \tau) \frac{\gamma^2 + \omega^2 - \gamma^2 \cos(2\omega \tau) - \gamma \omega \sin(2\omega \tau) - e^{-2\gamma \tau} \omega^2}{\gamma^2 + \omega^2} \]

\[ b = kT M \omega \csc(\omega \tau) \frac{\omega \cos(\omega \tau) \left(1 - e^{2\gamma \tau}\right) + \gamma \sin(\omega \tau) \left(1 + e^{2\gamma \tau}\right)}{e^{\gamma \tau} (\gamma^2 + \omega^2)} \]

\[ c = \frac{kTM}{2} \csc(\omega \tau) \frac{-\gamma^2 - \omega^2 + e^{2\gamma \tau} \omega^2 + \gamma^2 \cos(2\omega \tau) - \gamma \omega \sin(2\omega \tau)}{\gamma^2 + \omega^2} \]

and

\[ K_1 = -\frac{M\gamma}{2} + \frac{M\omega}{2} \cot(\omega \tau) \]

\[ K_2 = +\frac{M\gamma}{2} + \frac{M\omega}{2} \cot(\omega \tau) \]

\[ L = \frac{M\omega}{2 \sin(\omega \tau)} e^{-\gamma \tau} \]

\[ N = \frac{M\omega}{2 \sin(\omega \tau)} e^{\gamma \tau}. \]

Acknowledgments

I am grateful to the Department of Physics of the University of California/Santa Barbara, were part of this work was carried out and the Deutsche Forschungsgemeinschaft for supporting this research by funds. I would particularly like to thank Jim Hartle for many useful conversations over a long period of time.

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