Exact Solutions of the Caldeira-Leggett Master Equation: A Factorization Theorem For Decoherence

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Abstract

Exact solutions of the Caldeira-Leggett Master equation for the reduced density matrix $\langle x'|\rho(t)|x\rangle$ for a free particle and for a harmonic oscillator system coupled to a heat bath of oscillators are obtained for arbitrary initial conditions. The solutions prove that the Fourier transform of $\rho(t)$ with respect to $\frac{(x+x')}{2}$ factorizes exactly into a part depending linearly on $\rho(0)$ and a part independent of it. The theorem yields the exact initial state dependence of $\rho(t)$ and its eventual diagonalization in the energy basis.

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I. Introduction – Feynman and Vernon[1] pioneered the 'influence functional technique' in which a quantum system of interest and its environment are represented by a single Hamiltonian and the time development of the reduced density matrix ρ of the system is computed by tracing out the degrees of freedom of the environment. Using this technique on the total Hamiltonian

$$H = \frac{p^2}{2m} + V(x) + x\sum_k c_k R_k + \sum_k \Big(\frac{p_k^2}{2M} + \frac{1}{2}M\omega_k^2 R_k^2\Big), \tag{1}$$

in which the environment is modeled as a thermal bath of oscillators with co-ordinate co-ordinate coupling to the system coordinate x, Caldeira and Leggett[2] derived the following high-temperature master equation for the reduced density operator:

$$\frac{\partial\rho}{\partial t} = -\frac{i}{\hbar}\big[H_R, \rho\big] - \frac{i\gamma}{\hbar}\Big(\big[\frac{1}{2}\{p, x\}, \rho\big] + \big[x, \rho p\big] - \big[p, \rho x\big]\Big) - \frac{D}{4\hbar^2}\big[x, \big[x, \rho\big]\big], \tag{2}$$

where H_R is the renormalized system Hamiltonian, γ is the relaxation rate and

$$D = 8m\gamma k_B T, \tag{3}$$

where k_B is the Boltzmann constant and T is the temperature of the bath. The same master equation has also been derived from completely different approaches and approximations[3, 4]. In particular, for

$$H_R = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{4}$$

Agarwal's approximations yield Eq(2) with

$$D = 8m\gamma\hbar\omega(\bar{n} + \frac{1}{2}), \tag{5}$$

where

$$\bar{n} = \Big[\exp\Big(\frac{\hbar\omega}{k_B T}\Big) - 1\Big]^{-1}, \tag{6}$$

which has been used even at zero temperature by some authors[5]. In that case, at all temperatures,

$$D \geq 4m\gamma\hbar\omega. \tag{7}$$

For an open system, coupling with this environment may lead to near diagonalization of the reduced density matrix in some preferred basis. Such decoherence has obvious conceptual interest in understanding the transition from quantum to classical behaviour[6]. In addition, advances of technology have increased the propsects of tests of decoherence by producing superpositions of macroscopically distinguishable states[7]. On the other hand, maintenance of quantum coherence is crucial to the success of quantum computation, cryptography and teleportation[8].

The purpose of the present work is a rigorous study of quantum decoherence by means of exact solutions of the Caldeira-Leggett equation. Some interesting questions which have been stimulated by the work of Zurek, Habib and Paz[9] in the weak coupling approximation

are: which initial states are least susceptible to loss of quantum coherence, and which are the likely end states. We are able to give precise answers to these questions without making the weak coupling approximation due to a factorization property of the initial state dependence of the exact solutions of the master equation. We begin by proving the factorization theorem.

II. Exact Solution of the Master Equation

A. Oscillator case − In the position representation we denote

$$\langle x'|\rho(t)|x\rangle = \rho(R, r, t), \tag{8}$$

where

$$R = \frac{x + x'}{2}, r = x - x' \tag{9}$$

The master equation then becomes:

$$
\begin{aligned}
\frac{\partial \rho(R, r, t)}{\partial t} &= \Big[-\frac{i\hbar}{2m}\Big(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2}\Big) - \gamma(x - x')\Big(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}\Big) - \frac{D}{4\hbar^2}(x - x')^2 \\
&\quad + \frac{m\omega^2}{2i\hbar}(x'^2 - x^2)\Big]\rho(R, r, t) \\
&= -\Big[\frac{i\hbar}{m}\frac{\partial^2}{\partial r\partial R} + 2\gamma r\frac{\partial}{\partial r} + \frac{Dr^2}{4\hbar^2} + \frac{m\omega^2 rR}{i\hbar}\Big]\rho(R, r, t).
\end{aligned}
\tag{10}
$$

A Fourier transform with respect to R reduces it to a first order partial differential equation. Defining

$$
\begin{aligned}
\rho(R, r, t) &= \int \frac{dp\,dp'}{2\pi} \exp\big(i(p' - p)R - i(p + p')r/2\big)\langle p'|\rho(t)|p\rangle \\
&\equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dK\, e^{iKR}\tilde{\rho}(K, r, t), \quad K = p' - p,
\end{aligned}
\tag{11}
$$

we obtain

$$\frac{\partial\tilde{\rho}(K, r, t)}{\partial t} + \Big[(2\gamma r - \frac{\hbar K}{m})\frac{\partial}{\partial r} + \frac{m\omega^2 r}{\hbar}\frac{\partial}{\partial K} + \frac{Dr^2}{4\hbar^2}\Big]\tilde{\rho}(K, r, t) = 0. \tag{12}$$

To integrate this by Lagrange's method (of characteristics) note that on a curve $K = K(s), t = t(s), r = r(s)$, the equation becomes

$$\frac{d\tilde{\rho}}{ds} + \frac{Dr^2}{4\hbar^2}\tilde{\rho} = 0, \tag{13}$$

with

$$ds = \frac{dt}{1} = \frac{dr}{2\gamma r - \frac{\hbar K}{m}} = \frac{dK}{rm\omega^2/\hbar} = \frac{d\tilde{\rho}}{(-Dr^2/(4\hbar^2))\tilde{\rho}} \tag{14}$$

We readily obtain the three integrals

$$U_{\pm} = C_{\pm}, \quad U_3 = C_3, \tag{15}$$

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where $C_\pm$ and C_3 are integration constants and

$$U_\pm = (K - \frac{r}{\lambda_\pm}) \exp\left(\frac{-\hbar t}{m\lambda_\pm}\right), \tag{16}$$

$$U_3 = \tilde{\rho}(K, r, t) \exp\left[\frac{D}{32m\hbar(\gamma^2 - \omega^2)}\left(\lambda_+(K - \frac{r}{\lambda_+})^2\right.\right. \tag{17}$$

$$\left.\left. -\frac{2\hbar}{m\gamma}(K - \frac{r}{\lambda_+})(K - \frac{r}{\lambda_-}) + \lambda_-(K - \frac{r}{\lambda_-})^2\right)\right],$$

and $\lambda_\pm$ are constants defined by

$$\lambda_\pm = \frac{\hbar}{m\omega^2}(\gamma \pm \sqrt{\gamma^2 - \omega^2}). \tag{18}$$

If (K, r, t) and $(K', r', 0)$ are points on the curve (15), Eqs. (16) yield K', r' in terms of $U_\pm$

$$K' = \frac{U_+\lambda_+ - U_-\lambda_-}{(\lambda_+ - \lambda_-)}, \quad r' = (U_+ - U_-)\frac{\lambda_+\lambda_-}{\lambda_+ - \lambda_-}. \tag{19}$$

Eq. (17) then yields the general solution,

$$\tilde{\rho}(K, r, t) = \tilde{\rho}(K', r', 0) \exp(\alpha Z), \tag{20}$$

where

$$\alpha = \frac{D}{16m^2(\gamma^2 - \omega^2)}, \tag{21}$$

and

$$Z = \frac{1}{\gamma}(K - \frac{r}{\lambda_+})(K - \frac{r}{\lambda_-})(1 - e^{-2\gamma t}) \tag{22}$$

$$-\frac{m\lambda_+}{2\hbar}(K - \frac{r}{\lambda_+})^2(1 - e^{-\frac{2\hbar t}{m\lambda_+}})$$

$$-\frac{m\lambda_-}{2\hbar}(K - \frac{r}{\lambda_-})^2(1 - e^{-\frac{2\hbar t}{m\lambda_-}}).$$

Eq. (20) is the factorization theorem: the exact solution at an arbitray time is equal to the initial reduced density operator with shifted arguments (K', r') times the function $\exp(\alpha Z)$ which is independent of the initial conditions. It may be verified by direct substitution that the expression (20) solves Eq.(12). With $\tilde{\rho}(K, r, t)$ known, a Fourier transform yields $\rho(R, r, t)$ explicitly.

B. Free Particle Case – Starting from Eq. (10) with $\omega = 0$, or by taking the $\omega \to 0$ limit of Eqs(20)-(22), we obtain,

$$\tilde{\rho}(K, r, t) = \tilde{\rho}(K', r', 0)\left(\exp - \frac{D}{16m^2\gamma^2}\left[K^2 t + \frac{m(r - r')}{\hbar}\left((r + r')\frac{m\gamma}{\hbar} + K\right)\right]\right) \tag{23}$$

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where,

$$K' = K, r' = \frac{\hbar K}{2m\gamma} + (r - \frac{\hbar K}{2m\gamma})e^{-2\gamma t}. \tag{24}$$

The general solution (23) valid for arbitrary initial conditions agrees with the particular solution for an initial Gaussian wavepacket obtained earlier in Ref [11] except that γ should be replaced by 4γ in the solution quoted there.

III. Energy Basis Via Decoherence

A. Oscillator case – The decoherence mechanism during the system-bath interaction is known to suppress the off-diagonal elements of the reduced density matrix of the system in an appropriate basis, making all information on the system classically interpretable in that basis. For simplified models where the self-Hamiltonian of the system has either been ignored or considered co-diagonal with the interaction Hamiltonian, the preferred basis in which the density matrix becomes nearly diagonal has been believed to be the one that commutes with the interaction Hamiltonian. In the Caldeira-Leggett Model studied here, the coupling to the bath is a coordinate-coordinate coupling. Consider the solutions, Eq(20) and Eq(23) for the oscillator and the free particle, respectively, at long times ($\gamma t >> 1$) [12]. For the oscillator the solution at $t \to \infty$ for the overdamped case ($\gamma >> \omega$) is:

$$\tilde{\rho}(K, r, \infty) = \tilde{\rho}(0, 0, 0) \exp\left[-\frac{D}{16m^2\omega^2\gamma}\left(K^2 + \frac{m^2\omega^2 r^2}{\hbar^2}\right)\right]. \tag{25}$$

This limiting density matrix is actually independent of the initial density matrix $\rho(0)$ provided that $\rho(0)$ is normalized, because then

$$\tilde{\rho}(0, 0, 0) = \frac{\text{Tr}\rho(0)}{\sqrt{2\pi}} = 1/\sqrt{2\pi}.$$

The final density matrix is not diagonal in the position basis or momentum basis. For example, in the position basis we find,

$$\langle x'|\rho(\infty)|x\rangle = A \exp(-\alpha_+(x^2 + x'^2) - 2\alpha_- xx'), \tag{26}$$

where

$$A = 4mw\sqrt{\frac{\gamma}{4\pi D}}, \quad \alpha_\pm = \frac{m^2w^2\gamma}{D} \pm \frac{D}{16\hbar^2\gamma}. \tag{27}$$

Since $\rho(\infty)$ is Hermitian, we seek an orthonormal complete set of states $|\phi_n\rangle$ s.t.

$$\rho(\infty)|\phi_n\rangle = \lambda_n|\phi_n\rangle, \tag{28}$$

and

$$\rho(\infty) = \sum_n \lambda_n|\phi_n\rangle\langle\phi_n|. \tag{29}$$

Using the relation [13],

$$\int_{-\infty}^{\infty} e^{-(x-y)^2} H_n(\alpha x)dx = \sqrt{\pi}(1 - \alpha^2)^{n/2} H_n\left(\frac{\alpha y}{\sqrt{1 - \alpha^2}}\right), \tag{30}$$

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we find the solutions ϕ_n of (28) to be,

$$\langle x|\phi_n\rangle = A_n e^{-x^2\left(\frac{mw}{2\hbar}\right)} H_n\left(x\sqrt{\frac{mw}{\hbar}}\right), \tag{31}$$

where $H_n(x)$ are the Hermite Polynomials, and A_n are normalization constants. We also find the eigenvalues

$$\lambda_n = \frac{8m\gamma\hbar w}{D + 4m\gamma\hbar w}\left(\frac{D - 4m\gamma\hbar w}{D + 4m\gamma\hbar w}\right)^n. \tag{32}$$

Thus the final density matrix is diagonal in the basis of energy eigenstates of the oscillator (Eq. (31)). The eigenvalues λ_n form a convergent geometric series due to the inequality (7) and yield $\text{Tr}\rho(\infty) = 1$.

The Wigner function corresponding to the final density matrix is easily seen to be of Gaussian form (in agreement with a theorem of Tegmark and Shapiro [14]),

$$\begin{aligned}
W(x, p, t = \infty) &= \int_{-\infty}^{\infty} \frac{dy}{2\pi\hbar}\langle x - \frac{y}{2}|\rho(\infty)|x + \frac{y}{2}\rangle e^{ipy/\hbar} \\
&= \frac{4m\gamma w}{\pi D}\exp\left(-x^2\frac{4m^2\gamma w^2}{D} - p^2\frac{4\gamma}{D}\right).
\end{aligned} \tag{33}$$

It yields the position and momentum uncertainties

$$\Delta x = \sqrt{\frac{D}{8m^2\gamma w^2}}, \ \Delta p = \sqrt{\frac{D}{8\gamma}}, \tag{34}$$

and

$$\Delta x \Delta p = \frac{D}{8\gamma m w} > \frac{1}{2}\hbar. \tag{35}$$

The linear entropy corresponding to the final density matrix is,

$$S = \text{Tr}(\rho(\infty) - \rho^2(\infty)) = 1 - \frac{4m\gamma\hbar w}{D} > 0. \tag{36}$$

Since the density matrix for $t \to \infty$ is independent of the initial state, the final uncertainty product $\Delta x \Delta p$ and the entropy production (36) are also independent of the initial state. At intermediate times the exact density matrix (20) shows a factorized dependence on the initial density matrix which we hope to study in detail later.

B. Free Particle Case – Eq. (23) shows that due to the factor $\exp(-Dk^2t/(16m^2\gamma^2))$ on the right-hand side, the density matrix is driven to a diagonal matrix in momentum space for $t \to \infty$. Further, the diagonal elements $(K = p' - p = 0)$ become

$$\tilde{\rho}(o, r, t) \xrightarrow[t \to \infty]{} \frac{1}{\sqrt{2\pi}}\exp\left[-Dr^2/(16\gamma\hbar^2)\right].$$

Since momentum being diagonal implies energy being diagonal for a free particle, the energy basis emerges in this example too as the preferred basis for $t \to \infty$.

Conclusion – We have obtained exact solutions of the Caldeira-Leggett Master equation for the reduced density matrix for an oscillator and for a free particle for arbitrary initial conditions in a compact factorizable form. The solutions for both cases studied show that the density matrix eventually diagonalizes in the energy basis at long times though the coupling to the bath is via position. Our conclusion is in tune with the recent result of Paz and Zurek [10] where they show that eigenstates of energy emerge as pointer states, but we do not use any weak coupling approximation. The $t \to \infty$ form of our Wigner function agrees with a theorem of Tegmark and Shapiro [14]. We hope to study later the intermediate time behavior of the density matrix using the factorised exact solution obtained here.

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