THERMAL EQUILIBRIUM FROM THE
HU-PAZ-ZHANG MASTER EQUATION

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ABSTRACT: The exact master equation for a harmonic oscillator coupled to a heat bath, derived recently by Hu, Paz and Zhang, is simplified by taking the weak-coupling, late-time limit. The unique time-independent solution to this simplified master equation is the canonical ensemble at the temperature of the bath. The frequency of the oscillator is effectively lowered by the interaction with the bath.

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arXiv:hep-th/9210034v1 7 Oct 1992

INTRODUCTION

The evolution of the density matrix of a quantum harmonic oscillator linearly coupled to a heat bath is a fundamental problem, but it has only recently been solved exactly[1]. Physical quantum mechanical systems have often been idealized as isolated, with the sole effect of the environment being the maintenance of a finite temperature. The non-trivial role of the environment in decohering the excitations of a weakly-coupled system is currently still being explored; as a complement to this research, this letter examines the ground state of a harmonic oscillator weakly coupled to a heat bath.

If a system is in equilibrium with a thermal environment, to which it is weakly coupled, it has long been assumed that the reduced density matrix for the system is given by the canonical ensemble at the environmental temperature. Using the density matrix evolution equation ('master equation') derived in Reference [1], this letter confirms this assumption in the case of the harmonic oscillator. The discussion assumes familiarity with the results of Reference [1] (hereafter denoted HPZ), which will not be derived here.

THE HPZ MASTER EQUATION AT
WEAK COUPLING AND LATE TIME

In HPZ, the following master equation is derived, for the time evolution of the density matrix $\rho(x, x')$ of a simple harmonic oscillator, with the position variable x

coupled linearly to a heat bath:

$$i\frac{\partial}{\partial t}\rho = -\frac{1}{2}\left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2} - \Omega_0^2(x^2 - x'^2)\right]\rho$$
$$+ (x - x')\left[A(t)(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}) + B(t)(x + x')\right]\rho \qquad (1)$$
$$- i(x - x')\left[C(t)(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}) + D(t)(x - x')\right]\rho .$$

Here $\hbar$ and the oscillator mass have been set equal to 1. The time-dependent real co-efficients defined in HPZ have been renamed A, B, C, and D. The terms in (1) proportional to A and D are responsible for diffusive effects in the evolution of ρ. B could be considered a time-dependent addition to the effective frequency of the oscillator, while C has the effect of a time-dependent dissipation constant.

Equation (1) is derived using an initial quantum state that is a direct product of the initial oscillator and (thermal) environment states; the authors of HPZ suggest that some features of their master equation may be artifacts of this actually rather implausible initial condition. In order to avoid the spurious time dependences introduced by the artificial assumption that the oscillator and heat bath are uncorrelated at time $t = 0$, the co-efficients will be replaced by their asymptotic forms at late times: $A(t) \to A_\infty \equiv A(\infty)$, etc. Setting the RHS of (1) equal to zero, one obtains an equation for the time-independent state into which the open harmonic oscillator might be expected to settle down at late time. Equivalently, this equation can be considered to describe the ground state of a simple harmonic oscillator in the presence of a thermal environment:

$$0 = -\frac{1}{2}\left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2} - \Omega_0^2(x^2 - x'^2)\right]\rho$$
$$+ (x - x')\left[A_\infty(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}) + B_\infty(x + x')\right]\rho \qquad (2)$$
$$- i(x - x')\left[C_\infty(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}) + D_\infty(x - x')\right]\rho .$$

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The time-independent co-efficients have simple forms in the weak-coupling limit, where only terms of up to second order in the bath-oscillator coupling constant are retained[HPZ, eq. 2.46]. In the notation of the present letter,

$$
\begin{aligned}
A_\infty &= g^2 \frac{1}{\Omega_0} \lim_{t\to\infty} \int_0^t ds \int_0^\Gamma d\omega\, I(\omega) \coth \frac{\beta\omega}{2} \cos \omega s \sin \Omega_0 s \\
B_\infty &= -g^2 \lim_{t\to\infty} \int_0^t ds \int_0^\Gamma d\omega\, I(\omega) \sin \omega s \cos \Omega_0 s \\
C_\infty &= g^2 \frac{1}{\Omega_0} \lim_{t\to\infty} \int_0^t ds \int_0^\Gamma d\omega\, I(\omega) \sin \omega s \sin \Omega_0 s \\
D_\infty &= g^2 \lim_{t\to\infty} \int_0^t ds \int_0^\Gamma d\omega\, I(\omega) \coth \frac{\beta\omega}{2} \cos \omega s \cos \Omega_0 s \;.
\end{aligned}
\tag{3}
$$

$I(\omega)$ is the spectral density of the environmental heat bath, and g is the bath-oscillator coupling constant. It is assumed that $I(\omega)$ is cut off at some high frequency Γ and vanishes at least linearly at zero frequency, so that, as long as the limit $t \to \infty$ is taken last, the order of the s and ω integrals is arbitrary. The temperature of the bath is $kT = \beta^{-1}$, where k is the Boltzman constant.

In solving (2) to first order in g^2, the co-efficient B_∞ will be split into two terms:

$$
B_\infty \equiv \Omega_0 \tanh \frac{\beta\Omega_0}{2} A_\infty + \Omega_0 \delta\Omega \;.
\tag{4}
$$

The first term is chosen to provide a cancellation shown below, while the second term is a renormalizing correction to the effective frequency of the oscillator, proportional to g^2. ($\delta\Omega$ will be determined in the next section of this letter.) Define the renormalized frequency to be $\Omega \equiv \Omega_0 + \delta\Omega$.

A standard representation of the delta function allows one to write

$$
\begin{aligned}
C_\infty &= \frac{g^2 \pi}{2\Omega_0} I(\Omega_0) \simeq \frac{g^2 \pi}{2\Omega} I(\Omega) \\
D_\infty &= \frac{g^2 \pi}{2} \coth \frac{\beta\Omega_0}{2} I(\Omega_0) \simeq \frac{g^2 \pi}{2} \coth \frac{\beta\Omega}{2} I(\Omega) \;.
\end{aligned}
\tag{5}
$$

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One can therefore re-write (2) in the final form

$$
\begin{aligned}
0 = & -\frac{1}{2}\Big[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2} - \Omega^2(x^2 - x'^2)\Big]\rho \\
& + (x - x')A_\infty\Big[(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}) + \Omega\tanh\frac{\beta\Omega}{2}(x + x')\Big]\rho \\
& - i(x - x')\frac{g^2\pi}{2\Omega}I(\Omega)\Big[(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}) + \Omega\coth\frac{\beta\Omega}{2}(x - x')\Big]\rho \, ,
\end{aligned}
\tag{6}
$$

keeping only terms of up to first order in g^2. This is the weak-coupling, infinite-time limit of the exact time-independent master equation of HPZ.

Define the thermal density matrix

$$
\rho_\beta(x, x') = (1 - e^{-\beta\Omega}) \sum_{n=0}^{\infty} e^{-n\beta\Omega}\, \psi_n(x)\psi_n(x') \, ,
\tag{7}
$$

where $\psi_n(x)$ is the wave function for the nth excited state of the harmonic oscillator with frequency Ω. It will now be verified that $\rho = \rho_\beta$ is a solution to (6). The verification is straightforward, and proceeds line by line.

The first line of (6) is simply $[\hat{H}_x - \hat{H}_{x'}]\rho_\beta$, for $\hat{H}$ the harmonic oscillator Hamiltonian in the position representation, and so equals zero.

The second line is proportional to

$$
\begin{aligned}
& \sum_{n=0}^{\infty} e^{-n\beta\Omega}\Big[\Omega^{1/2}\sinh\frac{\beta\Omega}{2}(x + x') + \Omega^{-1/2}\cosh\frac{\beta\Omega}{2}(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'})\Big]\psi_n(x)\psi_n(x') \\
& = \frac{1}{\sqrt{2}}\sum_{n=0}^{\infty} e^{-n\beta\Omega}\Big[e^{\frac{\beta\Omega}{2}}(\hat{a} + \hat{a}') - e^{-\frac{\beta\Omega}{2}}(\hat{a}^\dagger + \hat{a}'^\dagger)\Big]\psi_n(x)\psi_n(x') \\
& = \frac{e^{\frac{\beta\Omega}{2}}}{\sqrt{2}}\sum_{n=0}^{\infty} e^{-n\beta\Omega}\Big[\sqrt{n}\,\psi_{n-1}(x)\psi_n(x') - e^{-\beta\Omega}\sqrt{n+1}\,\psi_{n+1}(x)\psi_n(x') + [x \leftrightarrow x']\Big] \\
& = \frac{e^{-\frac{\beta\Omega}{2}}}{\sqrt{2}}\sum_{n=0}^{\infty} e^{-n\beta\Omega}\sqrt{n+1}\Big[\psi_n(x)\psi_{n+1}(x') - \psi_{n+1}(x)\psi_n(x') + [x \leftrightarrow x']\Big] \\
& = 0 \ .
\end{aligned}
\tag{8}
$$

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Here $\hat{a} = \frac{1}{\sqrt{2\Omega}}(\Omega x + \frac{\partial}{\partial x})$, $\hat{a}^\dagger = \frac{1}{\sqrt{2\Omega}}(\Omega x - \frac{\partial}{\partial x})$, the primes imply that x is replaced by x', and ψ_n satisfies

$$\hat{a}\psi_n = \sqrt{n}\,\psi_{n-1}$$

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\,\psi_{n+1}$$

$$\psi_{-1} \equiv 0\ .$$

Similarly, the third line of (6) is proportional to

$$\sum_{n=0}^{\infty} e^{-n\beta\Omega}\Big[\Omega^{1/2}\cosh\frac{\beta\Omega}{2}(x-x') + \Omega^{-1/2}\sinh\frac{\beta\Omega}{2}(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'})\Big]\psi_n(x)\psi_n(x')$$

$$=\frac{1}{\sqrt{2}}\sum_{n=0}^{\infty} e^{-n\beta\Omega}\Big[e^{\frac{\beta\Omega}{2}}(\hat{a}-\hat{a}') + e^{-\frac{\beta\Omega}{2}}(\hat{a}^\dagger - \hat{a}'^\dagger)\Big]\psi_n(x)\psi_n(x')$$

$$=\frac{e^{\frac{\beta\Omega}{2}}}{\sqrt{2}}\sum_{n=0}^{\infty} e^{-n\beta\Omega}\Big[\sqrt{n}\,\psi_{n-1}(x)\psi_n(x') + e^{-\beta\Omega}\sqrt{n+1}\,\psi_{n+1}(x)\psi_n(x') - [x \leftrightarrow x']\Big] \qquad (9)$$

$$=\frac{e^{-\frac{\beta\Omega}{2}}}{\sqrt{2}}\sum_{n=0}^{\infty} e^{-n\beta\Omega}\sqrt{n+1}\Big[\psi_n(x)\psi_{n+1}(x') + \psi_{n+1}(x)\psi_n(x') - [x \leftrightarrow x']\Big]$$

$$= 0\ .$$

The canonical ensemble at temperature $kT = \beta^{-1}$ is therefore a solution to the late-time, weak coupling, time-independent master equation. This equation is a hyperbolic partial differential equation in the two independent variables x and x'. Normalizability of ρ requires that ρ and its derivatives decay to zero for large $|x|$ or $|x'|$. Normalizability therefore imposes Cauchy initial, final, and boundary conditions on the master equation, which in general over-determine the solution[2]. The solution which has been found is therefore unique. (The terms "initial" and "final" are used by analogy, since either x or x' may be considered to play the role of the timelike variable usually involved in hyperbolic equations.)

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DETERMINATION OF $\delta\Omega$

From equations (3) and (4) one can determine the frequency correction $\delta\Omega$. Comparing the definitions of C_∞ and D_∞, one sees that

$$\delta\Omega = -\frac{g^2}{\Omega} \lim_{t\to\infty} \int_0^\Gamma d\omega\, I(\omega) \coth\frac{\beta\omega}{2}\, R(\omega,\Omega,t)\,, \tag{10}$$

where terms of order g^4 are neglected, and R is defined by

$$R(\omega,\Omega,t) \equiv \tanh\frac{\beta\omega}{2} \int_0^t ds\, \sin\omega s \cos\Omega s + \tanh\frac{\beta\Omega}{2} \int_0^t ds\, \cos\omega s \sin\Omega s\,. \tag{11}$$

R can be evaluated by expanding the hyperbolic tangents in Taylor series, and noting that, for integer $n > 0$,

$$
\begin{aligned}
R_n(\omega,\Omega,t) &\equiv \omega^{2n+1} \int_0^t ds\, \sin\omega s \cos\Omega s + \Omega^{2n+1} \int_0^t ds\, \cos\omega s \sin\Omega s \\
&= \frac{1}{\omega^2 - \Omega^2}\Big[(\omega^{2(n+1)} - \Omega^{2(n+1)})(1 - \cos\omega t \cos\Omega) \\
&\qquad\qquad - \omega\Omega(\omega^{2n} - \Omega^{2n})\sin\omega t \sin\Omega t\Big] \\
&= \frac{\omega^{2(n+1)} - \Omega^{2(n+1)}}{\omega^2 - \Omega^2} - \sum_{m=0}^{n} \omega^{2m}\Omega^{2(n-m)} \cos\omega t \cos\Omega t \\
&\qquad - \omega\Omega \sum_{m=0}^{n-1} \omega^{2m}\Omega^{2(n-1-m)} \sin\omega t \sin\Omega t\,.
\end{aligned}
\tag{12}
$$

One then has

$$\delta\Omega = -\frac{g^2}{\Omega} \lim_{t\to\infty} \sum_{n=0}^\infty A_n \left(\frac{\beta}{2}\right)^{2n+1} \int_0^\Gamma d\omega\, I(\omega) \coth\frac{\beta\omega}{2}\, R_n(\omega,\Omega,t)\,, \tag{13}$$

where A_n are the co-efficients in the Taylor series for the hyperbolic tangent.

The oscillating functions of t in the last two lines of (12) may in fact be ignored in the limit $t \to \infty$: since $I(\omega)$ vanishes (at least) linearly at $\omega = 0$, $I(\omega) \coth\frac{\beta\omega}{2}$

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may be expanded in a series of non-negative powers of ω, and explicit calculation will show that

$$\lim_{t\to\infty} \int_0^\Gamma dx\, x^m e^{itx} = 0 \tag{14}$$

for $m \geq 0$.

Ignoring the t-dependent part of $R_n(\omega, \Omega, t)$, one therefore has, to leading order in g^2,

$$\delta\Omega = -\frac{g^2}{\Omega} \int_0^\Gamma d\omega\, I(\omega) \coth\frac{\beta\omega}{2} \left[\frac{\omega \tanh\frac{\beta\omega}{2} - \Omega \tanh\frac{\beta\Omega}{2}}{\omega^2 - \Omega^2} \right] . \tag{15}$$

In the high temperature limit, this becomes

$$\delta\Omega \mid_{\beta\to zero} = -\frac{g^2}{\Omega} \int_0^\Gamma d\omega\, \frac{I(\omega)}{\omega} , \tag{16}$$

while in the low temperature limit it approaches

$$\delta\Omega \mid_{\beta\to\infty} = -\frac{g^2}{\Omega} \int_0^\Gamma d\omega\, \frac{I(\omega)}{\omega + \Omega} . \tag{17}$$

CONCLUSION

In recent years it has been argued that open quantum systems are generically decohered by the environment to which they are coupled, in such a way that the state of the system is rapidly driven towards a mixture of eigenstates of the interaction Hamiltonian[1,3,4,5]. This phenomenon is considered to occur on a short time scale; open quantum systems in equilibrium after a long period of time have received comparatively little attention. It is nevertheless of fundamental importance to confirm that the equilibrium state of a system whose position variable is weakly coupled to a

heat bath is indeed the canonical ensemble, and not a mixture of position eigenstates. This is true at all temperatures, and is independent of the spectral density of the heat bath, to leading order in the coupling g^2.

At higher order in g^2, this result probably no longer holds. Heuristic arguments justifying the canonical ensemble typically assume weak coupling between the system and its environment. Presumably the equilibrium solution for ρ depends at higher orders in g^2 on the specific form of the spectral density $I(\omega)$.

The infinite-time limit of the master equation derived using uncorrelated initial states at $t = 0$ may be conjectured to be equivalent to the master equation one would obtain at finite times using more realistic initial conditions. The canonical ensemble is an explicit example of a state which does not (at leading order in the coupling constant) suffer wave-function collapse onto the pointer basis determined by the coupling to the environment. This supports the suggestions by several previous researchers that the role of the initial conditions in decoherence and environmentally-induced superselection needs further investigation.

ACKNOWLEDGEMENTS

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