Exact derivation of the Langevin and master equations
for harmonic quantum Brownian motion

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A many particle Hamiltonian, where the interaction term conserves the number of particles, is considered. A master equation for the populations of the different levels is derived in an exact way. It results in a local equation with time-dependent coefficients, which can be identified with the transition probabilities in the golden rule approximation. A reinterpretation of the model as a set of coupled harmonic oscillators enables one to obtain for one of them an exact local Langevin equation, with time-dependent coefficients.

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I. INTRODUCTION

The master and Langevin equations are the standard approaches to deal with irreversible phenomena. However, it is an old problem of physics to obtain such macroscopic irreversible equations departing from the reversible microscopic laws without appealing, a priori, to approximations or extra-dynamical hypotheses.

The simplest systems for which the origin of irreversibility can be studied on a microscopic basis are the harmonic linear ones [1,2], since one is able to reduce the Hamiltonian to normal modes, for which the dynamical evolution becomes trivial. With this purpose we consider many particle systems with Hamiltonians of the form

\[ H = \sum_{n=0}^{N} \sum_{m=0}^{N} \langle \psi_n | h | \psi_m \rangle b_n^\dagger b_m, \]  

(1)

which conserve the total number of quanta. For this kind of system it can be proved by a straightforward calculation that the time evolution of the creation operators is given by

\[ b_n^\dagger(t) = e^{-iHt} b_n^\dagger(0) e^{iHt} = \sum_m A_{nm}(t) b_m^\dagger(0), \]  

(2)

being \( A_{nm}(t) = \langle \psi_m | e^{-iHt} | \psi_n \rangle \) the transition amplitude between one-particle states.

From Eq. (2) the exact “Langevin” and “master” equations can be derived. This work is devoted to study these equations in order to trace the origin of

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1The meaning of Eq. (2) is clarified applying to both members of the equality the vacuum state. This means that the operator \( b_n^\dagger(t) \) creates states \( |\psi_n(t)\rangle \).
macroscopic irreversibility. In this route we show, from the reversible evolution of the system, which are the simplest, *a posteriori*, extra-dynamical hypotheses needed to understand the irreversible behavior.

II. THE MASTER EQUATION

For systems described by a Hamiltonian such as those of Eq. (1) we can obtain an exact master equation for the mean occupation number \( \langle N_n \rangle = \langle b_n^\dagger b_n \rangle \), corresponding to the state \( |\psi_n\rangle \) of the one-particle Hamiltonian \( h \), namely

\[
\frac{d \langle N_n(t) \rangle}{dt} = \sum_k W_{nk}(t) \langle N_k(t) \rangle ,
\]

or equivalently in the form of a kinetic balance equation

\[
\frac{d \langle N_n(t) \rangle}{dt} = \sum_{m \neq n} [W_{nm}(t) \langle N_m(t) \rangle - W_{mn}(t) \langle N_n(t) \rangle].
\]

The time-dependent (non-symmetrical) coefficients \( W_{nm}(t) \) are given by

\[
W_{nk}(t) = \sum_m \dot{P}_{nm}(t) P_{mk}^{-1}(t),
\]

where \( P_{nm}(t) = |A_{nm}(t)|^2 \) is the probability to find a quantum in the state \( |\psi_m\rangle \) at time \( t \) if it was in the state \( |\psi_n\rangle \) at \( t = 0 \).

We can prove Eq. (2) as follows: First, from (4), it can be checked that

\[
\langle N_n(t) \rangle = \sum_m P_{nm}(t) \langle N_m(0) \rangle ,
\]

\[\text{Eq. (3) has a simple interpretation. The mean number of quanta at the level } n \text{ at a given time } t \text{ can be obtained as a sum of the initial populations of different levels times the transition probabilities at } t \text{ from these levels (including the own } n) \text{ to the level } n.\]
provided we assumed a privileged initial condition which represents the absence of initial correlations:

\[ \langle b_m^\dagger(0)b_n(0) \rangle = \delta_{mn} \langle N_m(0) \rangle. \] (7)

Finally, as is well known, departing from the solution we can form a differential equation by derivation and eliminating the integration constants. That is, derivating (6) with respect to time and inverting this linear system to eliminate \( \langle N_m(0) \rangle \), we finally obtain (3).

III. THE LANGEVIN EQUATION

Until now the basis \( \{|\psi_n\rangle\}_{n=0,...,N} \) is any complete set of the one-particle space. In this section we consider the case in which the basis \( \{|\psi_n\rangle\}_{n=0,...,N} \) diagonalizes the unperturbed one-particle Hamiltonian \( h_0 \ (h = h_0 + v) \), such that \( H = H_0 + V \) can be thought as a set of interacting harmonic oscillators. \( H_0 \) represents the set of uncoupled oscillators and \( V \) is a linear interaction among them. Splitting the summation in such a way that one oscillator is identified as a Brownian particle and the rest as a bosonic reservoir, redefining the notation by \( \{|\psi_0\rangle, |\psi_n\rangle\}_{n=1,...,N} = \{|\Omega\rangle, |\omega_n\rangle\}_{n=1,...,N} \), \( b_0 = B \), we have \( (\hbar = 1) \)

\[ H_0 = \Omega B^\dagger B + \sum_{n=1}^{N} \omega_n b_n^\dagger b_n, \] (8)

and

\[ V = \langle \Omega|v|\Omega \rangle B^\dagger B + \sum_{n=1}^{N} \sum_{m=1}^{N} \langle \omega_n|v|\omega_m \rangle b_n^\dagger b_m + \sum_{n=1}^{N} \left( \langle \omega_n|v|\Omega \rangle b_n^\dagger B + \langle \Omega|v|\omega_n \rangle B^\dagger b_n \right). \] (9)

\(^3\)The last hypothesis has the same status as the random phase approximation.
In this case we can derive a generalized form of the Langevin equation for the position operator \( X = \frac{1}{\sqrt{2M\Omega}} (B + B^\dagger) \) of the oscillator with frequency \( \Omega \) departing from the exact solution (2) with \( n = 0 \), namely

\[
X(t) = a(t)X(0) + b(t) \frac{P(0)}{M\Omega} + f(t),
\]

(10)

\[
A_{\Omega\Omega}(t) = a(t) + ib(t), \quad f(t) = \frac{1}{\sqrt{2M\Omega}} \sum_{m=1}^{N} [A_{\Omega m}(t)b_m^*(0) + \text{h.c.}].
\]

As in this case we have two constants of integration and a particular solution \( f(t) \), \( X(t) \) satisfies a second-order differential equation like

\[
\ddot{X}(t) + \Omega^2(t)X(t) + \Gamma(t) \dot{X}(t) = F(t),
\]

(11)

with an inhomogeneous term given by

\[
F(t) = \ddot{f}(t) + \Omega^2(t)f(t) + \Gamma(t) \dot{f}(t),
\]

which represents the analogue of the stochastic acceleration in the standard Langevin equation. The unknown coefficients \( \Omega^2(t) \) and \( \Gamma(t) \), are the analogues of the time-dependent square frequency and damping factor, respectively. They can be easily determined by solving the linear system which results in replacing the two independent solutions of the homogeneous equations:

\[
\ddot{a}(t) + \Omega^2(t)a(t) + \Gamma(t) \dot{a}(t) = 0,
\]

\[
\ddot{b}(t) + \Omega^2(t)b(t) + \Gamma(t) \dot{b}(t) = 0.
\]

That is

\[
\Omega^2(t) = \frac{A_{\Omega\Omega}A_{\Omega\Omega}^* - A_{\Omega\Omega}^*A_{\Omega\Omega}}{A_{\Omega\Omega}A_{\Omega\Omega}^* - A_{\Omega\Omega}^*A_{\Omega\Omega}}, \quad \Gamma(t) = -\frac{A_{\Omega\Omega}A_{\Omega\Omega}^* - A_{\Omega\Omega}^*A_{\Omega\Omega}}{A_{\Omega\Omega}A_{\Omega\Omega}^* - A_{\Omega\Omega}^*A_{\Omega\Omega}}.
\]

(12)

\(^4\)However, its deterministic character is obvious from its definition.
IV. PERTURBATIVE CALCULATIONS

The coefficients of the master equation are in general time-dependent. We can evaluate the transition probabilities involved in these coefficients using time-dependent perturbation theory. The Fermi golden rule gives $P_{nm} = \delta_{nm} + \Gamma_{nm} t$, where

$$\Gamma_{nm} = 2\pi |\langle \psi_n | v | \psi_m \rangle|^2 \delta_t (\omega_n - \omega_m), \quad \text{for } n \neq m,$$

$$\Gamma_{nn} = -\sum_{n \neq m} 2\pi |\langle \psi_n | v | \psi_m \rangle|^2 \delta_t (\omega_n - \omega_m),$$

being $\delta_t (\alpha) = \frac{\sin^2 \alpha t}{\alpha t}$ an approximating of the Dirac delta for very long times. Using the last expressions for calculating coefficients $W_{nm}(t)$, neglecting higher order terms in the perturbation, we have the time-independent symmetrical coefficients $W_{nm}(t) = \sum_k \Gamma_{nk} (\delta_{km} - \Gamma_{km} t) = \Gamma_{nm}$, in agreement with standard results. In the case of the coefficients of the Langevin equation we must evaluate up to the second order the survival amplitude of the state $|\Omega\rangle$.

For very long times an exponential contribution dominates its time evolution, $A_{\Omega\Omega}(t) = e^{-i(\Omega + \delta \Omega - i \gamma t)t}$, with a frequency shift and a damping factor given by

$$\delta \Omega = \langle \Omega | v | \Omega \rangle + P \sum_{k=1}^{N} \frac{|\langle \omega_k | v | \Omega \rangle|^2}{\Omega - \omega_k}, \quad \gamma = 2\pi |\langle \Omega | v | \Omega \rangle|^2.$$

A straightforward calculation shows that in the exponential decay regime the coefficients of Eq. (12) are given by $\Omega(t) = \Omega + \delta \Omega$ and $\Gamma(t) = \gamma$.

V. CONCLUSIONS AND FURTHER REMARKS

We have shown that from reversible quantum mechanical laws we can obtain equations of motion as if they represented stochastic processes. However, our equations (3) and (11) describe the exact dynamical evolution of the system and in this sense they are equivalent to the Schrödinger and/or
Heisenberg equations. We also stress the fact that Eqs. (3) and (11) are local in time in contrast with the standard non-Markovian master and Langevin equations. In our case all memory effects are reduced to the knowledge of the initial conditions. The time-dependent coefficients of Eqs. (3) and (11) are uniquely determined for the amplitudes $A_{nm}(t)$ of the one-particle sector. Evaluating these amplitudes through perturbation theory, retaining up to the second order in the Dyson expansion, we retrieve the standard irreversible equations with time-independent coefficients. In Ref. [2] we have considered a particular model in which there is not interaction among bath oscillators ($\langle \omega_n | v | \omega_m \rangle = 0$). This choice allows us to reduce $H$ to normal modes (a set of uncoupled harmonic oscillators), which in the one-particle sector means that $h$ is diagonal: $h = \sum_{\nu=0}^{N} \alpha_\nu |\alpha_\nu\rangle \langle \alpha_\nu|$. In this case the transition amplitudes can be analytically obtained as

$$A_{nm}(t) = \sum_{\nu=0}^{N} e^{-i\alpha_\nu t} \langle \psi_m | \alpha_\nu \rangle \langle \alpha_\nu | \psi_n \rangle ,$$

which will allow us to extend the previous analysis beyond the perturbative calculations and determine its range of applicability in a further work.

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