

Master Langevin equations: Origin of asymptotic diffusion

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We extend the master-equation treatment of dynamical evolution of a system-plus-reservoir configuration including the propagation of initial correlations as a noise source. Specializing into the quantum harmonic oscillator coupled to a fermionic heat bath, we develop a model for the diffusion matrix in the space of diagonal density operators. It can be shown that mean values of observables undergo Langevin-like motion and, in particular, that the mean value and dispersion of the oscillator quanta approach the canonical equilibrium values. A final interpretation of the characteristics and role of the noise source is given.

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I. INTRODUCTION

The irreversible dynamics of two coupled components of a macroscopic, isolated system is a well-known textbook subject in statistical physics [1]. The most popular and useful realizations of such a situation are the Brownian particle—eventually subjected to a conservative external force field—in its thermal reservoir and the single particle in an environment of identical partners, to which it couples through a two-body interaction. The standard probabilistic approaches lead one to formulate the above problem in terms of the density matrix or the distribution function of the selected particle, whose evolution is governed by a master equation in the case of the Brownian object, and by a kinetic equation for the N -body system [2, 3]. Accordingly, the expectation values of the observables of interest satisfy damped equations of motion, whose solutions exhibit asymptotic decay towards the thermodynamic equilibrium values. Complementary to the dissipative behavior of the mean values, the covariances and dispersions bring into evidence the diffusive action of the heat bath, whose strength is related to the intensity of the damping through a fluctuation-dissipation relationship [4–7]. Such effects have been extensively investigated for both the classical and the quantal Brownian motion; however, a statement of the fluctuation-dissipation theorem in the quantal case has not been made for general thermal environments surrounding the macroscopic particle.

More recently, due to the increasing amount of experimental work devoted to extract information of far-from-equilibrium dynamics in N -fermion systems such as nuclei, new insights have been put forward regarding the role of the reservoir. The initial cluster correlations [8] seem to be very substantial in the process of fragment formation preceding the disassembly of a hot nucleus, and the so-called phase-space fluctuations [9, 10] are capable of accounting for a variety of dynamical effects involving the moments of the one-body distribution function. In this context, and in the same spirit of for-

mer authors such as Bixon and Zwanzig [11] and Van Kampen [12], Ayik and Grègoire [9] have recently developed an extension of the Boltzmann-Uehling-Uhlenbeck (BUU) kinetic equation that attempts to incorporate the initial two-body correlations with which the N -body system is constructed, in the manner of a fluctuating source appearing in the above equation of motion. The distribution function in the Wigner representation then becomes a stochastic variable in distribution space, and this character is transmitted to every mean value of dynamic observables. This view has been complemented by the approach of Randrup and Remaud [10], who derive the same evolution equations in phase space stemming from a Fokker-Planck description of the stochastic Wigner function. While several numerical experiments have been already published [13, 14] along these lines, the manifestations of the noise upon the collective variables have been also investigated [15] in the close-to-equilibrium regime, giving rise to a clear Brownian behavior with a well-identified fluctuation-dissipation relationship.

In the standard derivation of the master equation, the initial system-reservoir correlations are usually disregarded; such a procedure is valid insofar as one is interested in the asymptotic regime, since usually the lifetime of microscopic correlations is short in a macroscopic environment. However, as in the N -particle system, initial correlations may be relevant in the small time scale, where their propagation gives rise to stochastic kicks on the evolving density matrix of the Brownian particle. It is then of interest to take a deeper view on the characteristics of the noise associated to the initial system-reservoir correlations and attempt to achieve an interpretation of the origin of their fluctuation-dissipation relationship.

For this sake, in this work we adopt Ayik and Grègoire's point of view and develop a model for the fluctuating source in the master equation of a quantal harmonic oscillator in a fermionic heat bath [16–19]. This is presented in Sec. II. In Sec. III, we discuss the effects of this noise on the oscillator observables and dispersions; in particular, we give a prescription to extract the diffusion

coefficient for any quantity, once the diffusion matrix in probability space is known. The whole procedure is illustrated computing the correct dispersion in the phonon number. The discussion and final summary is presented in Sec. IV.

II. STOCHASTIC BROWNIAN MOTION MODEL

The physical problem under consideration is the relaxation of a system S due to its coupling to a heat reservoir \mathcal{R} . Let H be the total Hamiltonian of the combined system-plus-reservoir configuration,

$$H = H_S + H_R + H_{SR}, \quad (1)$$

with H_{SR} the driving interaction and let, at any time t ,

$$\rho(t) = \rho_S(t)\rho_R(t) + \rho_{SR}^{(c)} \quad (2)$$

be the total density operator, with $\rho_{SR}^{(c)}$ the correlated, i.e., nonfactorizable, contribution to the statistical matrix. The well-known reduction-projection techniques [16] lead to the master equation for the reduced density matrix of the system in the form

$$\begin{aligned} \dot{\rho}_S(t) = & -i[H_S + \text{Tr}_R H_{SR} \rho_R(t), \rho_S(t)] \\ & + \int_0^t d\tau \text{Tr}_R [H_{SR}, [H_{SR}, \rho_S(t-\tau)\rho_R(t)]] \\ & -i \text{Tr}_R [H_{SR}, e^{-iHt} \rho_{SR}^{(c)}], \end{aligned} \quad (3)$$

where H_{SR} denotes the interaction Hamiltonian in Heisenberg representation and Tr_R indicates a tracing operation on the heat bath variables. A symmetric equation holds for the thermal reservoir; however, in most applications the latter is an extended object assumed to be in thermodynamical equilibrium at any stage of the time evolution of the system S , i.e. $\rho_R(t) = \rho_R(0) = \rho_R^{\text{eq}}$.

In commonly investigated situations appearing in quantum optics and nuclear or condensed matter physics, the last term on the right-hand side of Eq. (3) plays no role, either because one assumes that no initial correlations have been built in the total system, or due to the additional hypothesis that, even if such correlations had been present, they would have damped away within a time scale much shorter than the actual observation time t . It is then clear that within the lifetime associated to the evolution kernel e^{-iHt} , the macroscopically large diversity of choices for the irreducible matrix $\rho_{SR}^{(c)}$, which remains an unknown entity for an observer concentrated on the system S , permits one to regard the propagating correlations as some external stochastic noise. In this sense, the reduced density $\rho_S(t)$ is a stochastic process in Liouville space that undergoes Brownian motion according to the functional Langevin equation (3).

In order to fix ideas, we consider a quantum harmonic oscillator coupled to an arbitrary heat reservoir. The master equation for the occupation probability ρ_n of the n th oscillator state is well known; thus in the Markovian limit one can write

$$\begin{aligned} \dot{\rho}_n(t) = & W_+ [(n+1)\rho_{n+1} - n\rho_n] \\ & + W_- [n\rho_{n-1} - (n+1)\rho_n] + \delta K_n(t), \end{aligned} \quad (4)$$

where

$$\delta K_n(t) = -i \langle n | \text{Tr}_R [H_{SR}, e^{-iHt} \rho_{SR}^{(c)}(0)] | n \rangle \quad (5)$$

is the contribution of the noise source to the time derivative of the population. A more elaborate description of the fluctuating kernel (5) depends on the specific choice of the interaction H_{SR} , which in turn determines the structure of the downwards and upwards transition rates, respectively, W_+ and W_- in Eq. (4). In favor of a definite illustration, we select the quantal Brownian motion (QBM) [16–19] model that considers the coupling of the oscillator to a fermionic heat bath. The QBM interaction is

$$H_{SR} = \sum_{\alpha, \mu} (\lambda_{\alpha\mu} \Gamma^\dagger b_\mu^\dagger b_\alpha + \lambda_{\alpha\mu}^* \Gamma b_\mu^\dagger b_\alpha), \quad (6)$$

where Γ^\dagger and b^\dagger (Γ and b) are boson and fermion creation (annihilation) operators, respectively. The transition rates read as

$$W_\pm = 2\pi \sum_{\alpha, \mu} |\lambda_{\alpha\mu}|^2 \delta(\mathbf{k}_\alpha - \mathbf{k}_\mu - \mathbf{q}) \times \begin{cases} \rho_\mu(1 - \rho_\alpha) \\ \rho_\alpha(1 - \rho_\mu) \end{cases}, \quad (7)$$

where \mathbf{k}_i , ε_i , and ρ_i are the momentum, the single particle, and the Fermi-Dirac population of the fermion state $|i\rangle$, and Ω and \mathbf{q} are the energy and momentum of an oscillator quantum, related by the dispersion law

$$\Omega = c_s |\mathbf{q}| \quad (8)$$

with c_s the speed of sound in the macroscopic environment. Furthermore, one has the detailed balance relationship

$$\frac{W_-}{W_+} = e^{-\Omega/T} \quad (9)$$

at any temperature T ; the transition rates (7) can be explicitly computed for a free Fermi gas [20], assuming constant coupling matrix elements $\lambda_{\alpha\mu} = \lambda$, giving

$$\begin{aligned} W_+ = & \frac{m |\lambda|^2}{q \lambda_T^2} \ln \frac{1 + \exp[-\beta(\frac{1}{2}mc_s^2 + \frac{1}{8m}q^2 - \frac{1}{2}\Omega - \mu)]}{1 + \exp[-\beta(\frac{1}{2}mc_s^2 + \frac{1}{8m}q^2 + \frac{1}{2}\Omega - \mu)]} \\ & \times (1 + \bar{n}_1), \end{aligned} \quad (10)$$

$$W_- = W_+ \frac{\bar{n}_1}{1 + \bar{n}_1}. \quad (11)$$

In these expressions, $\lambda_T = (2\pi/mT)^2$ is the thermal wavelength of fermions of mass m , \bar{n}_1 is the mean number of oscillator quanta at temperature T ,

$$\bar{n}_1 = \frac{1}{e^{\Omega/T} - 1}, \quad (12)$$

and μ is the fermion chemical potential. Moreover, introducing the effective decay rate

$$\nu = W_+ - W_-, \quad (13)$$

we realize that

$$W_+ = \nu(1 + \bar{n}_1), \quad (14)$$

$$W_- = \nu\bar{n}_1. \quad (15)$$

Now considering the interaction (6), after some algebra one finds the following simple appearance for the noise source in Eq. (5):

$$\begin{aligned} \delta K_n(t) = & -i \sum_{\alpha, \mu} [\lambda_{\alpha\mu} \sqrt{n} \langle n-1, \alpha | \rho_{SR}^{(c)} | n, \mu \rangle \\ & - \lambda_{\alpha\mu}^* \sqrt{n+1} \langle n, \alpha | \rho_{SR}^{(c)} | n+1, \mu \rangle] e^{-i(\Omega - \epsilon_\alpha + \epsilon_\mu)t}. \end{aligned} \quad (16)$$

As in previous developments of the QBM model [16–20], the notation here employed for matrix elements indicates a transition from a configuration with a given number of oscillator quanta and one labeled fermion state, to another configuration with plus or minus one boson and a different fermion state, the remaining $N-1$ fermions not undergoing any transition. If we now introduce an ensemble of initial conditions on which all fluctuating quantities may be averaged, it is clear that the noise source (5) averages to zero, i.e.,

$$\overline{\delta K_n(t)} = 0, \quad \forall n, \quad (17)$$

since the ensemble contains all possible matrix elements of $\rho_{SR}^{(c)}$ appearing in (16) with all possible phases.

One needs to know the correlation $\overline{\delta K_n(t) \delta K_{n'}^*(t)}$ in order to characterize the fluctuations. A computation of such a quantity for a quantum system has been performed by Ayik and Grègoire [9] in the frame of the Boltzmann-Langevin equations for fermions [actually, the so-called (BUU) kinetic equation enriched with the propagation of initial two-body correlations]. Their derivation is based on two major assumptions: (i) the two-body correlation operator ρ_2^c is expressed as the Hermitian adjoint of the two-body interaction; and (ii) the time correlation of ρ_2^c at time $t=0$ can be replaced by its value at a finite time

$$\begin{aligned} 2D_{nn'}(t) = & \delta_{nn'} \{ W_+ [(n+1)\bar{\rho}_{n+1} + n\bar{\rho}_n] + W_- [n\bar{\rho}_{n-1} + (n+1)\bar{\rho}_n] \\ & - \delta_{n-1, n'} n (W_+ \bar{\rho}_n + W_- \bar{\rho}_{n-1}) - \delta_{n+1, n'} (n+1) (W_+ \bar{\rho}_{n+1} + W_- \bar{\rho}_n) \}. \end{aligned} \quad (20)$$

In this expression, $\bar{\rho}_m$ is the averaged m th level population at time t , namely the solution of the deterministic master equation [21],

$$\dot{\bar{\rho}}_m = W_+ [(m+1)\bar{\rho}_{m+1} - m\bar{\rho}_m] + W_- [m\bar{\rho}_{m-1} - (m+1)\bar{\rho}_m]. \quad (21)$$

This reflects, on the one hand, the fact that the fluctuating kick at time t originates in a correlation propagated from some arbitrary previous instant. On the other hand, the diagonal term of $D_{nn'}$ exhibits the gain-plus-loss structure characteristic of diffusion processes [12], a structure that shows up as well in the sum of both off-diagonal terms. In particular, one may compute the diffusion matrix (20) at equilibrium; let

t . A test of the validity of this assumption is the fact that this correlation kernel gives the appropriate diffusion coefficients for one-body, momentum dependent observables [15]. In what follows, we briefly summarize the main steps and hypothesis of their procedure as applied to the present case, for which we interpret the correlation matrix elements in Eq. (16) as the transition amplitudes

$$\rho_{n\alpha, n+1\mu}^{(c)} = \langle \Phi_{SR}(n) | \Gamma^\dagger b_\alpha^\dagger b_\mu | \Phi_{SR}(n) \rangle, \quad (18)$$

where $|\Phi_{SR}(n)\rangle$ is the reservoir plus system state that involves n phonons:

(1) As one writes the noise correlation, i.e., $\delta K_n(t) \delta K_{n'}^*(t')$ in terms of (16), eight terms involving a product of two correlation matrices appear. One then assumes that the averaging procedure in the ensemble of initial conditions, denoted by the overbar, suppresses the intermediate generalized projector operator in the product $\overline{\rho^{(c)}(t) \rho^{(c)}(t')}$. In other words, a typical contribution is

$$\begin{aligned} & \overline{\rho_{n\mu, n-1\alpha}^{(c)}(t) \rho_{n'-1\alpha', n'\mu'}^{(c)}(t')} \\ & = \langle \Phi_{SR}(n) | \Gamma^\dagger b_\mu^\dagger b_\alpha \Gamma b_{\alpha'}^\dagger b_{\mu'} | \Phi_{SR}(n') \rangle. \end{aligned}$$

The indicated matrix element then becomes a product of boson and fermion occupation numbers. In addition, in the noise correlation, each term contains a phase factor, which for the above contribution is $e^{i(\Omega - \omega_{\alpha\mu})(t-t')}$.

(2) The noise correlation thus obtained is now integrated over the time difference $t-t'$. This gives rise to the energy conserving kernel $\delta(\Omega - \omega_{\alpha\mu})$ that appears in the transition probabilities in Eq. (7).

(3) Finally, one introduces an effective white noise,

$$\overline{\delta K_n(t) \delta K_{n'}^*(t)} = \delta(t-t') 2D_{nn'}(t) \quad (19)$$

whose correlation matrix $D_{nn'}(t)$ is the integrated correlation matrix of the actual noise, as arising from steps 1 and 2, where the occupation numbers have been taken at the current time t . Its expression is

$$\bar{\rho}_n^{\text{eq}} = \frac{1}{1 + \bar{n}_1} e^{-nx} \quad (22)$$

with $x = \Omega/T$ and \bar{n}_1 given in (12). One finds, recalling Eq. (13),

$$\begin{aligned} D_{nn'}^{\text{eq}} = & \nu e^{-nx} \{ \delta_{nn'} [(n+1)e^{-x} + n] - \delta_{n-1, n'} n \\ & - \delta_{n+1, n'} (n+1)e^{-x} \}. \end{aligned} \quad (23)$$

The role of $D_{nn'}(t)$ as the diffusion matrix for the population of oscillator quanta becomes clear on very simple grounds. Indeed, close to thermodynamic equilibrium the average occupation evolves as [21, 22]

$$\dot{\bar{\rho}}_n(t) = \rho_n^{\text{eq}} + e^{-\nu t} \rho_n(0) \quad (24)$$

with the decay rate ν given in (13). Thus the presence of an added fluctuating velocity δK_n [Eq. (24)] should be replaced by

$$\rho_n(t) = \rho_n^{\text{eq}} + e^{-\nu t} \rho_n(0) + \int_0^t dt' e^{-\nu(t-t')} \delta K_n(t'). \quad (25)$$

We can then compute the covariance of the occupation probabilities,

$$\sigma_{n,n'}^2(t) = \overline{\delta \rho_n(t) \delta \rho_{n'}(t)} \quad (26)$$

with $\delta \rho_n = \rho_n(t) - \overline{\rho_n(t)}$. A closed expression can be attained if we specialize $D_{n,n'}(t)$ into its equilibrium value (20); in such a case, we get an integrated formula,

$$\sigma_{n,n'}^2(t) = \frac{D_{n,n'}^{\text{eq}}}{\nu} (1 - e^{-2\nu t}) \quad (27)$$

valid for $\nu t \gg 1$.

III. BROWNIAN MOTION OF OBSERVABLES

Given the stochastic time evolution (4), any operator Q acting on the system coordinates that exhibits a diagonal part $\sum_n Q_n |n\rangle \langle n|$ in the Fock basis will undergo Brownian, Langevin-like evolution with multiplicative noise. Indeed, the expectation value

$$q(t) = \text{Tr}[Q \rho_s(t)] \quad (28)$$

$$= \sum_n Q_n \rho_n(t) \quad (29)$$

(where Tr means a tracing operation on the Hilbert space of the system) satisfies

$$\dot{q}(t) = K_q(t) + \delta K_q(t) \quad (30)$$

with $K_q(t) = \sum_n Q_n \bar{\rho}_n(t)$ a dissipative velocity and $\delta K_q(t) = \sum_n Q_n \delta K_n(t)$ a stochastic noise with correlation

$$\overline{\delta K_n(t) \delta K_{n'}(t')} = \sum_{n,n'} Q_n 2D_{nn'}(t) Q_{n'} \delta(t-t') \quad (31)$$

$$= \delta(t-t') 2D_Q(t) \quad (32)$$

being $D_Q(t)$ the diffusion parameter for this stochastic field. From (26), one may as well extract the dispersion of the observable

$$\sigma_Q^2 = \overline{\delta q^2(t)} = \overline{q^2(t)} - [\overline{q(t)}]^2. \quad (33)$$

In addition, we note that since the fluctuation $\delta q(t)$ is induced by $\delta \rho(t)$,

$$\delta q(t) = q(t) - \overline{q}(t) \quad (34)$$

$$= \sum_n Q_n \delta \rho_n \quad (35)$$

we have

$$\sigma_Q^2(t) = \sum_{n,n'} Q_n \sigma_{nn'}^2(t) Q_{n'}. \quad (36)$$

From (24), (27), and (30) we thus learn that in the close-to-equilibrium regime,

$$\sigma_Q^2(t) = \frac{D_Q^{\text{eq}}}{\nu} (1 - e^{-2\nu t}). \quad (37)$$

Moreover, in addition to arbitrary observables, one could consider the moments of the density operator ρ_S as stochastic processes. In other words, if

$$n_k(t) = \text{Tr}[n^k \rho_s(t)] \quad (38)$$

$$= \sum_n n^k \rho_n(t) \quad (39)$$

it is straightforward to show that Eq. (4) is equivalent to the coupled system [22, 23],

$$\begin{aligned} \dot{n}_k &= W_+ \sum_{p=0}^{k-1} (-1)^{k-p} \binom{k}{p} n_{p+1} \\ &+ W_- \sum_{p=0}^{k-1} \binom{k+1}{p} n_p + k W_- n_k \\ &+ \delta K_k(t) \end{aligned} \quad (40)$$

with the specific noise source

$$\delta K_k(t) = \sum_n n^k \delta K_n(t). \quad (41)$$

Since the analytical solution of the deterministic system for the ensemble averages \bar{n}_k is known, one might in principle fold the fluctuations (41) into that solution and obtain the fluctuating moments $n_k(t)$. A set of correlations $\sigma_{kk'}^2 = \overline{\delta n_k \delta n_{k'}}$ could be established in this manner; this is just an alternative to the covariance matrix $\sigma_{nn'}^2$ of Eq. (27). Being both a moment and an observable, the mean number of quanta \bar{n}_1 , proportional to the mean excitation energy of the oscillator, is specially interesting. One easily obtains from (40),

$$\dot{n}_1 = -\nu n_1 + W_- + \delta K_1(t) \quad (42)$$

whose fluctuating solution is

$$\begin{aligned} n_1(t) &= n_1(0) e^{-\nu t} + \bar{n}_1 (1 - e^{-\lambda t}) \\ &+ \int_0^t dt' e^{-\nu(t-t')} \delta K_1(t') \end{aligned} \quad (43)$$

keeping in mind the relation (15).

The boson occupation number \bar{n}_1 is then recovered as the equilibrium ensemble averaged first moment; its covariance (33), (36) is

$$\sigma_{n_1}^2(t) = \frac{D_1^{\text{eq}}}{\nu} (1 - e^{-\nu t}), \quad (44)$$

while a straightforward calculation of the diffusion coefficient defined in Eq. (23) gives, at any time,

$$2D_1(t) = W_- + (W_+ + W_-) \bar{n}_1(t). \quad (45)$$

Using (13), we readily obtain

$$D_1^{\text{eq}} = \nu \bar{n}_1 (1 + \bar{n}_1), \quad (46)$$

i.e.,

$$\sigma_{n_1}^{\text{eq}} = \bar{n}_1 (1 + \bar{n}_1). \quad (47)$$

Equation (47) expresses a well-known relationship for the dispersion of the mean photon number in a fluctuating electromagnetic field with detailed balance (see, for example, Refs. [22, 23] and references therein), while Eq. (46) is the particular fluctuation-dissipation relationship for a boson system. The specific nature of the driving mechanism and the thermal environment appear in the dissipation rate ν , which for a fermionic reservoir reads [cf. Eqs. (10) and (13)] as

$$\nu = \frac{m |\lambda|^2}{q \lambda_T^2} \ln \frac{1 + \exp[-\beta(\frac{1}{2}mc_s^2 + \frac{1}{8m}q^2 - \frac{1}{2}\Omega - \mu)]}{1 + \exp[-\beta(\frac{1}{2}mc_s^2 + \frac{1}{8m}q^2 + \frac{1}{2}\Omega - \mu)]}. \quad (48)$$

IV. SUMMARY AND CONCLUSIONS

In this work we have analyzed the temporal evolution of the QBM model (i.e., a fermionic system coupled to a bosonic heat reservoir) when the effects of the initial correlations between the system of interest and the bosonic bath are taken into account.

These correlation terms give rise to a noise source whose statistical properties are given by its mean value (over the ensemble) and its temporal correlation. The latter has a structure of the type gain+loss which is characteristic of the diffusion process. This term is of primary importance because it appears in the evaluation of the fluctuations of the observables.

At this point, it is interesting to summarize the way in which this term is calculated. First, using the standard techniques developed for the resolution of the QBM model one obtains an expression for the time correlation of the noise source. This result already contains a specific selection of the system-plus-reservoir correla-

tion operator. Next, one sums up all the contributions for all times and then one makes the assumption introduced in Ref. [9] that at any time t the correlation of the noise source can be replaced by an effective white Gaussian one with the same diffusion matrix. This is the expression that we use to calculate the fluctuations of the observables; in particular, when the observable is the occupation number \bar{n}_1 the correct asymptotic limit is obtained.

It must be stressed that the above procedure is in fact equivalent to replacing the true initial (nonkinetic [2]) correlation by some kinetic one which gives the same diffusion matrix in density matrix space. In this way one does not keep track of uncontrollable correlations; instead, one contemplates in the description only the strictly kinetic ones appearing in the collision kernel corresponding to the close to equilibrium evolution, which of course produce the correct asymptotic regime. This means that although some extra degree of stochasticity has been introduced in the description, it is not related to the early history of the system but is a manifestation of the dynamics itself in the long-time run.

The results here encountered support the idea that the kinetic correlations are those responsible for the asymptotic diffusive behavior of real systems, once the initial nonkinetic ones have been washed away by the collisions.

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