Fluctuations of Quantum Currents and Unravelings of Master Equations

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Abstract The very notion of a current fluctuation is problematic in the quantum context. We study that problem in the context of nonequilibrium statistical mechanics, both in a microscopic setup and in a Markovian model. Our answer is based on a rigorous result that relates the weak coupling limit of fluctuations of reservoir observables under a global unitary evolution with the statistics of the so-called quantum trajectories. These quantum trajectories are frequently considered in the context of quantum optics, but they remain useful for more general nonequilibrium systems. In contrast with the approaches found in the literature, we do not assume that the system is continuously monitored. Instead, our starting point is a relatively realistic unitary dynamics of the full system

Keywords Weak coupling limit · Quantum stochastic calculus · Quantum fluctuations

1 Introduction

Certain aspects in the combination of nonequilibrium physics with quantum theory are often more problematic than their counterparts in nonequilibrium *classical* statistical mechanics. An important reason is that in statistical mechanics one often starts from fluctuation theory and from estimates of statistical deviations. But in the quantum case, even for *equilibrium* statistical mechanics, there is no standard large deviation theory (although recently progress

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was made in [23, 32, 39] and in the nonequilibrium case in [1]). For nonequilibrium purposes one wants to go beyond first order perturbation theory around equilibrium, i.e. beyond covariance estimates. The question then emerges what one accepts as the definition of (also large) fluctuations of heat, work and currents.

As it is often the case, such questions are more prone to confusion when working in the quantum formalism. Since recent developments in nonequilibrium physics have focused on fluctuations (of entropy production), quantum analogues have been attempted by many different groups, etc. [20, 21, 30, 36–38, 42, 43, 45].

Throughout this article, we choose the setup of a system connected to heat reservoirs and the fluctuations we study, are fluctuations of the heat currents.

In Sect. 2, we present two possible approaches to fluctuations in a Hamiltonian setup. These approaches have appeared repeatedly in the above-quoted articles. We remark that they are equivalent as far as the mean and the variance are concerned.

In Sect. 3, we put the Hamiltonian description aside in favor of an effective model—a quantum master equation derived in the so-called weak coupling limit. In the framework of this master equation, we can again distinguish different approaches. One of these is the formalism of quantum trajectories, which is discussed in Sect. 4. In Sect. 5, we combine the Hamiltonian description with the effective model. Our main result is contained in formula (5.1). It states that the fluctuations calculated by quantum trajectories are limits of the fluctuations in the Hamiltonian description. This result supplements the well-known derivation of the master equation, be it its rigorous form, as in [14], or a more heuristic derivation, as in [12].

One can further remark that both the fluctuations in the quantum trajectory picture [43] and the fluctuations in our Hamiltonian description satisfy the celebrated Gallavotti-Cohen fluctuation theorem, see [41] for a discussion. However, stressing this point would be misleading because one does not need the weak-coupling limit to state the Gallavotti-Cohen fluctuation theorem.

The work is mostly inspired by and based on [18, 43]. Section 6 presents a summary of mathematical arguments and states the main message of this paper as a theorem.

2 What is a Current Fluctuation?

2.1 Question

Imagine several heat reservoirs R_k, indexed by $k \in K$. Each reservoir is in thermal equilibrium at inverse temperatures β_k and well separated from the others. All heat reservoirs are connected with a small system S through a coupling term proportional to a small coupling constant λ. Formally, the composite system is described by a quantum Hamiltonian

$$H_\lambda = H_S + \sum_{k \in K} H_{R_k} + \lambda \sum_{k \in K} H_{S-R_k}, \qquad (2.1)$$

in which one assumes a clear separation between the reservoir Hamiltonians H_{R_k} and the interaction H_{S-R_k}. The dynamics of the full system $S + \sum_k R_k$ is given by the unitary group $e^{-it H_\lambda}$ on a Hilbert space of the form "system $\otimes$ reservoirs." Imagine that the coupling between the system and the reservoirs starts at a certain initial moment. We take the initial state represented by a density matrix ρ_0 of the form

$$\rho_0 = \rho_S \otimes \left[\bigotimes_{k \in K} \rho_{k, \beta_k} \right], \qquad (2.2)$$

where the states ρ_{k,β_k} are equilibrium states at β_k on the kth reservoir, and ρ_S is an arbitrary density matrix on S.

We want to ask how much energy has flown out of/into the different reservoirs after some time t, and how this quantity fluctuates. In the classical setup, there is no ambiguity as to what that means: There one has a phase space X for the total system with a Hamiltonian flow $x \mapsto x_t$ and the object of interest is the variable (function on X)

$$x \mapsto H_{R_k}(x_t) - H_{R_k}(x), \tag{2.3}$$

where H_{R_k} now also represents the energy of the reservoir. Usually (but not necessarily), one starts from an initial distribution ρ_0, rather than from a fixed phase space point $x \in X$, such that the above variables are actually random variables subject to some overall constraints like total energy conservation. A natural method to study the fluctuations of (2.3) is to proceed via its characteristic function, for $\kappa \in \mathbb{R}^{|K|}$, with coefficients κ_k:

$$\int \rho_0(\mathrm{d}x) \mathrm{e}^{-\mathrm{i}\sum_{k \in K} \kappa_k (H_{R_k}(x_t) - H_{R_k}(x))}. \tag{2.4}$$

Often, this formula is expressed in terms of a time-integrated current.

We now switch back to the quantum case. It seems that there is more than one way to generalize (2.4), as has been remarked by several authors.

2.2 Answer 1

The question amounts to choosing a quantization of the observable contained in (2.4). Following the usual quantum dictionary one is tempted to introduce a "current operator"

$$I_k(t) := -\mathrm{i}U^{\lambda}_{-t}[H_{\lambda}, H_{R_k}]U^{\lambda}_t, \tag{2.5}$$

where $U^{\lambda}_t := \mathrm{e}^{-\mathrm{i}t H_{\lambda}}$ is the dynamics generated by the total Hamiltonian H_{λ} and H_{R_k} is the free Hamiltonian of the kth reservoir only. Obviously,

$$U^{\lambda}_{-t} H_{R_k} U^{\lambda}_t - H_{R_k} = \int_0^t \mathrm{d}u \, I_k(u) \tag{2.6}$$

and one might set out to study fluctuations of the heat by considering fluctuations of the operator (2.6). This amounts to replacing (2.4) directly with

$$\rho_0 \left[\mathrm{e}^{-\mathrm{i}\sum_{k \in \mathcal{K}} \kappa_k (U^{\lambda}_{-t} H_{R_k} U^{\lambda}_t - H_{R_k})} \right]. \tag{2.7}$$

The expression (2.7) looks rather elegant but we do not know of any experiment or theoretical consideration where this quantity enters naturally. Observe for example that $U^{\lambda}_{-t} H_{R_k} U^{\lambda}_t$ does not in general commute with H_{R_k}, hence their difference does not seem to be easily measurable. We therefore prefer a more operational definition that we present in the next section. Nevertheless, the current operator as defined through (2.5) has its place in the literature, e.g. in the quantum formulation of the Green-Kubo relations [26, 46]. As we remark in Sect. 2.4, the definition (2.5) coincides in the first and second order with the definition which we present below. Hence, for the Green-Kubo relation, it does not matter which definition of current fluctuations one chooses.

2.3 Answer 2

A quantity that seems more relevant practically is the following: Assume for simplicity that $(H_{R_k})_{k \in K}$ have discrete spectrum, indicating that we have not taken the thermodynamic limit and let $x \in X$ label a complete set of eigenvectors $|x\rangle$ of $(H_{R_k})_{k \in K}$ with eigenvalues $(H_{R_k})_{k \in K}(x)$. The corresponding spectral projections are denoted $P_x := |x\rangle\langle x|$ and, by a slight abuse of notation, we use the same symbol P_x to denote $1 \otimes P_x$, where 1 is the identity on $\mathcal{H}_S$. Then we define the characteristic function as

$$\chi(\kappa, t, \lambda, \rho_0) := \sum_{x,y \in X} \text{Tr}\left[P_y U_t^\lambda P_x \rho_0 P_x U_{-t}^\lambda P_y \right] e^{-i \sum_{k \in \mathcal{K}} \kappa_k (H_{R_k}(y) - H_{R_k}(x))}. \quad (2.8)$$

The idea behind this formula is clear: measure the reservoir energies (thereby projecting the reservoirs on the eigenstates x), at time $s = 0$ switch on the interacting time evolution U_s^λ, at time $s = t$ switch the interaction off, and finally measure again the reservoir energies (projecting on the eigenstates y).

We now use that the initial state ρ_0 is diagonal in the basis $|x\rangle$ to rewrite (2.8) as

$$\chi(\kappa, t, \lambda, \rho_0) = \rho_0 \left[e^{-i \sum_{k \in \mathcal{K}} \kappa_k H_{R_k}} U_t^\lambda e^{i \sum_{k \in \mathcal{K}} \kappa_k H_{R_k}} U_{-t}^\lambda \right]. \quad (2.9)$$

Actually, we take the expression (2.9) just as our starting point. Our main result is valid only after taking thermodynamic limit, in which the operators $(H_{R_k})_{k \in K}$ have continuous spectrum and the definition of the state ρ_0 has to be reconsidered. Nevertheless we will see further on that (2.9) has a well defined thermodynamic limit.

Usually, when considering a system interacting with reservoirs, it is assumed that only system observables can be measured, since the reservoirs are very large and difficult to control. Equation (2.9) does not follow this rule: it involves measuring reservoir observables H_{R_k}. Note, however, that H_{R_k} are reservoir observables of a special kind: they commute with H_0, and hence they are constants of motion for the free dynamics, which acts outside the time interval $[0, t]$. Measuring of H_{R_k} at times 0 and t is conceivable even if the reservoirs are large (but finite), since to do this we have an infinite amount of time: $s \in]-\infty, 0]$ for the initial measurement and $s \in [t, \infty[$ for the final one. Therefore, in our opinion, (2.9) can be viewed as measurable in realistic experiments, even though it involves reservoir observables.

This approach to fluctuations was already used in [30] for fluctuations of heat, in [42] and very recently in [45] for fluctuations of work, and, most widespread, starting in [33, 34], for fluctuations of charge transport. Note also the elegant approach to statistics of charge transport in [7, 29].

2.4 Comparison

As we have seen, the question "what is a current fluctuation?" does not have a unique answer. In any case, both definitions of current fluctuations we have discussed above coincide in the first and second moment. In other words, the first and second derivatives with respect to κ of expressions (2.7) and (2.9) coincide and are equal to

$$\rho_0 \left[\int_0^t I_k(u) du \right], \quad \rho_0 \left[\int_0^t I_k(u) du \int_0^t I_{k'}(u') du' \right] \quad (2.10)$$

or, alternatively, to

$$\rho_0 \left[U_{-t} H_{R_k} U_t - H_{R_k} \right], \quad \rho_0 \left[(U_{-t} H_{R_k} U_t - H_{R_k})(U_{-t} H_{R_{k'}} U_t - H_{R_{k'}}) \right]. \tag{2.11}$$

This can be easily checked (disregarding possible subtleties due to unboundedness of operators) by using that $[H_{R_k}, H_{R_{k'}}] = 0$ and that ρ_0 is diagonal in H_{R_k}, i.e. for all operators A:

$$\rho_0 \left[H_{R_k} A \right] = \rho_0 \left[A H_{R_k} \right]. \tag{2.12}$$

Conclusion: If one is interested in second order fluctuations, for example Green-Kubo and Onsager relations, both generating functions (2.7) and (2.9) are equivalent.

Note that the equality between (2.7) and (2.9) up to second order depends crucially on the choice of the initial state. However, often in physics, one is interested in expressions which are independent of the initial state.

Assume that the dynamics $U_{-t} \cdot U_t$ admits a unique nonequilibrium steady state ρ_∞.[1] One expects that the covariance

$$\lim_{t \uparrow +\infty} \frac{1}{t} \rho_0 \left[\int_0^t du(I_k(u) - \rho_0 \left[I_k(u) \right]) \int_0^t du'(I_{k'}(u') - \rho_0 [I_{k'}(u')]) \right] \tag{2.13}$$

which is a combination (see also (2.15)) of the two expressions in (2.10) for $t \uparrow \infty$, is independent of the initial state and in particular equal to the correlation function

$$\int_{\mathbb{R}} du \rho_\infty \left[\left(I_k(u) - \rho_\infty [I_k(0)] \right) \left(I_{k'}(0) - \rho_\infty [I_{k'}(0)] \right) \right]. \tag{2.14}$$

Using the above reasoning and standard manipulations of the cumulant generating function, one easily checks that (2.14) equals

$$- \lim_{t \uparrow +\infty} \frac{\partial^2}{\partial \kappa_k \partial \kappa_{k'}} \frac{1}{t} \log \left[\text{Expression (2.7) or (2.9)} \right] \Big|_{\kappa=0}. \tag{2.15}$$

When ρ_∞ is an equilibrium state, hence all temperatures equal, then expression (2.14) with $\rho_\infty \left[I_k(0) \right] = 0$ features in the Green-Kubo relation, as stated rigorously in [26] and specifically for quasi-free systems in [3].

Having chosen a definition of a current fluctuation in a microscopic (Hamiltonian) description, we set out to consider an effective model, arising by a certain consistent approximation. The model we will be dealing with in the present paper is that of the quantum master equation which often arises in the so-called weak coupling limit. We give some reminders in the next section, and we continue the answer to our question in Sect. 4. In Appendix B, we outline the weak coupling limit of both generating functions (2.7) and (2.9).

3 Weak Coupling Limit

One of the aims of the present paper is to supplement the user's manual for one of the best known effective equations in the physics of open quantum systems: the master equation for the long-time evolution of the density matrix of a small system with discrete spectrum in

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[1]Obviously, one needs the thermodynamical limit for this assumption to be realistic.

contact with reservoirs. It is widely accepted that master equations gives a good description of the degrees of freedom of a small system in certain limiting regimes. In the physics literature, this limiting regime is characterized by the *Born-Markov* approximation and the *rotating wave* approximation, see [2, 12] for a review. Another name, common especially in the mathematical physics literature, is the *weak coupling limit*, which makes these two approximations exact. It goes back to [24] and was made precise in [14]. Reviews focusing on the mathematical aspects are [19, 31] We start with a formal sketch of the usual set-up.

The small system is modeled by a finite-dimensional Hilbert space S and a Hamiltonian H_S—a certain Hermitian matrix. It interacts with an environment, possibly containing several reservoirs indexed by $k \in K$. Let us think of each reservoir as an assembly of free oscillators. We use the well-known notation

$$d\Gamma(h_k) = \int_{\mathbb{R}^d} dq \, h_k(q) a_k^*(q) a_k(q), \tag{3.1}$$

where h_k is a dispersion function on $\mathbb{R}^d$, the so called one-particle Hamiltonian on the one-particle Hilbert space $\mathfrak{h}_k := L^2(\mathbb{R}^d)$ and $d\Gamma(h_k)$ acts on $\Gamma_s(\mathfrak{h}_k)$, the bosonic Fock space corresponding to $\mathfrak{h}_k$.

The coupling between the system and the environment is linear in the sense that

$$H_{S-R_k} = \int_{\mathbb{R}^d} dq \, V_k \otimes \left[f_k(q) a_k^*(q) + \overline{f_k(q)} a_k(q) \right], \tag{3.2}$$

where $f_k \in \mathfrak{h}_k$ and V_k are self-adjoint operators on $\mathcal{H}_S$. The total Hamiltonian is formally given by

$$H_\lambda = H_S \otimes 1 + \sum_{k \in K} 1 \otimes d\Gamma(h_k) + \lambda \sum_{k \in K} H_{S-R_k} \tag{3.3}$$

on the Hilbert space $\mathcal{H}_S \otimes [\otimes_{k \in K} \Gamma_s(\mathfrak{h}_k)]$. Observe that the prefactor λ measures the interaction strength.

The Hamiltonian H_λ generates a quantum evolution $U_\tau^\lambda = e^{-i\tau H_\lambda}$. The weak coupling limit concerns the convergence of the reduced dynamics on the small system. The coupling $\lambda \downarrow 0$ gets very weak as the time $\tau = t/\lambda^2$ goes to infinity. A well-known theorem by Davies [14] states the following result (which is written here in a formal way, one actually needs the framework of Sect. 6 or a limiting procedure like in Appendix A to give it a precise meaning):

$$\lim_{\lambda \searrow 0} \rho_0 \left[U_{\lambda^{-2}t}^\lambda U_{-\lambda^{-2}t}^0 (S \otimes 1) U_{\lambda^{-2}t}^0 U_{-\lambda^{-2}t}^\lambda \right] = \rho_S \left[e^{t\mathcal{L}} S \right] \tag{3.4}$$

for matrices S on $\mathcal{H}_S$. The initial state $\rho_0 = \rho_S \otimes [\otimes_{k \in K} \rho_{k,\beta_k}]$ is the product of an arbitrary state (density matrix) ρ_S on $\mathcal{H}_S$ and of thermal states ρ_{k,β_k} at inverse temperatures β_k in the respective reservoirs R_k. The superoperator (acting on matrices) $\mathcal{L}$ is the generator of a completely positive dynamics obtained in the weak coupling limit. It can be written in the so called Lindblad form [35], see (4.1) below. There are of course technical conditions for (3.4) to be true, which we skip here. One should realize that (3.4) is a non-trivial statement. It specifies conditions under which the (reduced) evolution on the small system S gets autonomous. The result is however somewhat rough, at least for nonequilibrium practice, as the resulting process is just a jump process between energy levels of the system. In particular, it does not allow us to track the interactions with a given reservoir. What follows is a way to remedy that, at least on a phenomenological level.

A first observation (which can be checked from the explicit construction given in Sects. 4 and 6) is that the generator splits naturally as

$$\mathcal{L} = \sum_{k \in K} \mathcal{L}_k, \tag{3.5}$$

where each $\mathcal{L}_k$ can be defined as the object that would emerge in the weak coupling limit from the microscopic Hamiltonian by cutting the interaction with all spaces $\mathfrak{h}_k$ except for $k' = k$.

Let us see how the decomposition (3.5) can inspire us further to answer the question of Sect. 2 in the case of master equations. One can define the time-evolved current operators

$$J_k(t) = e^{t\mathcal{L}}(\mathcal{L}_k(H_S)) \tag{3.6}$$

(much in the spirit of (2.5)), where we recall that H_S is the Hamiltonian of the small system.

Now, one might conjecture that the characteristic function

$$\rho_S \left[e^{-i \sum_k \kappa_k \int_0^t du\, J_k(u)} \right] \tag{3.7}$$

is the limit of the correlation function (2.7) in the weak coupling limit. That is actually not correct! Neither is it correct that (3.7) is the limit of (2.9). (3.7), however, coincides with the limits of both (2.7) and (2.9) as far as the mean current (first moment, i.e. first derivative in κ) is concerned.

Nevertheless, in [31], one starts from the current operators (3.6) and one obtains the correct Green-Kubo relations. This is due to the fact that one does **not** calculate the variance of the current via the characteristic function (3.7), but instead, one starts from the current-current correlation function which is an analogue of (2.14). (See [43] for a more general treatment of the Green-Kubo relations in the weak coupling limit.)

In the next section, we present another (better) way to identify the fluctuations in the weak coupling limit.

4 Quantum Trajectories

Let us look a bit closer at each of the components $\mathcal{L}_k$ of the weak coupling generator. They are given by

$$\mathcal{L}_k(S) = i[E_k, S] + \sum_{\omega \in \mathrm{sp}([H_S, \cdot])} c(\omega, k) \left(V_{\omega,k} S V_{\omega,k}^* - \frac{1}{2} \{ V_{\omega,k} V_{\omega,k}^*, S \} \right), \tag{4.1}$$

where $c(\omega, k)$ are positive constants, E_k are effective Hamiltonians, sometimes called *Lamb-shifts*, and

$$V_{\omega,k} := \sum_{e,e' \in \mathrm{sp} H_S, e-e'=\omega} P_e V_k P_{e'}, \tag{4.2}$$

where now P_e are spectral projections of H_S corresponding to the eigenvalue e. The summation in (4.1) is over all differences of eigenvalues of H_S (or equivalently, over all eigenvalues

of $[H_S, \cdot]$) and in what follows we write simply $\sum_\omega$ for $\sum_{\omega \in \mathrm{sp}([H_S, \cdot])}$ and $\sum_k$ for $\sum_{k \in K}$. One now decomposes $\mathcal{L}_k = \mathcal{L}_k^0 + \sum_\omega \mathcal{J}_{\omega,k}$ with

$$\mathcal{L}_k^0(S) = \mathrm{i}[E_k, S] - \frac{1}{2} \sum_\omega c(\omega, k)\{V_{\omega,k} V_{\omega,k}^*, S\}, \qquad \mathcal{J}_{\omega,k}(S) = c(\omega, k) V_{\omega,k} S V_{\omega,k}^*, \quad (4.3)$$

where $\mathcal{J}_{\omega,k}$ is called a jump operator. It is important to keep in mind that such a splitting $\mathcal{L}_k = \mathcal{L}_k^0 + \mathcal{J}_{\omega,k}$ is not uniquely given by the generator $\mathcal{L}_k$, instead we have used information about the operators H_S and V_k to define this splitting. (See [12] for extensive comments on this non-uniqueness.)

The final *unraveling* is written as

$$\mathcal{L} = \mathcal{L}_0 + \sum_{\omega,k} \mathcal{J}_{\omega,k}, \tag{4.4}$$

where $\mathcal{L}_0 = \sum_k \mathcal{L}_k^0$. We now introduce completely positive operations $\mathcal{W}_t(\sigma)$ and Λ_t^0 given by

$$\mathcal{W}_t(\sigma) := \Lambda_{t_1}^0 \mathcal{J}_{\omega_1,k_1} \Lambda_{t_2-t_1}^0 \cdots \Lambda_{t_n-t_{n-1}}^0 \mathcal{J}_{\omega_n,k_n} \Lambda_{t-t_n}^0, \qquad \Lambda_t^0 = \mathrm{e}^{t\mathcal{L}_0}, \tag{4.5}$$

for a "trajectory" σ that labels all the jump times and actions in $\mathcal{W}_t(\sigma)$:

$$\sigma = (t_1, k_1, \omega_1; t_2, k_2, \omega_2; \ldots; t_n, k_n, \omega_n), \quad 0 \le t_1 \le \cdots \le t_n \le t. \tag{4.6}$$

Via the (norm convergent) Dyson expansion corresponding to the splitting (4.4), we have

$$\mathrm{e}^{t\mathcal{L}} = \int \mathrm{d}\sigma \, \mathcal{W}_t(\sigma), \tag{4.7}$$

where the integral over σ is the abbreviation of the following expression:

$$\sum_{n=0}^{\infty} \sum_{k_1,\ldots,k_n} \sum_{\omega_1,\ldots,\omega_n} \int_0^t \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} \cdots \int_0^{t_2} \mathrm{d}t_1 =: \int \mathrm{d}\sigma.$$

The idea is now to interpret each contribution to the sum and integral as a *quantum trajectory*. In that philosophy, the map

$$S \mapsto \mathcal{W}_t(\sigma)(S) \tag{4.8}$$

gives the (unnormalized) evolution of the system, *conditioned* on the trajectory σ. This conditioning usually means that certain measurement outcomes were obtained and that these outcomes are represented by σ.

Taking this idea just one step further, one can obtain statistics of measurement outcomes (or, in our case, currents). Define the following probability distribution on all possible σ:

$$\mathrm{d}\mathbb{P}_{\rho_S}^t(\sigma) := \mathrm{Tr}[\rho_S \mathcal{W}_t(\sigma)(1)] \, \mathrm{d}\sigma, \tag{4.9}$$

and introduce the energy counting numbers n_k^t

$$n_k^t(\sigma) := \sum_i \delta_{k_i, k}(\sigma) 1_{(t_i < t)}(\sigma) \omega_i(\sigma), \tag{4.10}$$

where the index i runs over all jumps present in σ (i.e. from 1 to n in (4.6)) and $1_{(t_i < t)}$ is the indicator function of the event that in σ, the ith jump occurs before time t. The distribution of the random variables n_k^t is inherited from (4.9) and will be used throughout. The characteristic function of the joint distribution on $n_{k \in K}^t$ is defined as

$$\chi_{\text{w.c.}}(\kappa, t, \rho_S) := \int d\mathbb{P}_{\rho_S}^t(\sigma) \left[e^{-i \sum_k \kappa_k n_k^t(\sigma)} \right]. \tag{4.11}$$

Note that (4.11) characterizes the full distribution of $n_{k \in K}^t$. The study of fluctuations indeed amounts to more than characterizing covariances, as useful as that may be within linear response theory.

A further point concerns the "classical" nature of the variables $n_k^t(\sigma)$ and the use of standard probability theory. But that is exactly the point of the present paper: these variables characterize the "quantum" fluctuations, see further in (5.1).

In the quantum optics literature, this procedure of "unraveling master equations into trajectories" is generally accepted, see e.g. [12, 13] and the recent review [10], whereas the first source of unraveling is probably in [44].

From a more fundamental point of view, one could ask how quantum trajectories and, more specifically, the variables n_k^t emerge from microscopic dynamics. The usual justification of quantum unravelings found in the literature supposes that the system is described by a so-called quantum Langevin dynamics (the solution of a quantum stochastic differential equation (QSDE)). Even though it is a unitary dynamics, it can be viewed only as a very approximate description of realistic quantum systems quite far from "first principles". To justify the use of QSDE it is usually assumed that the unitary evolution is interrupted by measurements, which, in the limit of very short times between measurements, yields a quantum Langevin equation (originally introduced by [25] in a mathematical framework, see [4] for recent developments and [22] for a physical point of view). In many cases it amounts to supplementing the quantum evolution of the small system with a stochastic evolution of classical variables in the environment.

The quantum stochastic differential equation (QSDE) or stochastic Schrödinger evolutions, and their solutions, have been studied by many authors. The random variables n_k^t correspond there to the fluctuations of (linear combinations of) number operators in the reservoir spaces of the QSDE (see e.g. [43] or [9]). We will not elaborate on this point, since it is not our central subject (see however Appendix B).

Lately, a new class of models was considered, which give also rise to QSDE's. These are the so-called "repeated interaction models", where, instead of measuring the reservoir continuously, one refreshes it, see [5, 6].

5 Connecting Unravelings with the Hamiltonian Dynamics

Our paper describes an alternative justification of quantum unravellings that we believe is in many situations more satisfactory and does not explicitly introduce continual measurements, stochasticity or "refreshing of reservoirs". We start from a class of dynamics described in Sect. 3, which are often viewed as a relatively adequate description of realistic quantum systems. We prove that, after first applying the thermodynamic limit and then taking the weak coupling limit, the quantities (2.9) converge to quantum unravellings—expressions of the form (4.11). This idea, to our knowledge, is present in the literature only in a heuristic form. What we describe is a rigorous result.

Our proof of this result involves two steps. The first step is the theorem about the extended weak coupling limit obtained by two of us [18], which says that the microscopic dynamics converges in a certain sense to an appropriate quantum Langevin dynamics. The second step (which is well known in the literature) goes from the quantum Langevin dynamics to quantum unravellings.

There exists actually an alternative proof of our result that goes directly from the microscopic dynamics to quantum unravellings, without passing through a quantum Langevin dynamics. We will indicate it briefly in Remark 6.4.

Recall that

$$H_{R_k} = d\Gamma(h_k) = \int_{\mathbb{R}^d} dq \, h_k(q) a_k^*(q) a_k(q)$$

is the (second quantized) kth reservoir Hamiltonian, cf. (3.1). Remember also the characteristic function $\chi_{\text{w.c.}}(\kappa, t, \rho_S)$ from (4.11). Here comes the main result of the paper.

Under standard conditions of the weak coupling limit as in (3.4), and with the same remark about precision as in (3.4),

$$\chi_{\text{w.c.}}(\kappa, t, \rho_S) = \lim_{\lambda \searrow 0} \rho_0 \left[e^{-i \sum_k \kappa_k d\Gamma(h_k)} U_{\lambda^{-2}t}^\lambda e^{i \sum_k \kappa_k d\Gamma(h_k)} U_{-\lambda^{-2}t}^\lambda \right]. \tag{5.1}$$

The right-hand side is of course a general instance of the weak coupling limit of (2.9). This proves that quantum trajectories provide nonequilibrium fluctuations of the time-integrated heat dissipated in a given reservoir. In particular, the properties of the distribution of n_k^t, such as these related to fluctuation theories or to Green-Kubo relations, are related to the quantum fluctuations of energy currents in the sense of (5.1) and the arguments of Sect. 2. An extensive study of the distribution associated to (3.7) was performed in [43].

6 Mathematical Statement of the Results

The main result of the paper, formula (5.1), is a consequence of the more general and abstract results proven in [18]. For the convenience of the reader, we list some simple assumptions which allow to establish (5.1) and we specify what is the exact definition of the quantities appearing on the RHS (5.1). For simplicity of presentation, we choose a special form for the one-particle Hamiltonians h_k and we restrict the physical dimension of the reservoir space d to $d = 1$.

6.1 Formal Hamiltonian

Recall the formal Hamiltonian from (3.3):

$$H_\lambda = H_S + \sum_{k \in K} H_{R_k} + \lambda V_k \otimes (a_k^*(f_k) + a_k(f_k)), \tag{6.1}$$

where now

- $H_S = H_S^*$, $V_k = V_k^* \in \mathcal{B}(\mathcal{H}_S)$ with $\dim \mathcal{H}_S < \infty$;
- $H_{R_k} = d\Gamma(h_k)$, where h_k are the one-particle Hamiltonians on the Hilbert spaces $\mathfrak{h}_k = L^2(\mathbb{R}^+)$ acting as

$$(h_k g)(x) = x g(x); \tag{6.2}$$

- $f_k \in \mathfrak{h}_k$ are coupling functions;
- $a_k^*(f_k)/a_k(f_k)$ are creation/annihilation operators on the bosonic Fock space $\Gamma_s(\mathfrak{h}_k)$.

6.2 Effective Master Equation

Given the information of Sect. 6.1 and the inverse temperatures β_k, $k \in K$, one can construct the weak-coupling generator $\mathcal{L}$, which was introduced in Sect. 3 with unspecified parameters $c(\omega, k)$ and E_k. Define the functions

$$f_k^{\beta_k}(x) := \begin{cases} \dfrac{f_k(x)}{\sqrt{e^{\beta_k x} - 1}}, & x > 0, \\[2ex] \dfrac{f_k(-x)}{\sqrt{1 - e^{\beta_k x}}}, & x < 0. \end{cases} \tag{6.3}$$

The exact expressions for the parameters $c(\omega, k)$ and E_k are (see e.g. [18])

$$c(\omega, k) = \frac{1}{2\pi} |f_k^{\beta_k}(\omega)|^2, \tag{6.4}$$

$$E_k = \sum_\omega V_{\omega,k}^* V_{\omega,k} \, \Im \int_{\mathbb{R}^+} dt \, e^{i\omega t} \int_{\mathbb{R}} dx \, e^{-itx} |f_k^{\beta_k}(x)|^2. \tag{6.5}$$

6.3 Coupling to Thermal Reservoirs

One of the subtle points of quantum statistical physics is how to describe infinitely extended bosonic reservoirs at positive temperatures. Strictly speaking, the Hamiltonian H_λ defined in (6.1) describes the reservoirs only at zero temperature—but we are interested in the case of an arbitrary temperature. (This is why H_λ was called the "formal Hamiltonian".) We need the state ρ_0 in expressions (3.4) and (5.1) to be a thermal state (which cannot be represented by a density matrix in infinite volume). In expressions (3.4), (5.1), we pretended that this state can be defined on $\mathcal{B}(\mathcal{H}_S \otimes [\otimes_{k \in K} \Gamma_s(\mathfrak{h}_k)])$, or at least on its sufficiently large subalgebra preserved by the dynamics, but this could be problematic. (This would however be a good approach for fermions!)

Fortunately, there exists a formalism that allows us to describe a system interacting with reservoirs at positive temperatures in the thermodynamic limit rigorously. This formalism was used in standard works like [8, 27, 28]. The relevance of this construction has been argued e.g. in [15, 17]. Here we just present how one should modify the dynamics of the coupled system and we point to Appendix A for a justification.

One of the ingredients of this formalism are the so-called Araki-Woods representations of the CCR. To introduce them one needs to enlarge the Hilbert space. The enlarged Hilbert space is

$$\mathcal{H} := \mathcal{H}_S \otimes \Gamma_s(\oplus_{k \in K}(\mathfrak{h}_k \oplus \mathfrak{h}_k)). \tag{6.6}$$

We define the *free Liouvillian* of the kth reservoir on $\Gamma_s(\mathfrak{h}_k \oplus \mathfrak{h}_k)$ as

$$L_{R_k} = d\Gamma(h_k \oplus (-h_k)). \tag{6.7}$$

From now on, it will be convenient to identify $\mathfrak{h}_k \oplus \mathfrak{h}_k$ with $L^2(\mathbb{R})$ such that the one-particle operator $h_k \oplus (-h_k)$ acts by multiplication with $x \in \mathbb{R}$. The generator of the dynamics is chosen as the so-called *semi-Liouvillian* (see e.g. [16] for explanations about the terminology) and it equals

$$L_\lambda = H_S + \lambda \sum_{k \in K} V_k \otimes \left(a_k^*(f_k^{\beta_k}) + a_k(f_k^{\beta_k}) \right) + \sum_{k \in K} L_{R_k}. \tag{6.8}$$

This is a formal expression, but one can easily construct the operator L_λ rigorously (see [18]). Finally, let Ω stand for the vacuum vector in $\Gamma_s(\oplus_{k\in K}(\mathfrak{h}_k \oplus \mathfrak{h}_k))$ and define the vacuum state

$$\mathrm{Vac}[\cdot] = \langle \Omega, \cdot \Omega \rangle. \tag{6.9}$$

We can now define our object of interest:

$$\chi(\kappa, t, \lambda, \rho_S) = (\rho_S \otimes \mathrm{Vac})\left[\mathrm{e}^{-\mathrm{i}\sum_{k\in K} \kappa_k L_{R_k}} \mathrm{e}^{-\mathrm{i}t L_\lambda} \mathrm{e}^{\mathrm{i}\sum_{k\in K} \kappa_k L_{R_k}} \mathrm{e}^{\mathrm{i}t L_\lambda} \right]. \tag{6.10}$$

Remark that (6.10) arises from (2.9), that is

$$\chi(\kappa, t, \lambda, \rho_0) = \rho_0\left[\mathrm{e}^{-\mathrm{i}\sum_{k\in\mathcal{K}} \kappa_k H_{R_k}} U_t^\lambda \mathrm{e}^{\mathrm{i}\sum_{k\in\mathcal{K}} \kappa_k H_{R_k}} U_{-t}^\lambda \right], \tag{6.11}$$

by replacing $[\otimes_{k\in K} \rho_{k,\beta_k}]$ by Vac, H_{R_k} by L_{R_k} and H_λ by L_λ. One can check that in finite volume both expressions coincide—in particular, the positive temperatures of the reservoirs have been incorporated directly into the functions $f_k^{\beta_k}$. In fact, the vacuum state Vac represents the product of thermal states on the appropriate algebra of observables. More details and explanations can be found e.g. in [15].

In Appendix A, a limiting procedure which constructs expression (6.10) via finite-volume approximations is explained.

6.4 Main Result

We are ready to state rigorously our main result

Theorem 6.1 *Let $\chi_{\mathrm{w.c.}}(\kappa, t, \rho_S)$ be defined via (4.11) as in Sect. 4 and with parameters (6.4), (6.5). Assume that*

(1) *The reservoir correlation functions are integrable*

$$\int_{\mathbb{R}^+} \mathrm{d}t \left| \int_{\mathbb{R}} \mathrm{d}x \, |f_k^{\beta_k}(x)|^2 \mathrm{e}^{-\mathrm{i}tx} \right| < \infty. \tag{6.12}$$

(2) *The functions $f_k^{\beta_k}$ are continuous in a neighbourhood of $(\mathrm{sp}H_S - \mathrm{sp}H_S)$.*

Then for all $\kappa \in \mathbb{R}^{|K|}$,

$$\lim_{\lambda\downarrow 0} \chi(\kappa, \lambda^{-2}t, \lambda, \rho_S) = \chi_{\mathrm{w.c.}}(\kappa, t, \rho_S). \tag{6.13}$$

This theorem is a simple consequence of Theorem 5.7 in [18]. Essentially, one proves that $\mathrm{e}^{-\mathrm{i}t\lambda^{-2}L_\lambda}$ converges to a quantum Langevin dynamics and operators like $\mathrm{e}^{-\mathrm{i}\kappa_k\lambda^{-2}L_{R_k}}$ converge to $\mathrm{e}^{-\mathrm{i}\kappa_k N_k}$, where N_k is an appropriate linear combination of number operators (see also Appendix B). The link with unravelings of master equations belongs then to standard knowledge in quantum stochastic calculus (e.g. to be found in various forms in [9, 11, 43]).

Remark 6.2 The assumptions contain a mild infrared regularity requirement, since the assumption about $f_k^{\beta_k}$ implies that $x \mapsto x^{-1/2} f_k(x) \in L^2(\mathbb{R}^+)$.

Remark 6.3 Note that one would like to strengthen the statement of Theorem 6.1 For example, one would like to have convergence of the derivatives in κ. This is possible under stronger regularity assumptions on f_k. One can also prove a version of Theorem 6.1 allowing for complex κ_k, see [40].

Remark 6.4 Although the extended weak coupling limit in [18] gives valuable insight into the limit of fluctuations (see Appendix B), one does not really it to prove Theorem 6.1. One can also rewrite $\chi(\kappa, t, \lambda, \rho_0)$ as

$$\chi(\kappa, t, \lambda, \rho_0) = (\rho_S \otimes \text{Vac}) \left[e^{-itL_{\lambda,\kappa/2}} e^{itL_{\lambda,-\overline{\kappa}/2}} \right], \tag{6.14}$$

where

$$L_{\lambda,\kappa} = H_S + \sum_{k \in K} L_{R_k} + \lambda \sum_{k \in K} V_k \otimes \left(a_k^*(e^{-i\kappa_k(h_k \oplus -h_k)} f_k^{\beta_k}) + a_k(e^{-i\overline{\kappa}_k(h_k \oplus -h_k)} f_k^{\beta_k}) \right), \tag{6.15}$$

which, at least for $\Im\kappa = 0$, reduces technically to the usual derivation of the master equation.

Appendix A

We justify (6.10) from the physical point of view. We do that by arguing that (6.10) is the thermodynamic limit of finite volume versions of (6.11).

Let for each $n \in \mathbb{N}$, $\mathfrak{h}_{k,n}$ be finite-dimensional Hilbert spaces with one-particle Hamiltonians $h_{k,n}$ and coupling functions $f_{k,n} \in \mathfrak{h}_{k,n}$. Define the finite volume evolution reservoir Hamiltonians $H_{R_k,n}$ and full Hamiltonian $H_{\lambda,n}$ by

$$H_{R_k,n} = d\Gamma(h_{k,n}),$$

$$H_{\lambda,n} = H_S + \sum_{k \in K} H_{R_k,n} + \lambda \sum_{k \in K} V_k \otimes \left(a^*(f_{k,n}) + a(f_{k,n}) \right)$$

and the finite volume thermal states on $\mathcal{B}(\Gamma_s(\mathfrak{h}_{k,n}))$ as

$$\rho_{k,\beta_k,n}[\cdot] = \frac{1}{Z_{k,n}(\beta_k)} \text{Tr}\left[e^{-\beta_k H_{R_k,n}} \cdot \right], \qquad Z_{k,n}(\beta_k) = \text{Tr}\left[e^{-\beta_k H_{R_k,n}} \right]. \tag{A.1}$$

Assume that

(1) There is a $C < \infty$ such that for all $t \in \mathbb{R}$, $k \in K$ and $n \in \mathbb{N}$,

$$\left| \rho_{k,\beta_k,n} \left[a^*(e^{-ith_{k,n}} f_{k,n}) a(f_{k,n}) \right] \right| \le C.$$

(2) For each $t \in \mathbb{R}$ and $k \in K$,

$$\lim_{n \uparrow \infty} \rho_{k,\beta_k,n} \left[a^*(e^{-ith_{k,n}} f_{k,n}) a(f_{k,n}) \right] = \langle f_k, (e^{\beta_k h_k} - 1)^{-1} e^{-ith_k} f_k \rangle_{\mathfrak{h}_k},$$

$$\lim_{n \uparrow \infty} \rho_{k,\beta_k,n} \left[a(f_{k,n}) a^*(e^{-ith_{k,n}} f_{k,n}) \right] = \langle f_k, (1 - e^{-\beta_k h_k})^{-1} e^{-ith_k} f_k \rangle_{\mathfrak{h}_k}.$$

The notation on the RHS was introduced in Sect. 3.

Then the expressions

$$\chi_n(\kappa, t, \lambda, \rho_S) := (\rho_S \otimes [\underset{k \in K}{\otimes} \rho_{k, \beta_k, n}]) \left[e^{-i \sum_k \kappa_k H_{R_k, n}} e^{-it H_{\lambda, n}} e^{i \sum_k \kappa_k H_{R_k, n}} e^{it H_{\lambda, n}} \right] \tag{A.2}$$

converge as $n \uparrow \infty$ for all t and λ. This is checked by writing a Dyson expansion for (A.2), treating the terms in λ as a perturbation. The dominated convergence theorem can be applied since term-by-term convergence is implied by Assumption (2) above and a dominating bound follows from Assumption (1) above.

The connection with the setup in Sect. 6 is that, under the above assumptions

$$\lim_{n \uparrow \infty} \chi_n(\kappa, t, \lambda, \rho_S) = \chi(\kappa, t, \lambda, \rho_S). \tag{A.3}$$

Appendix B

In this appendix, we look more closely at what the "extended weak coupling limit" (as presented extensively in [18]) can tell us about the different fluctuation formulas that were proposed in Sect. 2.

Assume the notation introduced in Sects. 2 and 3. The result in [18] states that the unitary dynamics $U^\lambda_{\lambda^{-2}t}$ on $\mathcal{H}_S \otimes_k \Gamma_s(\mathfrak{h}_k)$ converges (in an appropriate sense) to a new unitary dynamics $\tilde{U}_t$ on $\mathcal{H}_S \otimes_{k, \omega} \Gamma_s(\tilde{\mathfrak{h}}_{k, \omega})$, where $\tilde{\mathfrak{h}}_{k, \omega}$ are modified one-particle spaces. The dynamics $\tilde{U}_t$, which is the solution of a Quantum Stochastic Differential Equation, is extensively discussed in [18, 43].

An important observation is the emergence of effective reservoir energy operators;

$$N_k := \sum_\omega d\Gamma(\omega 1_{\omega, k}), \tag{B.1}$$

where $1_{\omega, k}$ is the projector on $\tilde{\mathfrak{h}}_{k, \omega}$. One sees hence that the effective reservoir energy operator is more like a number operator. Its plays a role in the limits of respectively (2.7) and (2.9). One has, of course again under technical conditions,

$$\rho_0 \left[e^{-i \sum_{k \in \mathcal{K}} \kappa_k (U^\lambda_{-t} H_{R_k} U^\lambda_t - H_{R_k})} \right] \xrightarrow[\lambda \searrow 0]{} \tilde{\rho}_0 \left[e^{-i \sum_{k \in K} \kappa_k (\tilde{U}_{-t} N_k \tilde{U}_t - N_k)} \right] \tag{B.2}$$

and

$$\rho_0 \left[e^{-i \sum_{k \in \mathcal{K}} \kappa_k H_{R_k}} U^\lambda_t e^{i \sum_{k \in \mathcal{K}} \kappa_k H_{R_k}} U^\lambda_{-t} \right] \xrightarrow[\lambda \searrow 0]{} \tilde{\rho}_0 \left[e^{-i \sum_{k \in K} \kappa_k N_k} \tilde{U}_t e^{i \sum_{k \in K} \kappa_k N_k} \tilde{U}_{-t} \right], \tag{B.3}$$

where $\tilde{\rho}_0$ is a state which coincides with ρ_0 on $\mathcal{H}_S$ and which represents the thermal reservoir states on $\otimes_{k, \omega} \Gamma_s(\tilde{\mathfrak{h}}_{k, \omega})$. Although it is not obvious from these expressions, the expression (B.3) coincides with (4.11), this is the well-known connection between unravelings and quantum stochastic differential equations. To check that (B.2) and (B.3) coincide up to second order in κ, it suffices to know that

$$\tilde{\rho}_0[A N_k] = \tilde{\rho}_0[N_k A] = 0 \tag{B.4}$$

for all A, operators on $\mathcal{H}_S \otimes_{k, \omega} \Gamma_s(\tilde{\mathfrak{h}}_{k, \omega})$.

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