

# Quantum and classical fluctuation theorems from a decoherent histories, open-system analysis

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In this paper we present a first-principles analysis of the nonequilibrium work distribution and the free energy difference of a quantum system interacting with a general environment (with arbitrary spectral density and for all temperatures) based on a well-understood microphysics (quantum Brownian motion) model under the conditions stipulated by the Jarzynski equality [Jarzynski, *Phys. Rev. Lett.* **78**, 2690 (1997)] and Crooks' fluctuation theorem [Crooks, *Phys. Rev. E* **60**, 2721 (1999)] (in short, fluctuation theorems, FTs). We use the decoherent histories conceptual framework to explain how the notion of trajectories in a quantum system can be made viable and use the environment-induced decoherence scheme to assess the strength of noise that could provide sufficient decoherence to warrant the use of trajectories to define work in open quantum systems. From the solutions to the Langevin equation governing the stochastic dynamics of such systems we were able to produce formal expressions for these quantities entering in the FTs and from them prove explicitly the validity of the FTs at the high temperature limit. At low temperatures our general results would enable one to identify the range of parameters where FTs may not hold or need be expressed differently. We explain the relation between classical and quantum FTs and the advantage of this microphysics open-system approach over the phenomenological modeling and energy-level calculations for substitute closed quantum systems.

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## I. INTRODUCTION

Unlike in equilibrium statistical physics, few theorems of generality are established for nonequilibrium systems. Hence any valid statement with a broad spectrum of implications and wide range of applications is of great value. The fluctuation theorems (FTs) of Jarzynski [1] and Crooks [2] in nonequilibrium statistical mechanics are of such a nature and have stimulated intense research interest and activities in the past decade.<sup>1</sup> For earlier work on entropy fluctuation theorems, such as by Cohen, Evans, Searles, and others, see, e.g., [3]. FTs relate some equilibrium thermodynamic quantities of a physical system, like free energy differences, to the averages of mechanical quantities in nonequilibrium processes, like exponentiated work. For complex biological systems like proteins and DNAs the free energy differences are difficult to calculate, while the averages of work in nonequilibrium processes can be obtained from measurements in experiments or via numerical simulations.

### A. Background and basic issues

*How to define work in quantum physics.* The fluctuation theorems were originally derived for classical thermodynamic systems. It is natural to ask if they hold for quantum systems and, if not, under what conditions would they fail and whether there exist quantum fluctuation theorems (QFTs) different in form and content from the classical FTs. If this is not possible, can one find an approximate form in terms of corrections to the classical FTs? To our knowledge corrections have been derived but a full QFT that is valid for all conditions (e.g., non-Ohmic spectral density of the environments at low temperature) is still at large.

In these endeavors the main conceptual obstacle is how to make sense of work in a quantum setting. To begin with, work is not an observable [4], and as such, treating it as a quantum mechanical operator [5,6] is largely a computational convenience. Thus the foremost task is to find a physically meaningful definition and an operationally feasible way to calculate it. We will address this issue with the approach described below.

Let us try to appreciate the content of this pivotal point. In classical mechanics *exclusive work* [7] imparted to a system, say a particle, is defined as the integration of applied force on the system with displacement along a path. The force is exerted by an external agent that causes the system to move along a trajectory. Once one knows the trajectory, work can be calculated, but the difficulty for quantum systems is that particles do not follow trajectories; they are described by a wave function, which is a very different notion and entity from paths. The key challenge is to make sense of trajectories in quantum physics. We mention several approaches below and then present our own.

*Closed versus open quantum system.* If one restricts one's attention to closed quantum systems, i.e., isolated quantum systems having no interaction with any of their environments, one can define work via transitions between the system's energy levels (quantum jumps) [8,9], and general agreement seems to be reached. However, this is merely an idealization of realistic physical systems, which are more often open. The influence of their environments with which the system of interest interacts needs to be accounted for in the open system's evolution. Even in the simplest cases, when one talks about temperature or refers to (equilibrium) thermodynamic quantities, a heat bath (canonical ensemble) or a particle reservoir (grand canonical ensemble), which are open-system setups, is implicitly assumed.

Since for closed quantum systems fluctuation theorems can be easily derived, one can think of the system and environment as a closed system and work out the QFTs. This was done in

<sup>1</sup>By the FTs we refer specifically to Jarzynski's equality and Crooks's fluctuation theorem only.

[9–11]. However, this formulation has the innate shortcoming that the work defined therein requires the change in energy of the *combined* system, while the FTs refer to the work on the *open* system of interest (being a subsystem of the combined system, whose dynamics includes the back action from the other subsystems as its environment).

*Microscopic models for open system dynamics.* The use of a microphysics model, such as the quantum Brownian motion (QBM) model described below, could provide a rigorous basis for any phenomenological description. It makes explicit any assumption made in the phenomenological models, which enables one to clearly define the range of validity of the results derived from each model, as well as being able to provide the details in the derivations with or without the corresponding assumptions. Applying methods of nonequilibrium statistical mechanics, such as the Zwangzig-Mori-Nakajima projection operator or the Feynman-Vernon influence functional (IF) formalism, to a microscopic model consummates the objectives of quantum open-system treatment. Using these methods, one obtains a description of the open-system dynamics in terms of open-system variables alone, while the dynamics of the open system already factored in the back action of the environment. Environment-related quantities like heat can also be addressed within this framework. The IF is the method we have used before and prefer since it has the advantage of including the back action in a self-consistent manner and one can invoke field theory techniques (by way of the almost equivalent Schwinger-Keldysh closed time path formalism) to address nonequilibrium statistical mechanics issues.

Using microscopic models and open-system dynamics, several suggestions for trajectories have been made. For example, De Roeck [12] used the unraveling of the open-system master equation and compared his results to that of the closed-system approach. Deffner *et al.* [13] used the quantum Smoluchowski equation (QSE), which was derived from taking the high friction and high temperature limit in [14], as a starting point. They considered the solution to the QSE in terms of classical path integrals and interpreted these paths as trajectories. But these trajectories are difficult to interpret physically, being more in the nature of devices (to help solve a differential equation) than actual physical entities. By making the assumption that the reduced dynamics of a driven open-quantum subsystem is described by a quantum master equation Esposito and Mukamel [15] recast its solution in a representation that takes the form of a birth-death master equation (BDME) with time-dependent rates and used it to define “quantum” trajectories. But these QSE and BDME, just as the Pauli master equation, govern transition probabilities, are equivalent to a reduced density matrix with only diagonal elements, and thus contain no quantum phase information.<sup>2</sup>

<sup>2</sup>This may be viewed as the completely decohered end product of a decoherent histories or environment-induced decoherence process (complete diagonalization of the reduced density matrix), but as we shall explain in more detail below, it corresponds to the case of very strong noise acting on the subsystem, which is possible for high temperatures, and thus it falls under the parameter regime where the classical FTs are valid. In fact, for Gaussian systems, the QFTs

Alternatively, Crooks [16] proved the Jarzynski equality by considering the Markovian dynamics of a quantum system in the following setting: Instead of measuring the system, generalized measurement superoperators were used to represent measurements of heat flow. If the quantum environment is assumed to be large, to have rapidly decohered, and always to remain at thermal equilibrium in addition to being uncorrelated and unentangled with the system, then the change in energy of the bath can be measured without further disturbing the dynamics of the system.

In comparison with earlier work our approach is closest in spirit to that of Chernyak and Mukamel [5]. However, our methods (they use superoperators in Liouville space) and interpretations (they use von Neumann’s wave function collapse for quantum measurement) are different. We will detail the differences after we have a chance to describe our approach.

## B. Our approach and findings

For the sake of conciseness we just state what we do and name the ingredients in our approach here, leaving more detailed explanations for the next section.

In this paper we analyze the fluctuation theorems using the exactly solvable microscopic quantum Brownian motion model of a quantum harmonic oscillator coupled to a heat bath of  $N$  quantum harmonic oscillators with arbitrary spectral density function and for all temperatures. This is referred to as a “general” environment in [17], where an exact master equation for these full ranges was obtained and from which our discussions of the application of this model to QFTs are based.<sup>3</sup> The low temperature results are of special interest for the derivation of the QFT since it measures the deviation from the classical FTs.

*decoherent histories approach to define trajectories for quantum systems.* We resort to the conceptual framework of decoherent [18] or consistent [19,20] histories (dechis) and the key notion of decoherence for understanding the process of quantum to classical transition. We believe this is the most faithful and intuitive way of defining trajectories or explaining how they arise from quantum mechanics. To be more precise, these trajectories are actually stochastic classical paths in a quasiclassical domain as a result of decoherence in the histories. They arise from the action of noise, which is defined as variations in neighboring histories. (For a succinct explanation of the first point see, e.g., [19,21] and see [22] on the second point.)

*Environment-induced decoherence for explicit computations.* While the decoherent histories paradigm is conceptually clear for explaining the origin and mechanisms in the emergence of classical stochastic trajectories, it is less versatile in actual computations. The environment-induced decoherence

derived under these conditions have exactly the same form as the classical FTs.

<sup>3</sup>We advise against calling this a *non-Markovian environment* because non-Markovian refers to stochastic *processes*, not systems. Instead, use, e.g., *colored noise environments*, which can engender non-Markovian dynamics in the open subsystem.

(*envdec*) approach can be of more practical use. Here the approximate diagonalization of the reduced density matrix of the reduced or open system with respect to some basis is used as a signifier of decoherence of the quantum system in transit to classicality, whereby the notion of trajectory becomes viable. But which basis? This is the physically relevant issue. The quantum system is more readily decohered in the so-called “pointer basis” [23], which is affected by the form of interaction between the system and its environment. Here, with an explicit environment specified, it is easier to see how noise arises and its nature (colored, multiplicative [24]) than in the decoherent histories approach. The connection between these two approaches is discussed in [25]. An explicit model calculation (the QBM model) was given in the dechis approach [26], where one can compare these two approaches in operational details.

*Significance of stochastic regime between quantum and classical.* In reference to trajectories of quantum origin we notably attach the word “stochastic” to classical. This is because there is a stochastic component to them after the quantum histories decohere. They are described by a probability distribution function. Each such trajectory is a realization of this distribution. Taking the stochastic average of an ensemble of such trajectories will yield the unique classical path, which is a solution of a deterministic classical equation of motion.

Decoherence is due to noise, quantum or thermal or both. In the *envdec* scheme, one can see this explicitly from the stochastic equations governing the open (reduced) system. Noise is responsible for quantum diffusion, which brings forth decoherence. The stronger the noise is, the more complete the decoherence process is and the more classical the trajectories are. In fact for the QBM model there are two diffusion terms: a normal diffusion dominates at high temperatures, and an anomalous diffusion dominates at low temperatures. The latter is what one should focus on in marking the difference between the classical and the quantum FTs. Therefore the behavior of a system in the stochastic regime actually holds the key to quantum-classical transition or correspondence. It is particularly suitable for the exploration of FTs in open systems as they are also cast in a stochastic framework in terms of the probability distribution of work.

*Our findings.* In this paper we present a first-principles analysis of the nonequilibrium work distribution and the free energy difference of a quantum system interacting with a general environment (with arbitrary spectral density and for all temperatures) based on a well-understood microphysics (quantum Brownian motion) model under the conditions stipulated by the Jarzynski equality and Crooks’ fluctuation theorem. We use the decoherent histories conceptual framework to explain how the notion of trajectories in a quantum system can be made viable and use the environment-induced decoherence scheme to assess the strength of noise that could provide sufficient decoherence to warrant the use of trajectories to define work in open quantum systems. From the solutions to the Langevin equation governing the stochastic dynamics of such systems we were able to produce formal expressions for these quantities entering in the FTs and from them prove explicitly the validity of the FTs at the high temperature limit. At low temperatures our general results would enable one to identify

the range of parameters where FTs may not hold or need to be expressed differently. We explain the relation between classical and quantum FTs and the advantage of this microphysics open-system approach over the phenomenological modeling and energy-level calculations for substitute closed quantum systems.

## II. KEY POINTS AND MAIN IDEAS

Because we are seeking (a) a derivation of quantum fluctuation theorems in nonequilibrium physics by applying concepts and practices in (b) quantum foundation and measurement theory via decoherent histories and environment-induced decoherence with its ensuing classical stochastic equations, it might be useful to give a brief summary of the key ideas and procedures in this section for ease of cross-reference. For good reviews on these subjects we mention [9] for (a) and [19,20,27] for (b). Readers familiar with (a) can skip the first section, and readers familiar with (b) can skip the last section. Readers familiar with both may go to Sec. III.

### A. Fluctuation theorems

#### 1. Classical FTs

We briefly review the premises of these theorems in classical Hamiltonian dynamics.<sup>4</sup> Consider a classical system whose dynamics is governed by the Hamiltonian  $H(\lambda_t)$ , where  $\lambda$  is a deterministic parameter with a prescribed time dependence. At some initial time  $t_0$  that, without loss of generality, can be taken to be zero, the system is prepared in a thermal state  $\exp[-\beta H(\lambda_0)]/Z_0$ . Then the parameter  $\lambda$  is changed according to a protocol up to a final time  $\tau$ . Work done during this process is defined as

$$W = \int_0^\tau dt \frac{\partial H}{\partial \lambda} \dot{\lambda}(t), \quad (1)$$

where an overdot denotes derivative with respect to time.<sup>5</sup> Although the Hamiltonian dynamics of the system is entirely deterministic, due to the probabilistic nature of the initial conditions that are sampled from the thermal phase space density, work is described by a probability distribution  $\mathcal{P}(W)$ . Note that thermal equilibrium is only assumed at  $t = 0$  as part of the preparation. In general the evolved system is not in thermal equilibrium. Jarzynski equality is the following statement:

$$\langle e^{-\beta W} \rangle \equiv \int dW \mathcal{P}(W) e^{-\beta W} = e^{-\beta \Delta F}. \quad (2)$$

Here  $\Delta F \equiv F_\tau - F_0$ , where  $F_0$  and  $F_\tau$  are free energies of the system at thermal equilibrium at inverse temperature  $\beta$  with the parameter  $\lambda$  assuming values  $\lambda_0$  and  $\lambda_\tau$ , respectively. Equation (2) is remarkable in that it relates an average of a thermodynamical quantity over nonequilibrium processes to strictly equilibrium properties.

<sup>4</sup>For a recent review on classical FTs, see [28].

<sup>5</sup>For a discussion of various definitions of work, their relationship to each other, and how that affects the content and context of the fluctuation theorems, see [7].

For the statement of Crooks's fluctuation theorem one defines the reverse process in which the system is prepared initially at  $t = 0$  in the thermal state  $\exp[-\beta H(\lambda_\tau)]/Z_\tau$  and the parameter  $\lambda$  is changed in a time-reversed manner to assume the value  $\lambda_0$  at  $\tau$ . The probability distribution of work associated with this process is denoted by  $\mathcal{P}_R(W)$ . Crooks's fluctuation theorem states

$$\frac{\mathcal{P}_F(W)}{\mathcal{P}_R(-W)} = e^{\beta(W - \Delta F)}, \quad (3)$$

where the subscript  $F$  stands for forward process and  $\Delta F$  is defined as before. The Jarzynski equality follows from Eq. (3) by multiplying both sides by  $\mathcal{P}_R(-W)e^{-\beta W}$  and integrating over  $W$ .

## 2. Quantum FTs

The main difficulty in formulating fluctuation theorems for quantum mechanics is defining work. Except for closed systems there is no agreement on a definition of work in quantum mechanics. For closed systems there is general agreement on the following operational definition: (1) Measure the energy of the system using the Hamiltonian initially at  $t = 0$  to be  $E_n^0$ , thus "collapsing the wave function" to one of the eigenfunctions of the Hamiltonian at the initial time:  $H(0)|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle$ . (2) Let the system evolve under the time-dependent Hamiltonian according to the prescribed protocol. (3) At the end of the protocol measure the energy of the system using the Hamiltonian at  $t = \tau$  to be  $E_m^\tau$ , thus collapsing the wave function to an eigenfunction of the Hamiltonian at  $\tau$ :  $H(\tau)|\psi_m^\tau\rangle = E_m^\tau|\psi_m^\tau\rangle$ . Work for this specified realization is defined as  $W = E_m^\tau - E_n^0$ . Since the system is closed, one can interpret the change in energy of the system as work performed on the system. In classical mechanics of isolated systems work acquires a probabilistic feature only due to the sampling of the initial conditions since the dynamics is deterministic. In quantum mechanics work acquires an additional probabilistic feature from the dynamics:

$$\mathcal{P}(W) = \frac{1}{2\pi} \int du e^{-iuW} \text{Tr}[e^{iu\hat{H}_H(\tau)} e^{-iu\hat{H}_H(0)} \hat{\rho}_\beta], \quad (4)$$

where the subscript  $H$  indicates Heisenberg operators. Jarzynski equality and Crooks's fluctuation theorem can be proven in a few lines for a closed system with this definition of work.

In this paper we develop an alternative approach based on a microscopic model using the open quantum systems paradigm. First, consider a classical harmonic oscillator, without a bath. Initial position and momentum of the oscillator are sampled from the thermal phase space density. The rest of the trajectory is entirely determined by the protocol of how the external force is applied. Work is calculated using this deterministic trajectory according to Eq. (1). However, a deterministic trajectory is strictly a classical notion and cannot be applied to a general quantum mechanical system. A state that is sampled from the thermal density matrix in general does not have a well-defined position and momentum. Furthermore the time evolution usually causes the wave function to spread further. We cannot talk about the quantum oscillator being at one point in space having a certain velocity and moving in a deterministic continuous trajectory as a function of time.

Next, consider the same classical model with a heat bath. For each realization of the protocol, the initial data for both the system oscillator and the bath are sampled from the initial phase space density. The initial data for the bath determines the noise for that particular realization. The system oscillator follows a trajectory determined by a combined action of the deterministic force  $f(t)$  and the stochastic force  $\xi(t)$ . Although the noise is stochastic, each realization of the experiment corresponds to a unique noise and hence a unique trajectory. The definition of work in terms of trajectories is unaffected.

It is a simple yet subtle and deep point how the interaction with a bath would help to define a trajectory for a quantum particle. To understand this conceptually we adopt the decoherent or consistent histories viewpoint of quantum mechanics as described below.

## B. Trajectories in quantum mechanics

Trajectories that are well defined in classical mechanics are generally ill defined in quantum mechanics except under certain conditions. We shall spell out these conditions here. Let us begin with something simple, such as a quantum particle in motion. In a closed quantum system  $S$ , namely, a system subjected to no outside (environmental) influence except for its own quantum fluctuations, the closest entity to its "trajectory" is a wave packet moving with a certain group velocity but that also spreads in time due to the Heisenberg uncertainty relation between the variance of the canonical variables, position and momentum in this case. The same system at a finite temperature is no longer closed because for it to exist at finite temperature it must be or have been in contact with a source with energy exchange or a bath  $B$  kept at nonzero temperature. The influence of the environment  $E$  (we call  $E$  a bath  $B$  if it is described by a thermal density matrix with inverse temperature  $\beta$ ) has complicated and interesting consequences. This is the subject of open quantum systems.

There are at least two major effects an environment brings in "opening up" a closed quantum system: (a) it turns the original Hamiltonian (unitary) dynamics to dissipative (nonunitary) dynamics (this refers to energy flow from the system to the environment) and (b) fluctuations in the environment decohere the quantum system (this refers to quantum phases of the system being dispersed into the environmental variables). The latter is responsible for shaping the notion of trajectories in quantum system, and there are precise conditions pertaining to the features of the environment (e.g., Ohmic spectral density, high temperature) whereby it becomes physically well defined in a measurement. One way is to construct the reduced density matrix of the open quantum system and look at whether and how quickly its off-diagonal elements decay in time, leaving the system's statistical state describable by an approximately diagonal density matrix with respect to some physically meaningful basis (related to measurement instruments and interaction, such as Zurek's "pointer basis" [23]). This time, called decoherence time, marks the appearance of classical features because, after it is effectively decohered, this open system is adequately described by probabilities rather than amplitudes and its quantum phase information is lost (more accurately, dispersed into or shared by the multitude of environmental degrees of freedom). This process is captured



by stochastic equations; the most common forms are the master equation, the Langevin, and the Fokker-Planck equations.

What distinguishes these equations is the presence of noise or fluctuations in the environment and dissipative dynamics of the open (reduced) system, depicting the two distinct features of open-system dynamics. In general two kinds of noise exist in any quantum system, the intrinsic quantum noise entering in the Heisenberg relation, which exists for all systems even at zero temperature, and thermal noise from a finite temperature bath. Both contribute to decohering a quantum system, although the thermal noise usually overwhelms.

There are many ways to characterize a quantum system as approaching its classical limit. The familiar cases are the correspondence principle, the Bohr-Sommerfeld rules in quantum mechanics, the description of Maxwell-Boltzmann distribution as limits of the Fermi-Dirac and the Bose-Einstein distributions, or the more simplistic  $\hbar \rightarrow 0$  or at high temperature stipulations. One can show that the coherent state is the most classical of quantum states [29]. One can derive an uncertainty function at finite temperature [30] or equivalently calculate the entropy function and be able to demarcate the transition from the quantum noise-dominated regime to the thermal noise-dominated regime. There has been significant advance in the last two decades in our understanding of the quantum-classical correspondence. (See, e.g., [31].) Decoherence is at the heart of the quantum to classical transition issue, and the main cause of it is noise of all forms, either in the fluctuations of the environment or in the separation of neighboring coarse-grained histories and in the accuracy of the measurement devices and procedures. We will use the decoherent or consistent history [18–20] viewpoint for conceptual clarity, especially pertaining to the issue of trajectories, but we adopt the environment-induced decoherence scheme for computations, as it is technically easier to manipulate.

### 1. Decoherence functional in dechis and influence functional in envdec

The main idea of the dechis approach is to define a history  $\alpha$  by a set of projection operators  $P_\alpha(t_k)$  acting at times  $t_k$ . As a special case we consider projections in position basis. These kind of histories are naturally implemented in the path integral approach. The projectors are represented by window functions  $w_\alpha[x(t_k)]$ , which take on unit value if the instantaneous configuration satisfies the requirement of the history  $\alpha$  and vanish otherwise. As a limiting case we mention a fine-grained history, for which the path is specified exactly at all times and is assigned an amplitude  $\exp(iS/\hbar)$  as usual. It is useful to define the decoherence functional of two histories  $\alpha$  and  $\beta$  by [22]

$$\mathcal{D}[\alpha, \beta] = \int Dx Dx' e^{i(S[x] - S[x'])/\hbar} \rho(x(t_i), x'(t_i); t_i) \times \left\{ \prod_k w_\alpha[x(t_k)] \right\} \left\{ \prod_l w_\beta[x'(t_l)] \right\}. \quad (5)$$

The product over  $k$  and  $l$  can be discrete or continuous, as is the case in Sec. III. The probability of a given history  $\alpha$  is given by the diagonal element of the decoherence

functional:  $P[\alpha] = \mathcal{D}[\alpha, \alpha]$ . For classical trajectories it is required that the probability of a coarse-grained history be the sum of its constituents. For an arbitrary set of histories quantum interference effects lead to a violation of the probability sum rule:  $P[\alpha \vee \beta] = \mathcal{D}[\alpha, \alpha] + \mathcal{D}[\beta, \beta] + 2\text{Re}\mathcal{D}[\alpha, \beta] \neq P[\alpha] + P[\beta]$ . If a set of histories can be identified for which the real part of the off-diagonal elements of the decoherence functional vanishes (or are much smaller than the diagonal elements for approximate decoherence), probabilities can be assigned to individual histories. The challenge is to identify the conditions under which, and to what extent, the decoherence condition is satisfied.

Technically, the environment-induced decoherence program is easier to implement, and the relation between these two programs is explained or illustrated in [25,26]. This is what we will do by way of the QBM model presented in the next section. We will argue that for histories obtained by coarse graining the environment sufficiently and the system of interest to some extent (determined by the strength of noise), an approximate decoherence condition can be satisfied to a specified degree of accuracy. On the other end, if quantum interference between particle histories continues to play an overbearing role, decoherence is not consummated, the classical world is not reached, and the concept of trajectories is ill defined.

The quantum open-system formulation, via the influence functional, provides one with a clear perspective on the organic relation between the processes of fluctuations or noise, correlation, decoherence, and dissipation and how they enter in the transition from the quantum to the classical world with the intermediate stochastic and semiclassical regimes. While it is useful to explain this with the aid of stochastic equations, which we will derive below, the key idea can be put succinctly: The stronger the effect of noise in the environment is, the more efficient it decoheres the quantum system, and the more clearly the classical notion of trajectory can be defined and used for the description of a quantum particle. The important understanding is the existence of a stochastic regime between the quantum and the classical and how quantum features are expressed in terms of classical stochastic variables.<sup>6</sup>

### 2. World line influence functional formalism

Thus far we have learned that the decoherence of a quantum system due to the noise arising from a coarse-grained environment is instrumental in the emergence of a classical world. How strongly the system is coupled to its environment(s), the nature of the noise from the environment, and its temperature all enter in determining how completely the system is decohered, and there is always a stochastic component in the open system's dynamics governed by a Langevin equation or its (near) equivalent master or Fokker-Planck equations. Almost complete decoherence is a necessary condition for a classical description, which in this context, is what trajectories are predicated upon. Under this condition

<sup>6</sup>A famous case is the transcription of Gaussian quantum fluctuations in the environment as classical noise via the Feynman-Vernon identity [32].

a powerful approach called the world line (WL) influence functional formalism has been used effectively for more than two decades in nuclear and particle physics communities (see, e.g., [33]). We shall only mention its key features so as to bring out its relevance to the present problem and skip all the details.

The influence functional technique of Feynman and Vernon [32] and the closely related closed-time-path effective action method of Schwinger [34] and Keldysh [35] are initial value (in-in) formulations, which are particularly suitable for exploring the time evolution of many-body systems, unlike the  $S$ -matrix (in-out) formulation used for calculating scattering processes. In general this yields a nonlocal and nonlinear coarse-grained effective action (CGEA) for the system's motion. The CGEA may be used to treat the nonequilibrium quantum dynamics of interacting particles. Take, for example, the QBM model: When the particle trajectory becomes largely well defined as a result of effective decoherence due to interactions with the environment, with some degree of stochasticity caused by noise, the CGEA can be meaningfully transcribed into a stochastic effective action, describing stochastic particle motion. The evolution propagator for the reduced density matrix of the open system is dominated by the particle trajectory giving the extremal solution of the real part of the CGEA. Stochastic fluctuations around the decohered semiclassical trajectories are described by the imaginary part of the CGEA. For further technical details, see [36,37].

When the back action of the environment is taken into account, the dynamics of the open system will, in general, be non-Markovian, as it contains memories, and the noise in the environment is generally colored, as it contains many time scales characterized by its spectral density and varies with temperature. Dissipation in the open-system dynamics is controlled and balanced by the noise in the environment as manifested in the existence of fluctuation-dissipation relations between these two sectors. What is more important, because the influence action includes the back action of the environment in a self-consistent manner, the world line is not merely a prescribed classical entity or a simple solution to an equation of motion at the tree level (in truth, with an everpresent stochastic component) but, rather, a dynamical one, as the result of constant negotiation between the open system and its environments at all times. This is the special beauty of the IF method.

### III. THE QBM MODEL

In this section we describe the salient features of the bilinear QBM model with a general environment following [17] for non-Markovian dynamics and write down the solutions of the Langevin equation following [38]. We focus on the stochastic dynamics of the quantum open system, which incorporates the effects of the environment. This will play a crucial role in our formulation of FTs in the following section.

A closed quantum system can be partitioned into several subsystems according to the relevant physical scales. If one is interested in the details of one such subsystem, call it the distinguished, or relevant, system, that interacts with the other subsystems comprising the environment, the details of which are not of interest, one can coarse grain the information in the

environment but keep its overall influence on the distinguished subsystem of interest, thereby rendering it an open system. This influence is best captured by the influence functional technique of Feynman and Vernon [32], which we use here. Let us assume for simplicity the system  $S$  is composed of a simple harmonic oscillator with position and momentum  $(x, p)$  linearly coupled to a heat bath  $B$  consisting of  $N$  harmonic oscillators with positions and momenta  $(q_n, p_n)$  with  $n = 1, \dots, N$  and allow the system to be driven by a time-dependent external force  $f(t)$ . The Hamiltonian describing the dynamics of the combined system is given by

$$H_T = (H_S) + [H_B + H_I + H_R], \quad (6)$$

where

$$(H_S) = \frac{p^2}{2M} + \frac{1}{2}M\Omega^2 x^2 - f(t)x, \quad (7)$$

$$[H_B + H_I + H_R] = \sum_{n=1}^N \left[ \frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 \left( q_n - \frac{c_n}{m_n\omega_n^2} x \right)^2 \right].$$

The system oscillator is coupled to the bath via the linear interaction term  $H_I = (\sum_n c_n q_n)x$ . A renormalization of the potential via  $H_R = \sum_n \frac{c_n^2}{2m_n\omega_n^2} x^2$  preserves the physical (observed) frequency of the system oscillator for any system-bath coupling, as will be shown below. Without the renormalization term the potential might have no minimum, and the thermal state could not be defined. The remainder in the quantity in square brackets in the above equation is  $H_B$ . This is the QBM model.

The QBM model is used extensively in the open quantum systems literature thanks to its exact solubility and its generality. The solubility is due to the linearity of the model. The generality may not be immediately obvious. Representing the environment by a set of simple harmonic oscillators might appear to be a serious restriction to weak influences on the system because of its linearity. An argument for the generality of the model is given by Caldeira and Leggett [39].<sup>7</sup> The applicability of the model is limited to cases where the influence of the system on each bath mode is weak. This does not imply that the influence of the bath as a whole on the system is weak as well. The Brownian particle interacts with a very large number of environmental degrees of freedom. The effect of these interactions can add up to yield strong dissipation, fluctuations, and decoherence for the Brownian particle.

When the combined system is closed, the Hamiltonian  $H_T$  gives unitary evolution, and its density operator  $\rho$  obeys the von Neumann equation:

$$i\hbar \frac{\partial \rho(t)}{\partial t} = [H_T, \rho(t)]. \quad (8)$$

<sup>7</sup>“For most cases of interest, at least when the system variable is macroscopic, this assumption is physically reasonable; in that case the environment is usually also (geometrically) macroscopic and the interaction of the system with any one environmental degree of freedom is generally proportional to the inverse of the volume, while the characteristic energy of such a degree of freedom is volume-independent.”

An alternative description closer in spirit to (but should by no means be identified with) that of a trajectory in phase space that gives a full and equivalent description is by way of the Wigner function [40]. For a closed system such as  $S$  by itself, without any interaction with its environment,  $\mathcal{W}(X, p, t)$  is defined with the new variables  $X \equiv (x + x')/2$  and  $y \equiv x' - x$ :

$$\mathcal{W}(X, p, t) = \frac{1}{2\pi\hbar} \int dy e^{\frac{i}{\hbar}py} \rho(X - y/2, X + y/2, t). \quad (9)$$

Because of its appearance in phase space variables it is often said that the Wigner function is the quantum correspondence of the classical phase space density [41] and the peak of the Wigner function coincides with the classical trajectory in phase space. This is an erroneous statement. The Wigner function gives as complete a description as that provided by the density matrix because it contains full quantum phase information. As such it can take on negative values.<sup>8</sup>

However, what we are interested in is how the system  $S$  behaves under the influence of its environment, in this case a heat bath  $B$  at temperature  $1/\beta$ . The state of the open system at any one time is completely specified by the reduced density matrix  $\rho_r$ , which is obtained from the density matrix of the combined system by integrating out the bath degrees of freedom. In position representation it is given by

$$\rho_r(x, x', t) = \int \prod_n dq_n \rho(x, \{q_n\}, x', \{q_n\}, t). \quad (10)$$

Because it incorporates the back action of the environment, the time evolution of the reduced density matrix of the open system is nonunitary and, in general, non-Markovian. The reduced density matrix of the system oscillator at  $t_f$  can be obtained from the reduced density matrix at some earlier time  $t_i$  via [43]

$$\rho_r(x_f, x'_f, t_f) = \int dx_i dx'_i J(x_f, x'_f, t_f; x_i, x'_i, t_i) \rho_r(x_i, x'_i, t_i), \quad (11)$$

where  $J$  is the propagator. If the system and the bath are initially uncorrelated and the bath is in a Gaussian state, the propagator  $J$  can be calculated exactly:

$$J(x_f, x'_f, t_f; x_i, x'_i, t_i) = \int_{x(t_i)=x_i}^{x(t_f)=x_f} Dx \int_{x'(t_i)=x'_i}^{x'(t_f)=x'_f} Dx' e^{\frac{i}{\hbar}(S_S[x] - S_S[x'] + S_{IF}[x, x'])}. \quad (12)$$

<sup>8</sup>Under special conditions for Gaussian systems such as a free simple harmonic oscillator (closed system) or one that interacts bilinearly with an Ohmic bath at high temperature (an open system) the Wigner function is positive definite for all times. The quantum and classical dynamics have the same form in the equations of motion [42]. For more general conditions by including environmental influence the reduced Wigner function (defined later) may become positive definite at late times after the system has sufficiently been decohered. This can indeed be used as a criterion for the appearance of classicality and the condition for the trajectory notion to be safely adopted in a quantum open system.

Now we introduce the following notation: for functions  $A(s)$  and  $B(s)$  and kernel  $K(s, s')$  define

$$A \cdot K \cdot B \equiv \int_{t_i}^{t_f} ds \int_{t_i}^{t_f} ds' A(s) K(s, s') B(s'). \quad (13)$$

In terms of the new variables the exponent appearing in Eq. (12) can be written as

$$S_S[x] - S_S[x'] = -M\dot{X}(t_f)y_f + M\dot{X}(t_i)y_i + y \cdot L_0 \cdot X, \quad (14)$$

$$S_{IF}[x, x'] = -y \cdot \mu \cdot X + \frac{i}{2} y \cdot \nu \cdot y, \quad (15)$$

where  $L_0(t, t') = M(\frac{d^2}{dt^2} + \Omega^2)\delta(t - t')$ . The kernels  $\mu(s, s')$  and  $\nu(s, s')$  are called the dissipation and noise kernels, respectively. For the special case, when the heat bath is in a thermal state of the bath Hamiltonian  $H_B = \sum_{n=1}^N [\frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 x_n^2]$ , these kernels are given by

$$\mu(t, t') = \sum_{n=1}^N \frac{c_n^2}{m_n \omega_n} \sin[\omega_n(t - t')] \Theta(t - t'), \quad (16)$$

$$\nu(s, s') = \sum_{n=1}^N \frac{c_n^2}{2m_n \omega_n} \coth\left(\frac{\beta\hbar\omega_n}{2}\right) \cos[\omega_n(t - t')]. \quad (17)$$

In the equivalent description in terms of the Wigner function one defines a reduced Wigner function  $\mathcal{W}_r$  in terms of the reduced density matrix formally in the same way as in Eq. (9) (denoted by a subscript  $r$ ). Using Eqs. (9)–(12) it can be shown that the reduced Wigner function evolves from time  $t_i$  to a later time  $t_f$  via

$$\begin{aligned} \mathcal{W}_r(X_f, p_f, t_f) &= \frac{1}{2\pi\hbar} \int dy_f e^{\frac{i}{\hbar}p_f y_f} \int dx_i dx'_i \\ &\times \int_{x(t_i)=x_i}^{x(t_f)=X_f - y_f/2} Dx \int_{x'(t_i)=x'_i}^{x'(t_f)=X_f + y_f/2} Dx' \\ &\times e^{\frac{i}{\hbar}(S_S[x] - S_S[x'] + S_{IF}[x, x'])} \int dp_i e^{-\frac{i}{\hbar}p_i(x'_i - x_i)} \\ &\times \mathcal{W}_r\left(\frac{x_i + x'_i}{2}, p_i, t_i\right). \end{aligned} \quad (18)$$

First, we perform a functional change of variables from the variables  $x(t), x'(t)$  to  $X(t) = [x(t) + x'(t)]/2$ ,  $y(t) = x'(t) - x(t)$ . We also perform a regular change of variables from  $x_i, x'_i$  to  $X_i = (x'_i + x_i)/2$ ,  $y_i = x'_i - x_i$ . The Jacobian determinant for both changes of variables is 1. Then we use Eqs. (14) and (15) and define  $L = L_0 - \mu$  to obtain

$$\begin{aligned} \mathcal{W}_r(X_f, p_f, t_f) &= \int dX_i \int dp_i \mathcal{W}_r(X_i, p_i, t_i) \frac{1}{2\pi\hbar} \int dy_f e^{\frac{i}{\hbar}p_f y_f} \\ &\times \int dy_i e^{-\frac{i}{\hbar}p_i y_i} \int_{y(t_i)=y_i}^{y(t_f)=y_f} Dy \int_{X(t_i)=X_i}^{X(t_f)=X_f} DX \\ &\times e^{\frac{i}{\hbar}[-M\dot{X}(t_f)y_f + M\dot{X}(t_i)y_i + y \cdot L \cdot X - \frac{1}{2}y \cdot \nu \cdot y]}. \end{aligned} \quad (19)$$

The functional integral over  $y$  is Gaussian and can be evaluated formally to give

$$\int_{y(t_i)=y_i}^{y(t_f)=y_f} Dy e^{\frac{i}{\hbar}(y \cdot L \cdot X - \frac{1}{2}y \cdot \nu \cdot y)} = \sqrt{\frac{1}{\det(\nu/2\pi\hbar)}} e^{-\frac{1}{2\hbar}(L \cdot X)^T \cdot \nu^{-1} \cdot (L \cdot X)}. \quad (20)$$

For the type of noise kernels displayed in Eq. (17) the outcome of this functional integral is independent of the end points  $y_i$  and  $y_f$ , irrespective of the distribution of bath frequencies. As a result, the integral over  $y_i$  and  $y_f$  is trivial and gives  $(2\pi\hbar)^2 \delta[M\dot{X}(t_i) - p_i] \delta[M\dot{X}(t_f) - p_f]$ . We have

$$\begin{aligned} \mathcal{W}_r(X_f, p_f, t_f) &= \frac{2\pi\hbar}{\sqrt{\det(v/2\pi\hbar)}} \int dX_i \int dp_i \mathcal{W}_r(X_i, p_i, t_i) \\ &\times \int_{X(t_i)=X_i}^{X(t_f)=X_f} DX (2\pi\hbar)^2 \delta[M\dot{X}(t_i) - p_i] \\ &\times \delta[M\dot{X}(t_f) - p_f] e^{-\frac{1}{2}(L \cdot X)^T \cdot (\hbar v)^{-1} \cdot (L \cdot X)}. \end{aligned} \quad (21)$$

Next, we do another functional change from  $X(t)$  to  $\xi(t)$ , where

$$X(t) \rightarrow \{X_i = X(t_i), p_i = M\dot{X}(t_i), \xi(t) = (L \cdot X)(t)\}. \quad (22)$$

For linear change of variables the Jacobian functional determinant is independent of  $\xi$ . To ensure that the boundary condition at  $t_f$  is satisfied we need to place a  $\delta$  function inside the new path integral. The net effect of the functional change of variables is

$$\int_{X(t_i)=X_i}^{X(t_f)=X_f} DX \delta[M\dot{X}(t_i) - p_i] \rightarrow \int D\xi \delta[X_\xi(t_f) - X_f], \quad (23)$$

where  $X_\xi(t)$  is the solution of the Langevin equation  $(L \cdot X_\xi)(t) = \xi(t)$  with the initial conditions  $(X_i, p_i)$ . After this functional change we obtain

$$\begin{aligned} \mathcal{W}_r(X_f, p_f, t_f) &= \int dX_i \int dp_i \mathcal{W}_r(X_i, p_i, t_i) \int \frac{D\xi}{\sqrt{\det(2\pi\hbar v)}} \\ &\times e^{-\frac{1}{2}\xi^T \cdot (\hbar v)^{-1} \cdot \xi} \delta[M\dot{X}_\xi(t_f) - p_f] \\ &\times \delta[X_\xi(t_f) - X_f] \\ &= \int dX_i \int dp_i \mathcal{W}_r(X_i, p_i, t_i) \int D\xi P[\xi] \\ &\times \delta[M\dot{X}_\xi(t_f) - p_f] \delta[X_\xi(t_f) - X_f] \\ &= \langle \delta[M\dot{X}_\xi(t_f) - p_f] \delta[X_\xi(t_f) - X_f] \rangle_{(X_i, p_i), \xi}. \end{aligned} \quad (24)$$

Here  $\xi(t)$  is a random noise with Gaussian statistics and is characterized by its mean and variance:

$$\langle \xi(t) \rangle = 0, \quad (25)$$

$$\langle \xi(t) \xi(t') \rangle = \hbar v(t, t'). \quad (26)$$

Furthermore, since the system and bath are assumed to be uncorrelated initially,

$$\langle X_i \xi(t) \rangle = \langle p_i \xi(t) \rangle = 0. \quad (27)$$

Equation (24) has a clear interpretation. The dynamics of the reduced Wigner function is identical to the dynamics of the phase space density of a stochastic classical system described by the Langevin equation  $(L \cdot X_\xi)(t) = \xi(t)$ .

As argued in [38], the Langevin equation provides a more detailed description of the dynamics than the master equation, in the sense that the class of quantum correlation functions that may be retrieved from the Langevin equation is larger than the corresponding class for the master or Fokker-Planck

equations unless the dynamics is Markovian. Work as defined in Eq. (39) is an example of this kind of quantity since its statistics requires the calculation of multitime correlations.

It is important to realize that this method gives exact quantum mechanical results at any parameter regime, including arbitrarily low temperatures. The fact that solutions  $X_\xi$  of a classical Langevin equation are used in Eq. (24) should not be regarded as having made a semiclassical approximation, as was done in, e.g., [5].

The effect of environment-induced decoherence at work that validates the notion of a physical trajectory is implicitly contained in this method (depending on the temperature of the bath and its spectral density), not extrinsically introduced by hand. Since these processes are dynamically and self-consistently determined, no semiclassical approximation has been made specifically in the derivation. The real challenge is in the interpretation of the physical variables in light of quantum measurement theory, as we discussed previously. In the following section we discuss under what conditions physical trajectories emerge from the dechis formalism.

### A. Decoherence functional

We consider histories where the system variable  $X$  is specified to follow a trajectory  $\chi(t)$  with a given accuracy  $\sigma(t)$ , while the environment variables are left completely unspecified. For technical reasons it is convenient to use Gaussian, rather than sharp, window functions  $w_\chi[x(\cdot)]$ . In the path integral this roughly corresponds to using  $\exp\{-\int dt \frac{[x(t)-\chi(t)]^2}{2\sigma^2(t)}\}$  in Eq. (5). Furthermore we introduce window functions at every instance of time rather than at discrete time intervals. The set of Gaussian window functions with this property acts as a noise term in the influence action. This can be seen in Eq. (28) where the noise kernel always occurs in the combination  $v + (2\sigma^2)^{-1}$ . There is some error introduced due to the overlap of projectors defined as above. As a result, we will be talking about approximate decoherence. In addressing the diagonal and off-diagonal elements of the decoherence functional it is convenient to define  $U = (\chi' + \chi)/2$  and  $u = \chi' - \chi$ . In [44] it is shown that the decoherence functional for two histories  $\chi(t)$  and  $\chi'(t)$  defined via these projectors is approximately given by

$$\begin{aligned} |D[U - u/2, U + u/2]| &\sim \exp\left\{-\frac{1}{2}(L \cdot U)^T \cdot [v + (2\sigma^2)^{-1}]^{-1} \right. \\ &\quad \left. \cdot (L \cdot U) - \frac{1}{2}u \cdot (v^{-1} + 2\sigma^2)^{-1} \cdot u\right\}. \end{aligned} \quad (28)$$

Here we again used a compact notation as before and  $v$  is defined in Eq. (26). The off-diagonal elements vanish as a Gaussian for  $u \gtrsim \sqrt{v^{-1} + 2\sigma^2}$ . Hence an approximately consistent set of histories can be obtained by picking histories that differ by at least this amount. However, if the Langevin noise is weak such that  $v^{-1} \gg \sigma^2$ , we run into trouble because now the decoherence condition requires  $u \gtrsim \sqrt{v^{-1}} \gg \sigma$ . Histories of accuracy  $\sigma$  in a set do not interfere with each other only if they are separated by a distance much larger than  $\sigma$ . This suggests that we cannot account for all probabilities within such a set.

We conclude that the accuracy should be adjusted to the noise level by  $\sigma^2 \sim v^{-1}$ . Then the decoherence condition



requires that  $u \gtrsim \sigma$ . Now we can have a set of histories that decohere approximately and for which the resulting probabilities add up to 1. “A picture of the system evolution based on actual nearly classical trajectories may only result from a compromise whereby the accuracy of observations is adjusted to the noise level,  $\sigma^2 \sim \nu^{-1}$  where  $\sigma$  is the accuracy at which the trajectories are defined. Larger noise for a given  $\sigma$  means more decoherence but less predictability; for a weaker noise, predictability is only limited by the Heisenberg bounds, but individual trajectories will not decohere.”<sup>9</sup> If we are satisfied with predictability within the limits imposed by the Langevin equation, then in the strong noise limit we may consider individual trajectories as depicting physical reality.”<sup>10</sup> This condition is ordinarily satisfied at high enough temperatures where the quantum and classical trajectories agree, even for non-Markovian dynamics, as we will see below.

For a given accuracy  $\sigma$  the higher the temperature is, the stronger the noise is, and the more effectively it brings about decohering histories into trajectories. Thus even at moderate temperatures and for relatively weak noise by judicious choices of the coarse graining measure  $\sigma$  decoherence can be effective enough to warrant the notion of trajectories. It is in this regime where deviations from FTs can be identified using this method. At low enough temperatures when no reasonable set of histories decoheres and the notion of trajectories is not applicable, we cannot say the FTs are violated (even though it appears reasonable to doubt their validity) because the contents of FTs may be phrased without invoking trajectories. For completeness of technical presentation we provide a low temperature expansion in Sec. V A 2.

#### IV. SOLUTIONS OF THE LANGEVIN EQUATION

It is convenient to rewrite the Langevin equation as

$$M\ddot{X}_\xi(t) + 2M \int_{t_i}^t ds \gamma(t-s) \dot{X}_\xi(s) + M\Omega^2 X_\xi(t) = f(t) - 2M\gamma(t-t_i)X_i + \xi(t), \quad (29)$$

$$\gamma(t-s) = \frac{1}{M} \sum_{n=1}^N \frac{c_n^2}{2m_n\omega_n^2} \cos[\omega_n(t-s)], \quad (30)$$

where  $\gamma$  is the damping kernel defined as the antiderivative of the dissipation kernel  $\mu$  [17]. It is related to the noise kernel by the fluctuation-dissipation relation (59) (see [45,46] for further exposition of the meaning and respective roles of  $\nu$  and  $\gamma$ ). In the rest of the paper we will drop the subscript  $\xi$ . The Langevin equation (29) is a linear integro-differential equation. The effect of interactions of the system oscillator with the bath is contained in a nonlocal potential and renormalization of the potential. One can think of the nonlocal potential as the system oscillator interacting with its own past, where the interaction is mediated by the bath. A formal solution to this equation can be obtained in terms of the homogenous solutions to the left-hand side of Eq. (29) with  $t_i$  set equal

to zero. Let us call the two linearly independent homogenous solutions  $h(t)$  and  $g(t)$ , such that

$$h(0) = \dot{g}(0) = 1; \quad \dot{h}(0) = g(0) = 0. \quad (31)$$

The formal solution of the Langevin equation is then

$$X(t) = X(t_i)h(t-t_i) + p(t_i)g(t-t_i) + \int_{t_i}^t dt' g(t-t') \times [f(t') + \xi(t') - 2MX(t_i)\gamma(t'-t_i)]. \quad (32)$$

Here  $h(t)$  and  $g(t)$  can be calculated using the Laplace transforms:

$$\hat{h}(s) = \frac{2\hat{\gamma}(s) + s}{s^2 + 2s\hat{\gamma}(s) + \Omega^2}, \quad \hat{g}(s) = \frac{1/M}{s^2 + 2s\hat{\gamma}(s) + \Omega^2}, \quad (33)$$

where the hat indicates Laplace transform. These expressions show the relation between the two linearly independent homogenous solutions:

$$s\hat{h}(s) = 1 - M\Omega^2\hat{g}(s), \quad sM\hat{g}(s) = \hat{h}(s) - 2M\hat{\gamma}(s)\hat{g}(s), \quad (34)$$

$$\dot{h}(t) = -M\Omega^2 g(t), \quad M\dot{g}(t) = h(t) - 2M \int_0^t ds \gamma(t-s)g(s). \quad (35)$$

#### A. Initial state preparation

The derivation of classical mechanical FTs for closed systems requires the closed system to be in a thermal state. As pointed out earlier, our derivation of the Langevin equation (29) assumes an uncorrelated initial state in which the bath is in the thermal state of its own Hamiltonian  $H_B$ . Such a state is obviously not the thermal state of the combined system and it is not stationary for any choice of the system's initial state. For this reason the uncorrelated initial state is not appropriate for applications to FTs. This observation is valid even for the classical Brownian motion model and is therefore not due to a quantum mechanical effect.

Assume that the bath oscillator frequencies form a continuum. It is customary to define the spectral density of the bath as

$$J(\omega) \equiv \sum_n \frac{c_n^2}{2m_n\omega_n} \delta(\omega - \omega_n) \quad (36)$$

and interpret  $J(\omega)$  as a continuous function. The resulting Langevin dynamics is truly dissipative, in the sense that  $\lim_{t \rightarrow \infty} g(t), \gamma(t) = 0$ . Physically, true dissipation corresponds to a positive average heat rate at all times. If the spectrum of bath frequencies is discrete, the resulting damping kernel is oscillatory. This is the case even for an infinite but countable number of discrete frequencies. As a result, after some (possibly very long) time, there may be average heat flow from the bath into the system. By true dissipation we mean a definite arrow of time for all times. Under these assumptions it can be shown [47] that if the uncorrelated initial state is prepared at the infinite past, for times  $t > 0$  the dynamics of the system oscillator is indistinguishable from that of a combined system and bath thermal state preparation. In other words, the

<sup>9</sup>We will continue the exploration of this regime in a future presentation.

<sup>10</sup>Quoted from Ref. [44], p. 89.

effect of a thermal initial state can be achieved by allowing the uncorrelated system to thermalize for an infinite amount of time. At  $t = 0$  the system density matrix is Gaussian. Means and variances of position and momentum are equal to those of the combined thermal state of QBM given in [48]:

$$\sigma_{xx} = \frac{1}{M\beta} \sum_{r=-\infty}^{\infty} \frac{1}{\Omega^2 + \nu_r^2 + 2\nu_r \hat{\gamma}(n_r)}, \quad (37)$$

$$\sigma_{pp} = \frac{M}{\beta} \sum_{r=-\infty}^{\infty} \frac{\Omega^2 + 2\nu_r \hat{\gamma}(\nu_r)}{\Omega^2 + \nu_r^2 + 2\nu_r \hat{\gamma}(n_r)}, \quad (38)$$

where  $\nu_r = 2\pi r/\hbar\beta$  are the bosonic Matsubara frequencies. These variances differ from those corresponding to a Boltzmann distribution with respect to the system Hamiltonian alone. The differences start at second order in the coupling strength between the system and the bath. In the literature ignoring these differences is sometimes referred to as the *weak coupling approximation*. The results of this paper *do not* depend upon the weak coupling approximation in this sense.

It is worth emphasizing that the equivalence of ensemble preparations is not just on the level of reduced density matrices, which can give only single-time correlations for general non-Markovian dynamics. As pointed out before FTs require multitime correlations, which can be obtained via the Langevin equation. It is the equivalence of the trajectories for  $t > 0$  that can be shown exactly for the two preparations mentioned. This means that any quantum mechanical correlation function involving only the open system variables and times larger than zero will be identical in both preparations [47].

As a result, the trajectories we obtained in the previous section can be used to describe a thermal state as long as we take  $t_i \rightarrow -\infty$  and assume a continuous spectrum for the bath frequencies. The thermal state preparation procedure is as follows: at the infinite past the system and bath are in a product state; the bath is in the thermal state, and the system is in an arbitrary state. The combined system evolves in time under the Hamiltonian (6) with  $f(t) = f(0)$  for  $t < 0$ . At  $t = 0$  the force protocol is started as usual. Although the formulation of FTs is independent of the value of  $f$  after  $t = \tau$ , it proves convenient to define  $f(t) = f(\tau)$  for  $t > \tau$ .

## V. PROBABILITY DISTRIBUTION OF WORK AND THE FTs

With these conceptual and technical preparations we now can define work performed on the system in the time interval  $[0, \tau]$  in the QBM model using the trajectories given by the solutions of the Langevin equation (32) as

$$\begin{aligned} W &= \int_0^\tau dt \frac{\partial H_T}{\partial t} = - \int_0^\tau dt \dot{f}(t) X(t) \\ &= - \int_{-\infty}^\infty dt \dot{f}(t) X(t) \equiv -\dot{f}^T \cdot X. \end{aligned} \quad (39)$$

In the last equality we utilized the notation of Eq. (13), where we set the integration limits to plus and minus infinity. We will adopt this convention for the rest of the paper. The superscript  $T$  stands for transpose. Since we have extended the range of integration in the redefined  $f(t)$  to the entire real axis (see the

end of the previous section), this change does not introduce any error in the above equation.

We define the retarded Green's function as  $g_{\text{ret}}(t - t') = g(t - t')\theta(t - t')$ . Then, for positive times,

$$X(t) = [g_{\text{ret}} \cdot f](t) + [g_{\text{ret}} \cdot \xi](t), \quad (40)$$

$$\langle X(t) \rangle = [g_{\text{ret}} \cdot f](t), \quad (41)$$

$$\sigma_{xx}(t, t') \equiv \langle X(t)X(t') \rangle - \langle X(t) \rangle \langle X(t') \rangle = [g_{\text{ret}} \cdot \hbar\nu \cdot g_{\text{ret}}^T](t, t'), \quad (42)$$

$$W = -\dot{f}^T \cdot g_{\text{ret}} \cdot f - \dot{f}^T \cdot g_{\text{ret}} \cdot \xi. \quad (43)$$

That  $\sigma_{xx}(t, t')$  is a function of  $t - t'$  only will be verified explicitly later.

Work defined in Eq. (43) is linear in  $\xi(t)$ , and  $\xi(t)$  is a Gaussian random process. Thus  $W$  itself is a Gaussian random variable. As a result the first two moments of  $W$  specify its entire statistics given by

$$\mathcal{P}(W) = \frac{1}{\sqrt{2\pi\sigma_W^2}} e^{-(W - \langle W \rangle)^2 / 2\sigma_W^2}. \quad (44)$$

The mean of work is given by

$$\langle W \rangle = -\dot{f}^T \cdot g_{\text{ret}} \cdot f. \quad (45)$$

Integrating this by parts and defining  $\Delta F = -[f(\tau)^2 - f(0)^2]/2M\Omega^2$ , we get

$$\langle W \rangle = \Delta F + \frac{\dot{f}^T \cdot h_e \cdot \dot{f}}{2M\Omega^2}, \quad (46)$$

where we have defined  $h_e(t, t') \equiv h(|t - t'|)$  and used the symmetry of the integrand. The standard deviation of work is calculated as

$$\sigma_W^2 = \langle W^2 \rangle - \langle W \rangle^2 = \dot{f}^T \cdot \sigma_{xx} \cdot \dot{f}. \quad (47)$$

Jarzynski equality states that

$$\langle e^{-\beta W} \rangle = \int dW \mathcal{P}(W) e^{-\beta W} = e^{-\beta(\langle W \rangle - \beta\sigma_W^2/2)} = e^{-\beta\Delta F_T}, \quad (48)$$

where  $\Delta F_T$  is the difference in free energy of the combined system for two different values of the external force  $f$  calculated quantum mechanically. Due to the linearity of the QBM model  $\Delta F_T$  has the same form as  $\Delta F$  defined earlier, which is the classical result. Note that this is only true for the difference of the free energies since the quantum and classical free energies themselves are different even for the simple harmonic oscillator. The quantum mechanical free energy in the case of  $f = 0$  is given by

$$F_T = F_B - \frac{1}{\beta} \log \left( \frac{1}{\beta\hbar\Omega} \prod_{r=-\infty}^{\infty} \frac{\nu_r^2}{\Omega^2 + \nu_r^2 + 2\nu_r \hat{\gamma}(\nu_r)} \right), \quad (49)$$

where  $F_B$  is the free energy of the isolated bath. The corresponding free energy in the classical model is simply the sum of the free energies of the isolated system and bath.

The equality of the difference of free energies due to a driving force can be understood easily by noting that the main

effect of the linear driving force is to shift the energy levels. As a consequence, the Jarzynski equality is satisfied if and only if

$$\dot{f} \cdot \sigma_{xx} \cdot \dot{f} = \frac{\dot{f} \cdot h_e \cdot \dot{f}}{\beta M \Omega^2}. \quad (50)$$

Note that this equality should hold for any  $\dot{f}(t)$ . This condition can be stated mathematically as

$$\frac{\delta}{\delta \dot{f}(s)} \int_0^{t_f} dt \int_0^{t_f} dt' \dot{f}(t) \left[ \frac{h(|t-t'|)}{\beta M \Omega^2} - \sigma_{xx}(t-t') \right] \dot{f}(t') = 0, \quad (51)$$

$$\int_0^{t_f} dt \dot{f}(t) \left[ \frac{h(|t-s|)}{\beta M \Omega^2} - \sigma_{xx}(t-s) \right] = 0. \quad (52)$$

This equation should also be valid for any  $\dot{f}(t)$ . Differentiating one more time with respect to  $\dot{f}(s')$ , we get the condition

$$\sigma_{xx}(s-s') = \frac{h(|s-s'|)}{\beta M \Omega^2}. \quad (53)$$

For Crooks's fluctuation theorem we need to consider the reverse process, which corresponds to a reversed force protocol and an initial state with the force value  $f(\tau)$ . We will use a subscript  $R$  for the quantities associated with the reversed process and no subscript for the forward process.

$$f_R(t) = f(\tau - t); \quad \Delta F_R = -\Delta F. \quad (54)$$

The corresponding work distribution is again specified by its first two moments, which can be shown to be

$$\begin{aligned} \langle W \rangle_R &= \langle W \rangle - 2\Delta F, \\ (\sigma_W^2)_R &= \sigma_W^2. \end{aligned} \quad (55)$$

Note that the standard deviation of work is the same for the forward and reverse protocols. The probability distribution of work in the reversed process is given by

$$\begin{aligned} \mathcal{P}_R(W) &= \frac{1}{\sqrt{2\pi}(\sigma_W^2)_R} e^{-(W-\langle W \rangle_R)^2/2(\sigma_W^2)_R} \\ &= \frac{1}{\sqrt{2\pi}\sigma_W^2} e^{-[W-(\langle W \rangle-2\Delta F)]^2/2\sigma_W^2}. \end{aligned} \quad (56)$$

Consider the ratio

$$\frac{\mathcal{P}_F(W)}{\mathcal{P}_R(-W)} = e^{\frac{(\langle W \rangle - \Delta F)}{\beta \sigma_W^2/2} \beta(W - \Delta F)}. \quad (57)$$

Crook's fluctuation theorem is satisfied if

$$\langle W \rangle - \Delta F = \beta \sigma_W^2/2. \quad (58)$$

As expected this condition is equivalent to condition (53) for the validity of Jarzynski equality.

Let us now try to understand the nature and meaning of condition (53). Here  $h$  and  $g$  are solutions to the homogenous Langevin equation. As such they do depend on the damping kernel but not on the noise kernel. On the other hand,  $\sigma_{xx}$  depends on both the damping kernel via  $g$  and on the noise kernel. For this equality to hold there has to be a relation between the noise and dissipation kernels. The same conclusion can be reached by studying Eq. (58). The average of work is independent of the noise kernel but depends on the

damping kernel. On the other hand, the standard deviation of work does depend on both kernels.

There is indeed such a relationship between the damping and noise kernels: the fluctuation dissipation relation (FDR). It is most easily presented in terms of the Fourier transforms of the corresponding kernels.

$$\hbar \tilde{v}(\omega) = M \hbar \omega \coth(\beta \hbar \omega/2) \tilde{\gamma}(\omega). \quad (59)$$

However, the quantum mechanical FDR in general does not satisfy condition (53), and thus the FTs do not need to hold. To see this note that the damping kernel is independent of  $\hbar$ . As a result, the homogenous solutions of the Langevin equation,  $h$  and  $g$ , do not depend on  $\hbar$ . On the other hand,  $\sigma_{xx}$  in general is a function of arbitrarily large powers of  $\hbar$  via the coth term in the noise kernel. FTs are satisfied if  $\hbar$  is set to zero. Corrections to FTs are expected at  $O(\hbar^2)$ .

### A. High and low temperature regimes

As described above, the noise kernel is the only place where quantum effects are manifest, as can be seen by the appearance of  $\hbar$ . Assumptions made on the properties of the bath renders the quantum features associated with the initial state of the system oscillator at the infinite past completely irrelevant. In FTs the noise kernel appears only in the standard deviation of work  $\sigma_W^2$ . In this section we will investigate this term in the high and low temperature regimes.

Using the Fourier transform, one can show from Eq. (47) that

$$\sigma_W^2 = (2\pi)^2 \int_{-\infty}^{\infty} d\omega \tilde{f}_d(\omega) \tilde{\sigma}_{xx}(\omega) \tilde{f}_d(-\omega), \quad (60)$$

where  $\tilde{f}_d(\omega)$  denotes the Fourier transform of  $\dot{f}(t)$ . Recall that in our convention  $\dot{f}(t)$  vanishes outside the interval  $[0, \tau]$ ; thus the Fourier transform is well defined. Using the FDR (59), it can be shown that

$$\tilde{\sigma}_{xx}(\omega) = \hbar \omega \coth\left(\frac{\beta \hbar \omega}{2}\right) \frac{\tilde{h}_e(\omega)}{2M\Omega^2}. \quad (61)$$

#### 1. High temperature expansion

For frequencies satisfying  $\beta \hbar \omega < 1$ , coth can be expanded into a Laurent series:

$$\coth\left(\frac{\beta \hbar \omega}{2}\right) = \frac{2}{\beta \hbar \omega} + \sum_{k=1}^{\infty} \frac{2^{2n} B_{2n}}{(2n)!} \left(\frac{\beta \hbar \omega}{2}\right)^{2n+1}, \quad (62)$$

$$\tilde{\sigma}_{xx}(\omega) = \frac{\tilde{h}_e(\omega)}{\beta M \Omega^2} + \sum_{k=1}^{\infty} \frac{2^{2n} B_{2n}}{(2n)!} \left(\frac{\beta \hbar \omega}{2}\right)^{2n+2} \frac{\tilde{h}_e(\omega)}{\beta M \Omega^2}, \quad (63)$$

where  $B_n$  is the  $n$ th Bernoulli number. If we assume that either  $\tilde{h}_e(\omega)$  or  $\tilde{f}_d(\omega)$  decreases sufficiently fast for large frequencies such that  $\beta \hbar \omega \geq 1$ , the Laurent series is a good expansion. Hence the characterization of "high" temperature depends on two time scales: the intrinsic time scale of the oscillator (determined by its interaction with the bath as well as its natural frequency) and the time scale of the driving force. It is reasonable to assume that  $\tilde{h}_e(\omega)$  vanishes for frequencies larger than the bath cutoff. Usually, this is taken to be very large. We will assume that  $\tilde{f}_d(\omega)$  becomes negligible at frequencies

much smaller than this cutoff frequency, denoted as  $\omega_h$ . This is expected to be a reasonable assumption for typical driving forces. High temperature refers to the condition  $\beta\hbar\omega_h \ll 1$ .

If we keep only the first term in the expansion (63), we see that condition (50) for the validity of FTs is satisfied. Deviations from FTs to all orders of  $\hbar$  can be calculated to be

$$\frac{1}{\beta M \Omega^2} \sum_{n=1}^{\infty} \frac{2^{2n} B_{2n}}{(2n)!} \left( \frac{\beta\hbar\omega}{2} \right)^{2n+2} \dot{f} \cdot h_e^{(2n+2)} \cdot \dot{f}. \quad (64)$$

The superscript on  $h_e$  denotes the order of derivatives taken with respect to the argument. The correction term can also be written as

$$\frac{1}{\beta M \Omega^2} \sum_{n=1}^{\infty} \frac{2^{2n} B_{2n}}{(2n)!} \left( \frac{\beta\hbar}{2} \right)^{2n+2} f^{(n+2)} \cdot h_e \cdot f^{(n+2)}. \quad (65)$$

Note that the knowledge of the homogenous solution to the Langevin equation is enough to calculate the correction term to all orders of  $\hbar$ .

### 2. Low temperature expansion

Below we present the form of the standard deviation of work in a low temperature expansion but we will not go into the details of the low temperature expansion because the notion of trajectories will ultimately break down at sufficiently low temperatures. For high frequencies the following expansion of coth is more suitable than Eq. (62):

$$\coth\left(\frac{\beta\hbar\omega}{2}\right) = \text{sgn}(\omega) \left[ 1 + 2 \sum_{k=1}^{\infty} e^{-k\beta\hbar|\omega|} \right], \quad (66)$$

$$\tilde{\sigma}_{xx}(\omega) = \frac{\hbar}{2M\Omega^2} |\omega| \tilde{h}_e(\omega) \left[ 1 + 2 \sum_{k=1}^{\infty} e^{-k\beta\hbar|\omega|} \right]. \quad (67)$$

This expansion is convergent for all frequencies. However, convergence is fastest for  $\beta\hbar\omega \gg 1$ . If we assume that either  $\tilde{h}_e(\omega)$  or  $\tilde{f}_d(\omega)$  decreases sufficiently fast for  $\omega \rightarrow 0$  such that  $\beta\hbar\omega \leq 1$ , expansion (67) is a good one to use for Eq. (60). Hence the characterization of low temperature depends on two time scales: the intrinsic time scale of the oscillator and the time scale of the driving force. It is reasonable to assume that  $\tilde{h}_e(\omega)$  vanishes for frequencies lower than the lowest bath frequency. Usually, this is taken to be very small. We will assume that  $\tilde{f}_d(\omega)$  becomes negligible at frequencies much higher than the lowest bath frequency. (This condition can be violated by a very slowly changing driving force.) Let us denote this frequency by  $\omega_l$ . Low temperatures are defined by  $\beta\hbar\omega_l \gg 1$ .

### 3. High temperature conditions and Markovian dynamics

An important special case is the Ohmic bath characterized by the spectral density:

$$J(\omega) = \frac{2M\gamma_0}{\pi} \omega. \quad (68)$$

Without a high frequency cutoff, the damping kernel becomes local in time. The Langevin equation takes on the form

$$M\ddot{X}(t) + 2M\gamma_0\dot{X}(t) + M\Omega^2 X(t) = f(t) + \xi(t). \quad (69)$$

Physically, one would like to have a high frequency cutoff, which in turn makes the damping kernel nonlocal in time. The high frequency cutoff also cures the pathologies of the noise kernel that occur in the Ohmic case without cutoff. A large cutoff  $\Lambda$  ensures that the damping kernel is strongly peaked around zero. If the driving force  $f(t)$  does not change significantly on time scales of order  $1/\Lambda$ , the Markovian approximation can be justified.

However, Markovian dynamics is not the criterion for FTs to be satisfied; high temperature is. This is because even at high temperature if the bath is non-Ohmic the dynamics of the open system can be non-Markovian.

## VI. RELATION BETWEEN CLASSICAL AND QUANTUM FTs

It is a well-known fact that the dynamics of a quantum system with a quadratic Hamiltonian is identical to the classical dynamics of the same model [42]. This applies to the QBM model as well. One may wonder, if FTs are satisfied in classical dynamics, with the above observation, what is it then that causes the possible violation of QFTs at low temperatures? Although the dynamics is the same for quantum and classical models, initial conditions are not. The thermal state at low temperatures is different for both. The damping kernel does not depend on the initial conditions and thus is the same for both quantum and classical models. The noise kernel, on the other hand, depends on the initial state of the bath. As a result, it is the noise kernel that is different and could give rise to deviations from FTs.

In the previous section we have seen how the classical limit is reached at high temperatures. We identified high temperatures as the ones such that all the relevant bath modes are multiply occupied. By relevant bath modes we mean those that are within the range of frequencies of the external driving force. As is well known from elementary quantum mechanics multiply-occupied harmonic oscillators act classically. In this classical limit FTs are satisfied.

Alternatively, one can solve the classical version of the QBM model exactly, which is possible due to the linearity of the model. Moreover in the classical model one can use the thermal state of the combined system instead of resorting to the infinite time preparation.<sup>11</sup> The result is a Langevin equation in which the noise is correlated with the initial conditions of the system oscillator. One can define a new noise that is uncorrelated with the initial conditions of the system oscillator. This redefinition also gets rid of the slip term [45,48] in the Langevin equation, and one obtains the familiar form

$$M\ddot{X}(t) + 2M \int_0^t ds \gamma(t-s) \dot{X}(s) + M\Omega^2 X(t) = f(t) + \xi(t), \quad (70)$$

$$\langle \xi(t) \rangle = 0, \quad (71)$$

<sup>11</sup>Like the quantum model, in the classical model too the equivalence of both preparations can be proven exactly for any spectral density.



$$\langle \xi(t)\xi(t') \rangle = \frac{2M}{\beta} \gamma(t-t'), \quad (72)$$

$$\langle X_i \xi(t) \rangle = \langle P_i \xi(t) \rangle = 0, \quad (73)$$

where the initial conditions are sampled from the reduced phase space density of the system that is obtained from the thermal phase space density of the combined system by integrating out the bath degrees of freedom.

Equations (70)–(73) are the beginning point of the analysis of [49]. The authors of that paper start with the phenomenological Langevin equation that is identical to (70). They further assume a Gaussian noise with the classical FDR (72). Finally, they assume that the initial values of the system oscillator coordinates are sampled from the classical phase space density  $f_S(X_i, P_i, t_i) \propto \exp[-\beta H_S(X_i, P_i, t_i)]$ . This last point can be justified from the microphysics model:

$$\begin{aligned} f_S(X_i, P_i, t_i) &= \prod_{n=1}^N \int dx_{ni} \int dp_{ni} f(X_i, P_i; \{x_{ni}\}, \{p_{ni}\}; t_i) \\ &\propto \exp[-\beta H_S] \prod_{n=1}^N \int dx_{ni} \int dp_{ni} \\ &\quad \times \exp \left\{ -\beta \left( \sum_{n=1}^N \left[ \frac{p_{ni}^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 \right. \right. \right. \\ &\quad \left. \left. \left. \times \left( x_{ni} - \frac{c_n}{m_n \omega_n^2} X_i \right)^2 \right] \right) \right\} \\ &\propto \exp[-\beta H_S(X_i, P_i, t_i)]. \end{aligned}$$

Similarly, the change in free energy that appears in the Jarzynski equality and Crooks's fluctuation theorem is that of the combined system. However, the construction of the coupling and the renormalization term make it coincide with that of the isolated system oscillator. This clever scheme notwithstanding, we point out that in their phenomenological approach [49] the free energy difference is mistakenly interpreted as that of the free oscillator since there is not enough information to track down its origin. This kind of ambiguity and disconnectedness, often found in the phenomenological models in the literature, heightens the importance and advantage of using a first-principles approach based on microphysics models, as is adopted here.

Starting from a microscopic model, we were able to recover all the features of the phenomenological Langevin equation. From there on, using the same analysis as in [49] leads to the verification of FTs. However, it is crucial to make the following distinction: In the phenomenological theory there is no *a priori* reason why FTs should hold because the open-system dynamics is not Hamiltonian. As a result, one needs to show the validity of FTs explicitly. In our formalism, on the other hand, we start with a closed (system plus bath) Hamiltonian system in a thermal state (of the combined system). Hence all the premises of the FTs are satisfied, and one expects that they should hold. What needs to be done is to verify them from explicit calculations.

One might object to this claim by noting that an uncountably infinite bath is required for the preparation described in

Sec. IV. The proof of FTs for close Hamiltonian systems utilizes the Liouville theorem, for which we have seen only proofs for a finite number of degrees of freedom. In this sense our model, with infinite preparation time, does not trivially satisfy FTs and needs the explicit verification. On the other hand, for finite baths one can use the thermal state of the combined system at  $t = 0$ , and then the FTs follow trivially. This second procedure is very easy for the classical model, though somewhat complicated yet still straightforward for the quantum model. The important point is that the infinite time preparation is only introduced for technical convenience. It can be argued that for any relevant times  $t > 0$  the effect of an infinite bath can be approximated arbitrarily closely by a large but finite bath. Hence our results are insensitive to the unphysical assumptions about the bath we made in our derivation.

It is worth mentioning that Speck and Seifert [50] have shown that the Jarzynski relation holds for general classical ergodic systems governed by stochastic dynamics including non-Markovian processes. Ohkuma and Ohta [51] studied classical systems described by a nonlinear, non-Markovian Langevin equation with Gaussian colored noise. Both of these works are more general than our work when applied to classical systems because they are not restricted to linear models. On the other hand, both adopt a phenomenological approach without an underlying microscopic model, as we do.

## VII. DISCUSSION

### A. Comparison to previous work

As mentioned in Sec. I A there seems to be a consensus on how to define work in closed quantum systems [9]. Work is defined as the difference of the energy of the closed system measured at two different times. This method is less attractive when applied to open systems (treating the system plus the environment as the closed system) since it involves measuring the energy of the combined system. Furthermore work is restricted to the open system, and it is only a part of the total energy, which involves also heat exchange with the bath. This can lead to big errors if one calculates the work of the combined system since work is the difference of two large numbers.

In this paper we use the decoherent histories conceptual framework to explain how the notion of trajectories in a quantum system can be made viable and use them to define work for open quantum systems. These quantities are likely to be more easily accessible than the energy levels for practical purposes related to experiments, especially for open quantum systems. The classical mechanical definition of work in terms of trajectories is used in the formulation of FTs.

The work operator is another route taken [8], but there is no satisfactory definition of work as an operator [4]. Besides, the work operator approach does not place any limit on the range of validity of its predictions. Using the environment-induced decoherence scheme, we can assess how strong the noise in the environment needs to be to provide sufficient decoherence to warrant the use of trajectories so as to be able to define work in open quantum systems. The parameter range whereby this condition is not satisfied is likely related to the range where FTs

may not hold quantum mechanically. The question of whether deviations from FTs can be observed in low temperature experiments at all, and if so in which parameter range, requires more quantitative analysis. This will be treated in a future presentation.

Comparing with previous work in the literature, the approach of [5] is closest to ours in spirit. However, in substance our approach differs from theirs in several important ways, as numerated below. Foremost a theoretical justification of the use of and the derivation of the range of validity of the trajectory concept in quantum mechanics are necessary in the formulation of FTs. To this end the authors of [5] invoke continuous measurements and wave function collapse together with taking the semiclassical limit. We point out the key conceptual and procedural steps that we believe [5] are flawed.

*Conceptual flaws.* It is said in [5] that “the classical limit can be reproduced by using the Wigner function” and also that “ $Q_+$  (our  $X$ ) is a classical coordinate variable and  $Q_-$  (our  $y$ ) is a quantum coordinate.”

These wrong statements stem from, we believe, a lack of understanding of the central issues in quantum decoherence. Misconceptions like these were common but were addressed and clarified in the 1990s. See, e.g., [18,41].

*Quantitative differences.* The range of validity is not stated clearly in [5], and the generating functional of work given in their Eq. (9) is said to be valid at arbitrary temperature. We believe this is an overstatement.

In the dechis or envdec formalism trajectories emerge due to the influence of the environment, in particular, the strength of noise: The stronger the noise is, the more pronounced the trajectories that take shape are; the weaker the noise is, the more quantum features prevail. These conditions of classicality can be quantified clearly, and from them one obtains the criteria for determining the range of validity of quantum FTs, as we discussed in an earlier section.

Equation (13) of [5] gives the lowest order in  $\hbar$  correction to the Jarzynski equality. We provide the corrections to arbitrary orders of  $\hbar$  in our Eq. (65) in terms of the homogenous solutions to the Langevin equation. Furthermore we show that these corrections apply to both Crooks’s fluctuation theorem and Jarzynski’s equality. At the classical level we derive Crooks’s fluctuation theorem and Jarzynski’s equality for the Brownian motion model.

## B. New issues brought forth

The dechis and envdec approaches bring forth a number of new issues that were not so clearly noted before. We name three here.

*Initial state preparation.* Initial state preparation is an important aspect of FTs. Most of the literature on FTs for closed systems is usually clear on this aspect. However, a certain level of ambiguity exists in open-system treatments. In this work we considered an initial thermal state for the closed system made up of the subsystem plus its environment. However, for computational ease and clarity of exposition we developed an equivalent initial state preparation method based on product initial states for the system and the bath. Our initial state preparation replaces the system’s dependence on the initial state by the properties of noise statistics. As a result,

our preparation method has only one probabilistic element as opposed to two. This makes the analysis clearer and the identification of quantum effects easier.

*On the meaning of the average in Eq. (2).* The averages that are calculated using the statistics of noise can alternatively be expressed in terms of expectation values of quantum mechanical operators. The important point is that products of position and momentum operators need to be symmetrized owing to the properties of the Wigner function, which is used in the averaging process. In the specific case of the Jarzynski equality, we observe that the average over noise realizations can also be obtained by taking the expectation value of the quantum mechanical operators as

$$\begin{aligned} \langle e^{-\beta W} \rangle &= \int D\xi P[\xi] \int dx_0 dp_0 W_r(x_0, p_0, 0) e^{\beta \int_0^\tau dt \dot{f}(t) x_\xi(t)} \\ &= \text{Tr}_{S+B} [e^{\beta \int_0^\tau dt \dot{f}(t) \hat{x}_H(t)} \hat{\rho}_\beta]. \end{aligned} \quad (74)$$

In this special case symmetrization is achieved by the exponential function together with the fact that the dynamics is linear and work itself is a linear function of position. Consequently, we do not need to impose the symmetrization procedure explicitly. It is in this strict sense that the results that are obtained using the work operator  $\hat{W} \equiv -\int_0^\tau dt \dot{f}(t) \hat{x}_H(t) = \hat{H}_H(\tau) - \hat{H}_H(0)$  for the Jarzynski equality agree with our results obtained via trajectories.

*How to decide if possible violations to FTs can be observed.* The formulation of FTs involves averages over noise realizations, with idealized situations where trajectories are perfectly well resolved for each realization of noise. But, of course, in an experiment, even classically, there is only finite resolution. Let us assume that the resolution of the experiment is independent of temperature. This introduces an error to the FTs obtained from these data that is independent of the temperature.

In the quantum case the condition  $\sigma^2 \sim \nu^{-1}$  suggests that for stronger noise we can resolve the trajectory to a higher precision. As the noise weakens, such as at decreasing temperature, the stochastic features of classical trajectories are enhanced due to the decoherence condition, and measurement results on a particle’s trajectory become less precise. By further weakening the noise we will get to a point in which quantum, or “Heisenberg,” noise dominates [30]. Here lies a fundamental difference between classical and quantum systems. In quantum mechanics the ability of resolving trajectories is not only determined by the precision of the measurement device but also by the temperature. As a result, the error in FTs introduced by the resolution of trajectories increases constantly as the temperature is lowered, unlike in classical mechanics. Below a certain temperature, upon entering the quantum-dominated regime, the imprecision in measurements will become too large, rendering any free energy calculations using FTs meaningless.

The properties of noise acting on the quantum Brownian particle are different from the noise in the corresponding classical model, as was shown above. This introduces a deviation from FTs that is independent of the error introduced by the limited precision of measurements (discussed in the previous paragraph). The quantum corrections to the noise kernel become larger at lower temperatures. As a result, we expect to observe deviations from FTs at low temperatures.

However, as we learned before, trajectories are not well defined at arbitrarily low temperatures. Further quantitative analysis is necessary to establish the domain of validity of our approach and the magnitude of possible violations to FTs within this domain as a function of temperature.

### C. Work in progress

We mention two aspects that command our current attention on this problem.

(a) We want to be able to answer the following question: Is there a temperature range for which experiments done to the precision prescribed by the decoherent histories interpretation give answers different from the corresponding calculations based on classical mechanics with the same measurement precision imposed (theoretically, measurements in classical systems can have infinite precision)? If so, what are the form and size of these violations? Such a difference would be due to quantum mechanics exclusively, and this is what we mean

by violations of the FTs at low temperatures due to quantum mechanical effects.

(b) Unlike in other approaches to quantum FTs, the use of open quantum system concepts and especially the influence functional method adopted here enables us to define and quantify heat flow in terms of the dissipative dynamics of the open system that results from a self-consistent treatment of the back action from its environment. We want to take advantage of this approach to address questions about energy exchange between the system and the bath, where applications abound.

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