Stochastic Thermodynamics of a Quantum Dot Coupled to a Finite-Size Reservoir

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In nanoscale systems coupled to finite-size reservoirs, the reservoir temperature may fluctuate due to heat exchange between the system and the reservoirs. To date, a stochastic thermodynamic analysis of heat, work, and entropy production in such systems is, however, missing. Here we fill this gap by analyzing a single-level quantum dot tunnel coupled to a finite-size electronic reservoir. The system dynamics is described by a Markovian master equation, depending on the fluctuating temperature of the reservoir. Based on a fluctuation theorem, we identify the appropriate entropy production that results in a thermodynamically consistent statistical description. We illustrate our results by analyzing the work production for a finite-size reservoir Szilard engine.

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Introduction.—In nanometer scale systems in contact with an environment, fluctuations of physical quantities are ubiquitous. The ability to control and measure systems at such small scales has been a key driving force in the development of stochastic thermodynamics [1–8], which provides a theoretical framework for thermodynamics phenomena based on concepts such as stochastic entropy [9], as well as detailed [10–16] and integral [17–19] fluctuation theorems. Stochastic thermodynamics has over the last two decades successfully been employed to describe a large number of experiments on small scale systems, such as implementations of Maxwell's demon [20–24] and Szilard's engine [25,26], verifications of Landauer's principle [27–29], tests of fluctuation theorems [30–33], and determination of system free energies [31,34–36].

In all these experiments, the environment can to a good approximation be described as a bath, or reservoir, in thermal equilibrium. Thus, the reservoir is effectively of infinite size, such that the exchange of heat with the system does not affect the reservoir. However, in many nanoscale experiments, the reservoirs are themselves of finite sizes, with system back action inducing energy fluctuations within the reservoir [37–42]. Given a fast relaxation timescale, such a reservoir may then be described by a fluctuating temperature. Such temperature fluctuations were recently investigated in small metallic islands [43].

Theoretically, the effect of finite-size reservoirs with time-dependent (but not fluctuating) temperatures on thermodynamic and transport properties have been investigated in a number of systems [44–49]. Furthermore, average values of thermodynamic quantities have been investigated for finite-size reservoirs that exhibit energy fluctuations [50]. There is to date, however, no stochastic thermodynamics analysis of small scale systems coupled to finite-size reservoirs, fully accounting for the system-reservoir back action and the resulting, correlated fluctuations of their physical properties. While the formalism outlined in Ref. [51] could provide the basis of such an investigation, we focus here on scenarios where the reservoir may be described by a (fluctuating) temperature at all times.

In this Letter, we present such a stochastic thermodynamics analysis, focusing on a basic, experimentally realizable setup [38,42]—a single level quantum dot with a time-dependent level energy, tunnel coupled to a finite-size electronic reservoir that can be described by a fluctuating temperature. The dynamics of the system and the reservoir temperature is described by a Markovian master equation. Based on a fluctuation theorem, relating the probabilities for forward and backward trajectories for the system and the reservoir temperature, we identify the appropriate stochastic entropy production. This allows for a thermodynamically consistent description given the knowledge of the fluctuating reservoir temperature. This is in contrast to previous approaches describing finite-size reservoirs, where effective temperatures are defined based on averages of reservoir observables [51–53]. To illustrate the approach, we consider a Szilard engine and show that the performed work is smaller than the work of an ideal engine, where the reservoir is of infinite size.

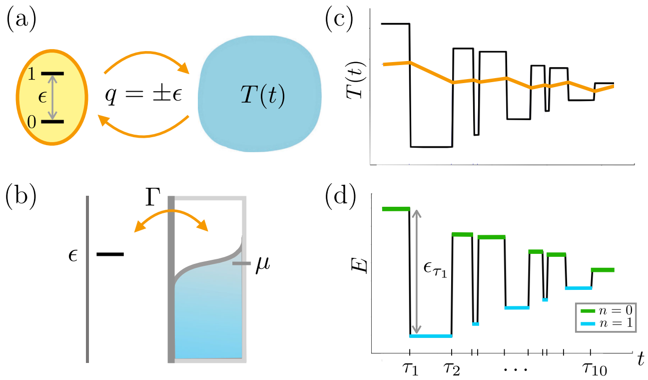

FIG. 1. (a) Sketch of a two-level system with an energy gap ϵ, coupled to a finite-size reservoir, the temperature of which being $T(t) \equiv T[E(t)]$. The system and reservoir exchange discrete amounts of heat $q = \pm\epsilon$ in a stochastic way. (b) Representation of the coupling between the dot system and the finite-size fermionic reservoir, where Γ is the tunneling strength. (c) Plot of the temperature $T(t)$ and the entropic temperature $T_{\mathrm{e}}(t)$ in orange for a linearly decreasing level energy ϵ_t. (d) Reservoir energy as a function of time. When an electron tunnels at time τ_j, the reservoir energy changes by ϵ_{τ_j}.

Entropy production conundrum.—The challenges with a stochastic thermodynamics description of small systems coupled to finite-size reservoirs can be compellingly illustrated by considering the basic setup in Fig. 1(a). A classical two-state system, with an energy difference $\epsilon > 0$ between the two states 0 and 1, exhibits stochastic state transfers due to the exchange of a discrete amount of heat $q = \pm\epsilon$ with a finite-size reservoir. Assuming that the reservoir temperature T increases monotonically with increasing reservoir energy, T will fluctuate between T_0 and $T_1 < T_0$, with superscripts denoting the system state. Naively employing the known result for infinite-size reservoirs, namely, that the entropy is given by the heat transferred divided by the reservoir temperature, one would assume that a transfer of heat into (out of) the reservoir leads to a production of entropy $\Delta s_{\mathrm{in}} = \epsilon/T_1$ ($\Delta s_{\mathrm{out}} = -\epsilon/T_0$) in the reservoir. For two subsequent heat transfers this leads to a reservoir entropy production

$$\Delta s_{\mathrm{in}} + \Delta s_{\mathrm{out}} = \epsilon(1/T_1 - 1/T_0) > 0. \tag{1}$$

Since the system is back in the same state after two transfers, the system does not contribute to the entropy. The result in Eq. (1) would thus imply that in equilibrium, stochastic heat fluctuations lead to a nonzero entropy production, which is physically nonsensical. From this reasoning, it is clear that entropy production in a reservoir with a temperature changing as a result of heat transfers between system and reservoir requires further understanding. To provide this, in the following we present a fully stochastic approach to the thermodynamics of an experimentally realistic implementation of the setup in Fig. 1(a).

System and master equation.—We consider a single level quantum dot with a time-dependent level energy ϵ_t, coupled to a finite-size electron reservoir via a tunnel barrier, characterized by a tunnel rate Γ, see Fig. 1(b). An electron tunneling from the dot to the reservoir (from the reservoir to the dot) at time t adds (removes) energy ϵ_t to (from) the reservoir. The stochastic nature of the tunneling process induces, in this way, fluctuations in time of the reservoir energy E. The electronic thermalization in the reservoir is considered to be so fast that, at all times, the electrons are effectively in a quasiequilibrium state, described by a Fermi distribution

$$f(\epsilon, E) = \frac{1}{1 + e^{\epsilon/k_{\mathrm{B}}T(E)}}. \tag{2}$$

The temperature $T(E)$ is related to E via the heat capacity $C(T) = C'T$ as

$$T(E) = \sqrt{\frac{2E}{C'}}, \tag{3}$$

where $C' = \pi^2 k_{\mathrm{B}}^2 \nu_0/3$, ν_0 being the density of states and k_{B} is the Boltzmann constant. As E fluctuates in time, $T(E)$ is a fluctuating temperature.

We describe the system's time evolution with the phenomenological, energy resolved master equation,

$$\frac{d}{dt}\begin{bmatrix} p_0(E) \\ p_1(E-\epsilon_t) \end{bmatrix} = \mathcal{W}\begin{bmatrix} p_0(E) \\ p_1(E-\epsilon_t) \end{bmatrix},$$
$$\mathcal{W} = \begin{bmatrix} -\Gamma_{\mathrm{in}}(\epsilon_t, E) & \Gamma_{\mathrm{out}}(\epsilon_t, E-\epsilon_t) \\ \Gamma_{\mathrm{in}}(\epsilon_t, E) & -\Gamma_{\mathrm{out}}(\epsilon_t, E-\epsilon_t) \end{bmatrix}, \tag{4}$$

where $p_n(E) \equiv p(n, E; t)$ is the probability that there are $n = 0, 1$ electrons on the dot and that the reservoir energy is E at time t. The probabilities satisfy the normalization condition $\int dE[p_0(E) + p_1(E)] = 1$, and the tunneling rates are given by [54,55]

$$\Gamma_{\mathrm{in}}(\epsilon, E) = \Gamma f(\epsilon, E), \qquad \Gamma_{\mathrm{out}}(\epsilon, E) = \Gamma[1 - f(\epsilon, E)], \tag{5}$$

see the Supplemental Material [56] for a motivation of these rates, as well as a discussion on charging effects and chemical potential fluctuations.

For a level energy that is constant in time, $\epsilon_t = \epsilon$, given a well-defined initial *total* energy for the system and reservoir (denoted by $\mathcal{E}$), the reservoir energy can only take on the values $\mathcal{E}$ and $\mathcal{E} - \epsilon$, for zero and one electron on the dot, respectively. This implies that the temperature fluctuates between $T(\mathcal{E})$ and $T(\mathcal{E} - \epsilon)$, and the stationary solution to Eq. (4) is given by $p_n(E) = \delta(E - \mathcal{E} + n\epsilon)p_n^{\mathrm{s}}(\epsilon|\mathcal{E})$ with

$$p_1^{\mathrm{s}}(\epsilon|\mathcal{E}) = 1 - p_0^{\mathrm{s}}(\epsilon|\mathcal{E}) = \frac{f(\epsilon, \mathcal{E})}{1 - f(\epsilon, \mathcal{E} - \epsilon) + f(\epsilon, \mathcal{E})}, \tag{6}$$

which reduces to $f(\epsilon, \mathcal{E})$ only when $T(\mathcal{E} - \epsilon) \simeq T(\mathcal{E})$.

Fluctuation theorem and entropic temperature.—For a stochastic thermodynamic description, we consider $n(t)$

and $E(t)$ as the stochastic system state and reservoir energy, respectively. A trajectory $\gamma = \{n(t), E(t)|0 \leq t \leq \tau\}$ may then be defined during a protocol, where the level energy may depend on time ϵ_t, as illustrated in Fig. 1(d). We denote the starting point of γ as $(n_0, E_0) \equiv [n(0), E(0)]$ and its endpoint as $(n_\tau, E_\tau) \equiv [n(\tau), E(\tau)]$. Note that $E(t)$ and $n(t)$ undergo abrupt changes at times τ_j, whenever an electron tunnels.

A fluctuation theorem relates the probability density $P(\gamma)$ for the trajectory to occur to the probability density $\tilde{P}(\tilde{\gamma})$ for the time-reversed trajectory $\tilde{\gamma}$ to occur under the time reversed protocol (where the level energy is changed as $\epsilon_{\tau-t}$)

$$\frac{P(\gamma)}{\tilde{P}(\tilde{\gamma})} = \exp\left[\frac{\sigma(\gamma)}{k_\mathrm{B}}\right], \tag{7}$$

where $\sigma(\gamma)$ is the total, stochastic entropy production along γ. We can write

$$\sigma(\gamma) = \Delta s(\gamma) + \Delta s_\mathrm{r}(\gamma), \tag{8}$$

where Δs, the change in system entropy, is given by

$$\Delta s(\gamma) \equiv k_\mathrm{B}[\ln p(n_0, E_0; 0) - \ln p(n_\tau, E_\tau; \tau)], \tag{9}$$

where $p(n_0, E_0; 0)$, $p(n_\tau, E_\tau; \tau)$ are the probabilities for the initial and final system states and reservoir energies. The term Δs_r, describing the stochastic entropy production associated to the reservoir, can be written as a stochastic integral along the trajectory γ (see the Supplemental Material [56])

$$\Delta s_\mathrm{r}(\gamma) \equiv -\int_\gamma \frac{dq(t)}{T_\mathrm{e}(t)}, \tag{10}$$

where $dq(t) = \epsilon_t dn(t)$ and we introduced the *entropic temperature* as

$$T_\mathrm{e}(t) \equiv T_\mathrm{e}(\epsilon_t, \mathcal{E}(t)) = \frac{\epsilon_t}{k_\mathrm{B}}\left[\ln\frac{\Gamma_\mathrm{out}(\epsilon_t, \mathcal{E}(t) - \epsilon_t)}{\Gamma_\mathrm{in}(\epsilon_t, \mathcal{E}(t))}\right]^{-1}, \tag{11}$$

where $\mathcal{E}(t) = E(t) + \epsilon_t n(t)$ denotes the total energy. Note that the entropic temperature is a stochastic variable taking on different values along different trajectories, just like $n(t)$ and $E(t)$.

The entropic temperature in Eq. (10) determines how the reservoir stochastic entropy changes along a given trajectory. In Fig. 1(c), we illustrate its behaviour in comparison to the actual temperature, $T(t) \equiv T[E(t)]$ which is obtained from the stochastic energy $E(t)$ via Eq. (3). We note that the entropic temperature is a continuous function with kinks when quanta of energy are exchanged via the tunneling process. This is due to the fact that the change in total energy is determined by the work performed on the system, which exhibits kinks because work is only performed when the dot is occupied (see below).

The entropic temperature becomes particularly simple for a constant level energy $\epsilon_t = \epsilon$ (again, assuming a fixed total energy)

$$T_\mathrm{e}(\epsilon, \mathcal{E}) = \frac{\epsilon}{k_\mathrm{B}}\left[\ln\frac{p_0^\mathrm{s}(\epsilon|\mathcal{E})}{p_1^\mathrm{s}(\epsilon|\mathcal{E})}\right]^{-1}, \tag{12}$$

where the entropic temperature is no longer a stochastic quantity. Furthermore, the stationary solution in Eq. (6) can be written as

$$p_1^\mathrm{s}(\epsilon|\mathcal{E}) = \frac{1}{1 + e^{\epsilon/k_\mathrm{B}T_e(\epsilon,\mathcal{E})}}. \tag{13}$$

The steady-state occupation of the dot is thus given by the Fermi-Dirac distribution if the entropic temperature is used. These observations further illustrate that it is the entropic temperature that determines the thermodynamics of the dot coupled to a finite-size reservoir.

Stochastic thermodynamics.—The stochastic internal energy of the system along the trajectory γ can be defined as

$$u(t) \equiv n(t)\epsilon_t. \tag{14}$$

The average internal energy is obtained by averaging this expression over the distribution for trajectories $P(\gamma)$,

$$U(t) = \langle n(t)\rangle\epsilon_t = p_1(t)\epsilon_t, \tag{15}$$

where $p_n(t) = \int dE p(n, E; t)$. According to the first law of thermodynamics, the system's internal energy changes can be divided into work and heat. Using Eq. (14), we identify heat and work as

$$du(t) = \epsilon_t dn(t) + n(t)\dot{\epsilon}_t dt = dq(t) + dw(t), \tag{16}$$

where the dot denotes a derivative with respect to t. In this way, the stochastic heat and work along the trajectory are given by

$$q \equiv \int_\gamma \epsilon_t dn(t), \qquad w \equiv \int_0^\tau dt\, n(t)\dot{\epsilon}_t. \tag{17}$$

Similarly to Eq. (15), we can write the first law in terms of the average heat, $Q \equiv \langle q\rangle$, and average work, $W \equiv \langle w\rangle$,

$$\Delta U \equiv U(\tau) - U(0) = W + Q, \tag{18}$$

where

$$Q = \int_0^\tau dt \dot{p}_1(t)\epsilon_t, \qquad W = \int_0^\tau dt p_1(t)\dot{\epsilon}_t. \tag{19}$$

Moreover, we can obtain the average entropy production by averaging the stochastic entropy production in Eq. (8)

$$\Sigma \equiv \langle \sigma(\gamma) \rangle = \Delta S - \left\langle \int_\gamma \frac{dq(t)}{T_{\rm e}(t)} \right\rangle, \tag{20}$$

where $\Delta S \equiv \langle \Delta s(\gamma) \rangle$. Using Eq. (7), the non-negativity of the Kullback-Leibler divergence [57] implies that

$$\Sigma = k_{\rm B} \left\langle \ln \frac{P(\gamma)}{\tilde{P}(\tilde{\gamma})} \right\rangle \geq 0. \tag{21}$$

Hence, Eq. (21) can be seen as a second law of thermodynamics for the dot system coupled to the finite-size reservoir. Note that, by considering the entropy production in Eq. (20) for a time-independent level energy $\epsilon_t = \epsilon$, it follows that $\Sigma = 0$ in equilibrium, as expected. Remarkably, we show in the Supplemental Material [56] that not only the average entropy production but also the stochastic entropy production in Eq. (8) is zero in equilibrium as well as in the quasi-static limit, where the system always approximately remains in equilibrium.

We note that Eqs. (20) and (21) look just like Clausius's second law [58], but with stochastic quantities and with temperature being replaced by the entropic temperature. The reason that the entropic and not the actual temperature enters the entropy production is because energy exchange happens in quanta. Indeed, we find that for $\epsilon_t \ll \mathcal{E}(t)$

$$T_{\rm e}(t) \approx \sqrt{\frac{2\mathcal{E}(t)}{C'}} - \sqrt{\frac{2\mathcal{E}(t)}{C'}} \frac{\epsilon_t}{4\mathcal{E}(t)}. \tag{22}$$

Thus, when the quantization of energy becomes negligible [and $\mathcal{E}(t) \approx E(t)$], the entropic temperature reduces to the actual reservoir temperature $T_{\rm e}(t) \approx T(t)$. In turn, a sizable ϵ_t leads to the disparity between the entropic temperature and the actual temperature. Our equations may thus be understood as a generalization of Clausius's second law that takes into account energy quantization in the exchange of heat.

In the Supplemental Material [56], we consider previously derived expressions for entropy production [52,59] which are expected to be positive in our scenario.

Work extraction.—To illustrate our approach, we first consider a basic protocol for work extraction. Starting at $t = 0$ with an empty dot at energy ϵ_0, we move the dot level down in energy with constant speed ν to zero, as $\epsilon_t = \epsilon_0(1 - \nu t)$. By simulating a large number of trajectories, we obtain the statistical properties of the thermodynamic quantities. In Fig. 2(a), the average extracted work $-W$, as well as the work extracted along individual trajectories, are shown as functions of time for different speeds. We see that $-W$, as well as the number of work extraction intervals, decrease for increasing ν.

The corresponding full probability distribution of extracted work is shown in Fig. 2(b). For the fast drive, a sizable fraction of trajectories display no electron tunneling and, hence, no work is extracted. For the slow drive the

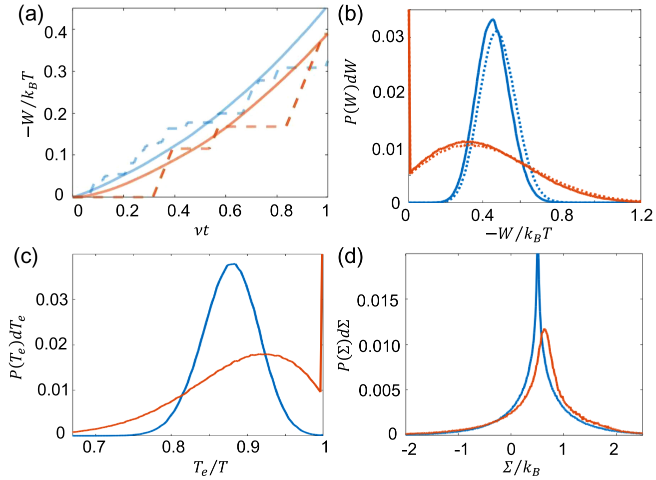

FIG. 2. Stochastic thermodynamic quantities. (a) The average extracted work $-W$ (solid lines) and the extracted work along a typical trajectory (dashed lines) as a function of time t. (b) The probability distribution of work extracted during the protocol. Solid (dashed) lines are for a finite (infinite) size reservoir. (c) The probability distribution of the entropic temperature T_e at the end of the protocol. (d) The probability distributions of the total entropy productions Σ during the protocol. In all panels the heat capacity $C(T) = 4k_{\rm B}$ and the dot level energy is driven as $\epsilon_t = \epsilon_0(1 - \nu t)$ with $\epsilon_0/k_{\rm B}T = 1.5$ and 10^6 trajectories have been generated. Initially, at $t = 0$, the dot is empty and the reservoir energy distribution is Gaussian, with average $2k_{\rm B}T$ and width $0.1k_{\rm B}T$. The drive speeds are $\nu = \Gamma/100$ (blue lines) and $\Gamma/10$ (red lines).

distribution becomes Gaussian shaped. Comparing to the work distribution of an infinite-size reservoir, the finite-size effects are most clearly visible for a slow drive, where they lead to a shift of the distribution towards smaller work values. Thus, the largest difference between the average work extracted with a finite and infinite-size reservoir seems to occur in the quasistatic regime.

In Fig. 2(c), the distributions of the entropic temperature $T_{\rm e}$ at the end of the protocol for the same parameters as in Fig. 2(b) are shown. Compared to the distribution for large speed, the small speed distribution is narrowed and shifted to lower temperatures. In Fig. 2(d) it is shown how the distribution of total entropy production is narrowed and shifted towards zero when the drive speed is decreased.

To highlight the effect of a finite-size reservoir on information to work conversion, we analyze a Szilard engine, following closely the quantum dot protocol in Ref. [26]. Initially, the dot level energy is put to zero, giving a dot occupation probability 1/2, and the reservoir energy is fixed to E_0. The occupation is then measured, with two possible outcomes: (i) If the dot is empty, the level energy is instantaneously increased to $\epsilon_{\rm i}$ and thereafter quasistatically taken back to zero. (ii) If the dot is instead occupied by an electron, the level energy is instantaneously decreased to $-\epsilon_{\rm i}$, and thereafter quasistatically increased back to zero. We note that the process is not completely

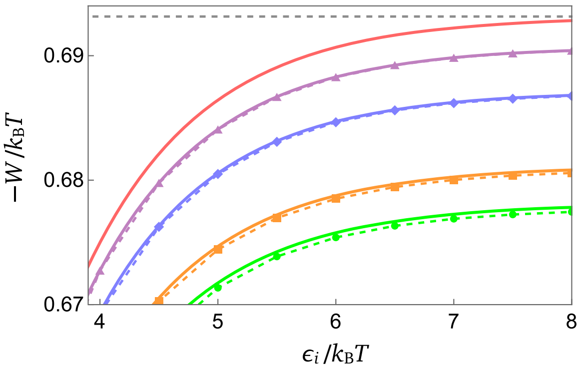

FIG. 3. Work extracted, $-W$, as a function of ϵ_i in a quasistatic cycle of the Szilard engine, for the following initial heat capacities $C[T(E_0)]$: $16k_B$ (green line), $20k_B$ (orange line), $40k_B$ (blue line), $100k_B$ (purple line). The full numerical solution (solid lines) and the expansion to first order in $1/C[T(E_0)]$ (dashed lines) are shown. The infinite-size reservoir case is shown with a solid, red line. The dashed, gray line corresponds to the upper bound on work extraction with an infinite-size reservoir in a cycle of the Szilard engine, which is $k_BT\ln 2$. Corresponding analytical expressions are given in the Supplemental Material [56].

cyclic, since the initial reservoir energy is well defined, while the final energy is a stochastic quantity. The average extracted work $-W$ as a function of ϵ_0, for different heat capacities, is shown in Fig. 3. We see that decreasing the size of the reservoir leads to a monotonically decreasing $-W$. This is in line with previous results showing that Landauer's upper bound on work extraction cannot be achieved with finite-size reservoirs [60].

Conclusion.—We provided a consistent thermodynamic description for a two-level system, namely, a quantum dot, coupled to a finite-size reservoir. In our approach, the reservoir entropy along a given trajectory is determined by the entropic temperature, which therefore dictates the thermodynamics of the system and finite-size reservoir. Notably, we found that the entropic temperature is required to describe the thermodynamics of the system and reservoir as long as energy exchange occurs in quanta. When energy quantization is negligible, the entropic temperature reduces to the actual temperature, and therefore a connection with Clausius's second law is established. We complete our analysis by defining work and heat, and by showing that the stochastic entropy production vanishes for each trajectory in the quasistatic limit. Our results are illustrated by a protocol for work extraction and for the Szilard engine.

Our results show how to describe the thermodynamics of a finite-size reservoir that can be described by a fluctuating temperature. While we focus on an electronic two-level system, our results can easily be generalized to other scenarios, e.g., a superconducting qubit coupled to an electro-magnetic environment [40,41] or an electron spin coupled to nuclear spins [39]. Of particular interest are systems, or reservoirs, which exhibit quantum coherence, such as double quantum dots [61] or squeezed bosonic reservoirs [62]. Furthermore, our approach can be adapted to include multiple reservoirs, allowing for transport scenarios.

Finally, we note that a microscopic derivation of our master equation in Eq. (4) would provide quantitative insight into the limitation of our approach and is left for future work. A starting point for such a derivation could be provided by the extended microcanonical master equation [50,63–67].

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Correction: Sign errors in two inline equations in the text preceding Eq. (1) have been fixed. A minor error in Eq. (1) has also been fixed.