Self-Consistent Microscopic Theory of Fluctuation-Induced Transport

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A Maxwell's demon type "information engine" that extracts work from a bath is constructed from a microscopic Hamiltonian for the whole system including a subsystem, a thermal bath, and a nonequilibrium bath of phonons or photons that represents an information source or sink. The kinetics of the engine is calculated self-consistently from the state of the nonequilibrium bath, and the relation of this kinetics to the underlying microscopic thermodynamics is established.

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Processes in which some of the energy in a nonequilibrium bath is transformed into work at the expense of increased entropy are of great interest in a number of important areas, but the study of the kinetics of such processes is complicated by the fact that no principles of the power and generality of those of equilibrium statistical mechanics exist for such cases. A number of semiheuristic type models have appeared recently that have served as illustrations that time correlated fluctuations interacting with a spatial asymmetry are sufficient conditions to give rise to transport [1–3]. An application of this idea has recently been utilized experimentally as a new type of molecular separation technique [4]. In addition, it is clear that spatial asymmetry is a necessary requirement only when all the odd moments of the fluctuations (including orders higher than first) vanish, and that transport will generally occur even in the absence of a spatial asymmetry if this requirement is not met [5].

These models, which come under the general heading of "fluctuation induced transport," are usually based on a reduced description of the noisy overdamped motion of a particle in a periodic potential. The nonequilibrium effects of the irreversible ($\delta S > 0$) interaction of the system with a nonequilibrium bath are modeled in various ways. A net current appears as a consequence of the nonequilibrium effects of the driving, even though the average driving force vanishes. In this way these nonequilibrium fluctuations can be used to do work.

This previous work has focused on phenomenology, and no attempt was made to formulate self-consistent models. Since the choice of the kinetics of the reduced system is somewhat arbitrary, it is often difficult to know whether such descriptions are appropriate, or even allowed by the microscopic laws of physics. In order to treat these models, self-consistently reduced descriptions need to be carefully derived from microscopic considerations since macroscopic equilibrium kinetics is no longer applicable. Here we construct a special microscopic model that contains an explicit description of the bath as well as the subsystem and allows a rigorous determination of the kinetics. This model can be used to more fully explore the question of what types of kinetic description are allowed by the underlying laws of physics and how these kinetic descriptions are related to the state of the bath and its fundamental thermodynamic properties.

We will consider a particle (subsystem) with position Q coupled to a thermal "Brownian" bath $\mathcal{A}$, representing the thermal background environment of the engine, and to a nonequilibrium bath $\mathcal{B}$. As we will demonstrate, *the nonthermal part of the energy in bath $\mathcal{B}$ can be viewed as a source or sink of negentropy (physical information) that allows the engine to operate, while the thermal parts of both baths provide the actual energy, as in the case of Maxwell's demon.* The Hamiltonian for the entire system will be given by

$$\mathcal{H} = \frac{M}{2}\dot{Q}^2 + U(Q) + \mathcal{H}_{\mathcal{A}} + \frac{1}{2}\sum_k(\dot{Y}_k^2 + \omega_k^2 Y_k^2) + \mathcal{H}_{\mathrm{int}\mathcal{A}} - \epsilon V(Q)\sum_k Y_k\,. \tag{1}$$

The first two terms on the right hand side describe the subsystem, where M is the mass of the subsystem. $\mathcal{H}_{\mathcal{A}}$ is the Hamiltonian for the Brownian bath. The fourth term describes the bath $\mathcal{B}$, which is represented as bath of linear oscillators, with frequency spectrum $\{\omega_k\}$. The last two terms are the interaction of the subsystem with the baths, where ϵ is a coupling constant. The form of the nonequilibrium bath $\mathcal{B}$, that of a set of phonons, was chosen for both simplicity and because of its generic relationship to many condensed matter type systems. Extensions of this approach to higher dimension (more gross variables) are straightforward.

The evolution of $\mathcal{B}$ is given by

$$Y_k(t) = A_k\cos(\omega_k t + \phi_k) + \frac{\epsilon}{\omega_k}\int_0^t d\tau\, V\big(Q(\tau)\big)\sin\omega_k(t-\tau)\,, \tag{2}$$

where A_k and ϕ_k are the initial amplitudes and phases of the oscillators. This equation can be used to eliminate the oscillator modes and to obtain a description of the variable Q [6]. We will assume that the interaction of the subsystem with $\mathcal{A}$ is that of a Brownian particle and that the frequency spectrum of the oscillator bath $\mathcal{B}$

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is quasicontinuous with a frequency density $\rho(\omega)$ of the Debye type

$$\rho(\omega) = \begin{cases} 3\omega^2/2\omega_c^3, & |\omega| \le \omega_c, \\ 0, & |\omega| > \omega_c, \end{cases} \quad (3)$$

which is regularized by a cutoff at high frequency ω_c that is assumed to be larger than any typical frequency of the gross variable. Since the bath is quasi-infinite, we can assume that the state of the bath does not change on time scales of interest as a result of its interaction with the subsystem. After elimination of the bath variables from the equations of motion we obtain a nonlinear Langevin equation for the subsystem,

$$M\ddot{Q} + \Gamma(Q)\dot{Q} + \tilde{U}'(Q) = \xi_{\mathcal{A}}(t) + V'(Q)\xi_{\mathcal{B}}(t), \quad (4)$$

where $\Gamma(Q) = \Gamma_{\mathcal{A}} + [V'(Q)]^2\Gamma_{\mathcal{B}}, \xi_{\mathcal{A}}(t)$ is Gaussian white noise,

$$\langle \xi_{\mathcal{A}}(t)\rangle = 0, \quad \langle \xi_{\mathcal{A}}(t)\xi_{\mathcal{A}}(s)\rangle = 2\Gamma_{\mathcal{A}}kT\delta(t-s), \quad (5)$$

and $\xi_{\mathcal{B}}(t)$ is a Gaussian noise with

$$\langle \xi_{\mathcal{B}}(t)\rangle = 0, \quad \phi(t) = \langle \xi_{\mathcal{B}}(t)\xi_{\mathcal{B}}(0)\rangle,$$

$$\Phi(\omega) = \int_{-\infty}^{\infty} dt\, \exp(i\omega t)\phi(t) = 4\Gamma_{\mathcal{B}}u(\omega), \quad (6)$$

where $u(\omega) = \langle \omega^2 A^2(\omega)\rangle/2$ is the energy density that depends explicitly on the preparation of the bath. In addition, the "bare" potential is now dressed by the oscillator bath $\tilde{U}(Q) = U(Q) - (\omega_c/\pi)\Gamma_{\mathcal{B}}V^2(Q)$. Here, for simplicity, we assume a random distribution of initial phases of the oscillators, which ensures that the noise is Gaussian. The only approximation that has been made in going from Eqs. (1)–(3) to Eqs. (4) and (5) is neglect of the Poincaré recurrence time of the system, and Eq. (7) follows from the random phase assumption.

For the purposes of this Letter we will consider only the overdamped ($\Gamma_{\mathcal{A}}/M \gg 1$) case, so that

$$\Gamma(Q)\dot{Q} = -\tilde{U}'(Q) + \xi_{\mathcal{A}}(t) + V'(Q)\xi_{\mathcal{B}}(t). \quad (7)$$

The inclusion of the thermal Brownian bath $\mathcal{A}$ plays an important role here since this description will break down when $\Gamma_{\mathcal{A}} = 0$. We will use this equation to study fluctuation induced transport in a system where $U(Q) = U(Q+\lambda)$ and $V(Q) = V(Q+\lambda)$, so that the Hamiltonian is invariant under the translation $Q \to Q + \lambda$. As a consequence, $\tilde{U}(Q) = \tilde{U}(Q+\lambda)$. A portion of a typical "dressed" ratchet potential $\tilde{U}(Q)$ is pictured in Fig. 1. Even though the average force on the particle vanishes, a net current will be produced, which if directed against a load force can be used to do work. The basic theoretical problem is to find the mean velocity $\langle \dot{Q}(t)\rangle$ in the subsystem given the shape of $U(Q)$ and $V(Q)$ and the properties of the noise terms $\xi_{\mathcal{A}}(t)$ and $\xi_{\mathcal{B}}(t)$.

Since we have started with an explicit microscopic (time reversible) Hamiltonian, if the system as a whole is in equilibrium the current must vanish. Therefore, a stationary current can appear only if the system is out of equilibrium. This is a basic consequence of the second law of thermodynamics, which requires that no net work can be extracted from a system in thermal equilibrium. Work can be extracted from the system via a Carnot type engine that runs off of two baths at different temperatures. Our system can operate as such an engine if $\mathcal{B}$ is prepared in a quasithermal state, that is, where the temperature of $\mathcal{B}$ is not necessarily equal to the temperature of the bath $\mathcal{A}(T \neq \overline{T})$. The equipartition of energy then gives $u(\omega) = k\overline{T}/2, \xi_{\mathcal{B}}(t)$ is Gaussian white noise with $\langle \xi_{\mathcal{B}}(t)\rangle = 0$, $\phi(t) = 2\Gamma_{\mathcal{B}}k\overline{T}\delta(t)$, and Eq. (7) is Markovian, and thus amenable to standard techniques. The evolution of the probability density $\rho(Q,t)$ for the system described by Eq. (7) is then given by the Fokker-Planck equation,

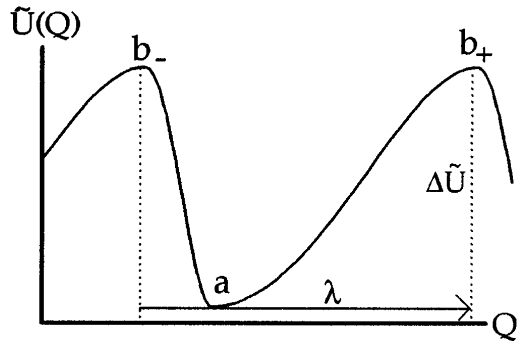

FIG. 1. Typical dressed ratchet potential $\tilde{U}(Q)$.

$$\partial_t\rho = \partial_Q\{\tilde{U}'(Q)/\Gamma(Q) + kT\partial_Q[\mathcal{D}(Q)/\Gamma(Q)]\}\rho,$$

$$\mathcal{D}(Q) = 1 + \frac{r(\Gamma_{\mathcal{B}}/\Gamma_{\mathcal{A}})[V'(Q)]^2}{1 + (\Gamma_{\mathcal{B}}/\Gamma_{\mathcal{A}})[V'(Q)]^2}, \quad (8)$$

where $r = (\overline{T} - T)/T$.

Equation 8 can be solved for the steady-state solution with periodic boundary conditions $\rho_s(x) = \rho_s(x+\lambda)$ and normalization $\int_x^{x+\lambda}\rho_s(x)\,dx = 1$ [7]. This yields an exact expression for the average velocity

$$\langle \dot{Q}\rangle = \frac{kT[1 - \exp(\delta/kT)]}{\int_0^\lambda dy\, e^{-\Psi(y)/kT}\int_y^{y+\lambda}dx\,\Gamma^2(x)e^{\Psi(x)/kT}/\mathcal{D}(x)}$$

$$\Psi(x) = \int^x \frac{U'(y)}{\mathcal{D}(y)}\,dy, \quad \delta = \Psi(0) - \Psi(\lambda). \quad (9)$$

It is easy to see from Eq. (9) that when the temperature difference between the baths is zero ($r = 0$), the current vanishes identically (since $\delta = 0$). This is to be expected and, of course, is a consequence of the second law. The current will also vanish in the limit $\Gamma_{\mathcal{B}}/\Gamma_{\mathcal{A}} \to 0$.

From this point on we will only consider cases where the characteristic noise intensities T and $D = \max\Phi(\omega)$ are small in comparison to the well depth $\Delta\tilde{U} = \tilde{U}(b) - \tilde{U}(a)$, which can be ensured by making the coupling between the system and the bath small enough. This situation is particularly interesting since analytic results are possible for both Markovian, and non-Markovian situations [2,8], and since the basics physics is illustrated most clearly.

For $T, D \ll \Delta\tilde{U}$, most of the time the system performs small-amplitude fluctuations about the minima of the potential. Occasionally it will "jump" from the minimum it occupied to the one on the right or left, with the probabilities per unit time W_+ and W_-, respectively. These jumps give rise to the average velocity $\langle\dot{Q}\rangle = \lambda(W_+ - W_-)$.

For the Markovian case described in Eq. (7) the transition rates can be calculated via standard techniques and evaluated by steepest descents. We obtain $W_\pm = W_K \exp(r\beta_\pm/kT)$, where

$$W_K = \frac{\sqrt{\tilde{U}''(a)|\tilde{U}''(b)|}}{2\pi} \exp(-\Delta U/kT) \tag{10}$$

is the Kramers activation rate, with $\Delta\tilde{U} = \tilde{U}(b) - \tilde{U}(a)$, and where for small $\Gamma_{\mathcal{B}}/\Gamma_{\mathcal{A}}$,

$$\beta_\pm = (\Gamma_{\mathcal{B}}/\Gamma_{\mathcal{A}}) \int_a^{b^\pm} U'(x)[V'(x)]^2\, dx. \tag{11}$$

These transition rates can be further expanded in powers of $\Gamma_{\mathcal{B}}/\Gamma_{\mathcal{A}}$, but, for our present purpose, this is not particularly enlightening. The mean velocity is given by

$$\langle\dot{Q}\rangle = \lambda W_K[e^{r\beta_+/kT} - e^{r\beta_-/kT}]. \tag{12}$$

This expression can also be obtained from the exact solution (9) by evaluating the integrals in the denominator via steepest descent. We see that the current will flow in one direction if $T < \overline{T}$ and in the opposite direction if $T > \overline{T}$. Thus, the system acts like Carnot engine, doing work by making use of two thermal baths at different temperatures.

The correlation ratchet, a system that is driven by the effects of colored noise, is obtained from Eqs. (6) and (7) by setting $u(0) = kT/2$. Thus, both $\mathcal{A}$ and $\mathcal{B}$ have "thermal parts" while $\mathcal{B}$ has a small part $u(\omega) - u(0)$ that deviates from equilibrium. If bath $\mathcal{B}$ has a nonthermal distribution over its modes, then $u(\omega)$ is not constant, and this manifest itself as time correlations [i.e., $\xi_{\mathcal{B}}(t)$ is no longer delta correlated] and a net current will arise.

When the bandwidth of the spectrum $\Phi(\omega)$ greatly exceeds the reciprocal relaxation time of the system $t_r^{-1} = \tilde{U}''(a)$, the transition probabilities $W_\pm$ can be calculated by an extension of the variational technique used in [2,8], where $W_\pm = W_K \exp[-\gamma_\pm F''(0)/kT]$ and

$$\gamma_\pm = \left(\frac{\Gamma_{\mathcal{B}}}{\Gamma_{\mathcal{A}}}\right)^2 \int_a^{b_\pm} \tilde{U}'[V'\tilde{U}'' + V''\tilde{U}']^2\, dx, \tag{13}$$

and where $F(\omega) = kT/4u(\omega)$, $F''(\omega) = d^2F(\omega)/d\omega^2$, with $|F''(0)/F(0)| \ll t_r^2$. The mean velocity

$$\langle\dot{Q}\rangle = \lambda W_K\Big[e^{-\gamma_+F''(0)/kT} - e^{-\gamma_-F''(0)/kT}\Big]. \tag{14}$$

We have neglected the small corrections to the prefactor in W_K due to the noise color and used the standard Kramers expression for this prefactor valid for white-noise driven systems.

The direction of the current is determined by the interplay of the shapes of the potential and energy density distribution $u(\omega)$. Just as the current in the thermal ratchet changes sign when r changes sign, the current in the correlation ratchet changes sign when $F''(0)$ changes sign. More details can be found in [2]. *These current reversals are a new phenomenon due to activation effects and are entirely unrelated to the current reversals found in* [3].

Although the corrections $\gamma_\pm F''(0)$ to the activation energy are small compared to the main term, they are not small compared to kT, and can change $W_\pm$ by orders of magnitude. Excepting the special case where $\tilde{U}(Q)$ is symmetric with respect to a, the transitions in one direction will typically dominate overwhelmingly over the transitions in the opposite direction. The optimal rate $\langle\dot{Q}\rangle = \lambda W_K$ is attained when all the thermally activated transitions are in one direction. Thus, while the vast majority of the energy in both $\mathcal{A}$ and $\mathcal{B}$ is thermally distributed in this near-equilibrium situation it is the relatively small amount of energy that is not distributed thermally, or equivalently the negentropy, that allows the engine to run. On the other hand, if the thermal energy were removed the engine would immediately stop running since virtually no transitions would ever occur. It should be clear from previous analysis that the force driving the particle comes overwhelmingly from the thermal parts of the baths. Therefore, we must conclude that while even a very small negentropic source or sink in $\mathcal{B}$ allows the engine to operate, the thermal fluctuations provide the energy.

As described in the preceding paragraph this system is an "information engine" analogous to a Maxwell's demon engine that extracts work out of a thermal bath by rectifying the thermal fluctuations of the system. Maxwell's demon is a "being" that uses information about the system to "choose" only those fluctuations that are helpful to make the engine run. This information, which can only be acquired if the demon is not in equilibrium with the bath [9], is used to rectify the energy already available, but otherwise inaccessible, in the thermal bath. As shown by Szilard [10], the information is acquired at the expense of an entropy increase of the demon, an observation that salvages the second law. Similarly it is clear from the approach used here that our system does work at the expense of the total increase of entropy of the baths and operates because of the physical information contained in the nonthermal energy of the bath, while the energy is paid predominately in the currency of the thermal fluctuations.

In the example given by Brillouin in [9] the demon uses light photons to determine the location of a particle and then uses this information to extract work from the system. The demon needs a source of light that is not in equilibrium with the bath in order to distinguish the

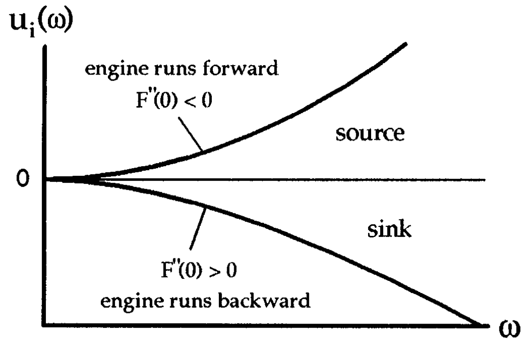

FIG. 2. Physical information $u_i(\omega)$ density near zero frequency. The generic cases where the phonon bath acts as an information source and the engine runs forward and where it acts as a sink and the engine runs backward are shown.

signal from the thermal background radiation. The model presented here can be regarded as a simplified picture of a bath of photons coupled to a particle in a thermal bath. By adding or removing photons (energy) from a system in thermal equilibrium an information source or sink is created of the same type as described by Brillouin. The subsystem in this case plays the role of the demon and allows the information to be converted to work.

This observation is made precise in the following way. Once the energy density over the frequency spectrum of the phonon bath $u(\omega) = \langle \omega^2 A^2(\omega) \rangle / 2$ is known, thermodynamic quantities can be calculated. Near equilibrium, as is the case for the above approximation, nearly all of the energy in the two baths is in a thermal state, and any entropy increase δS will not change the temperature. In this case the physical information (negentropy) in the phonon bath is given isothermally by $H_b = \int_0^{\omega_c} d\omega\, u_i(\omega)$, where $u_i(\omega) = u(\omega)/T - k/2$ is the information density. Since we have set $\Phi(0) = 2\Gamma_{\mathcal{B}} kT$, the sign of the information contained in the low frequency part of the spectrum is determined by the curvature of the information density at zero frequency, $u_i''(0) = -kF''(0)$ as illustrated in Fig. 2. The situation $F''(0) < 0$ implies a low frequency "source" of information in $\mathcal{B}$, and while $F''(0) > 0$ a "sink" in $\mathcal{B}$ as is illustrated in Fig. 2. As was shown above, the engine will run in opposite directions in these two cases. When $H_b > 0$ information flows out of $\mathcal{B}$ and the engine turns in one direction. The first is just thermodynamics, while the second is a result of the previous calculations. Just the opposite is the case when $H_b < 0$ and when the system is in equilibrium $H_b = 0$. Thus the semiheuristic treatments of [2,8] can be made self-consistent, and the relationship between thermodynamic quantities and reduced kinetic descriptions such as Eq. (4) can be established.

The free energy of the whole system is given by $\mathcal{F} = \tilde{U} + TH_b$. However, in the nonequilibrium case $\mathcal{F}$ is generally not sufficient to calculate rates, as should be clear from the above example. While (near equilibrium) the free energy does play the role of a stochastic Lyapunov function, it does not necessarily play a kinetic role analogous to the one the energy plays in equilibrium systems, and consequently the kinetics usually cannot be determined from thermodynamics quantities of the bath. In addition, when more than one gross variable is considered and when the bath is not in thermal equilibrium the reduced description *need not possess a local "energy-type" function of the gross variables in the Langevin equations* (i.e., the mean "force" is not necessarily curl free) [11]. This is true in our example *even when the state of the bath can be described by a scalar thermodynamic quantity,* such as in the quasithermal situation discussed above.

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