A Simple Model for Maxwell’s Demon Type Information Engine

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Abstract

We have investigated the recently proposed self-consistent theory of fluctuation-induced transport. In this framework the subsystem under study is coupled to two independent baths at different temperatures. In this non-equilibrium system one can extract energy at the expense of increased entropy. This is a simple model of Maxwell’s demon engine that extracts work out of a non-equilibrium bath by rectifying internal fluctuations. We point out the errors in the earlier results. We have obtained an analytical expression for the fluctuation-induced transport current in a non-equilibrium state and various cases of physical interest have been elucidated.

PACS Numbers: 05.60, +w, 05.40.+j, 87.10.+e.

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From thermodynamics, it is well-known that useful work cannot be extracted from equilibrium fluctuations [1]. In a thermal equilibrium state the principle of detailed balance ensures that no net particle current can flow in the presence of external potential of arbitrary shape. In contrast, in a non-equilibrium situation, where detailed balance is lost, net current flow is possible, i.e., one can extract energy at the expense of increased entropy. Several models have been proposed recently in this direction [2-6]. The motion of a heavily damped Brownian particle, in the presence of asymmetric static external potential and under non-white or correlated fluctuations, is a simple example of a non-equilibrium system. In such a system induced current or directed motion appears, eventhough the average of the driving fluctuations vanishes. It turns out that the preferred direction of motion and the magnitude of induced current depends sensitively on the shape of the potential as well as on the statistics of the fluctuations. Moreover, to obtain induced current the strength of non-white noise must exceed a certain minimum value and the magnitude of induced current shows a maximum value at an intermediate value of the noise strength. These models [2-7] of engines to obtain coherent response (or rectification) from unbiased forcing come under the common denomination of “thermal ratchets” or “fluctuation - induced transport systems”. The idea of thermal ratchets has been utilized recently for molecular separation [8]. One of the major motivations of these studies comes from molecular biophysics, where ratchet like mechanism is proposed to explain unidirectional movement of macromolecules or molecular motors. This is a physical example of preferred directional motion of Brownian particles (macromolecules) along periodic structures in the absence of obvious driving potentials, such as chemical potential gradients or thermal gradients.

In a physically well motivated recent work [9], Millonas points out that all the proposed earlier models [2-6] are basically phenomenological in nature and no attempt has
been made to formulate the problem from first principles. Millionas in his treatment
[9] constructs a Maxwell’s demon-type information engine that extracts work from non-
equilibrium bath and allows a rigorous determination of kinetics consistent with the under-
lying laws of physics. He explicitly writes down a microscopic Hamiltonian including
the subsystem and two thermal baths at different temperatures. An existing inequality
of temperature can be exploited to do useful work. After eliminating bath variables one
obtains non-linear Langevin equation for the subsystem variable $Q$: namely
\begin{equation}
M \ddot{Q} + \Gamma(Q) \dot{Q} + U'(Q) = \xi_A(t) + \sqrt{f(Q)} \xi_B(t),
\end{equation}
where $\Gamma(Q) = (\Gamma_A + \Gamma_B f(Q))$, $\xi_A(t)$ and $\xi_B(t)$ are two independent Gaussian white-noise
fluctuating forces with statistics given by
\begin{equation}
< \xi_A(t) >= 0, \quad < \xi_A(t) \xi_A(t') >= 2 \Gamma_A kT \delta(t - t'), \quad (2.a)
\end{equation}
and
\begin{equation}
< \xi_B(t) >= 0, \quad < \xi_B(t) \xi_B(t') >= 2 \Gamma_B kT \delta(t - t'), \quad (2.b)
\end{equation}
$T$ and $\bar{T}$ are temperatures of the two baths A and B, respectively. Henceforth we set
Boltzmann constant $k$ to be unity. The bath B is characterised by a space dependent
friction coefficient $\Gamma_B f(Q)$. In eq.(1) $U'(Q)$ is an external force (correspondingly $U(Q)$ is
an external potential) and we have used expression $f(Q)$ for $[V'(Q)]^2$ of ref.[9]. The final
calculations in ref.[9] are done in an overdamped limit by simply neglecting $\ddot{Q}$ term in
eqn.(1). We have shown elsewhere that such a procedure is incorrect [10]. The resulting
Fokker-Planck equation (eqn.(8) of ref.[9]), turns out to be inconsistent. For example, in
an equilibrium situation ($T = \bar{T}$), when the potential $U(Q)$ is unbounded and positive,
i.e., $U(Q) \to \infty$ as $Q \to \pm \infty$, the equilibrium distribution comes out to be
\begin{equation}
P_c(Q) = C \Gamma(Q) e^{-U(Q)/T},
\end{equation}
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where $C$ is the normalization constant. This distribution function is incorrect because in equilibrium $P_e(Q)$ must have the form

$$P_e(Q) = Ne^{-U(Q)/T}, \quad (4)$$

where $N$ is the position independent normalization constant. Also, if we set $\Gamma_A = 0$ (i.e, the particle is coupled to a single bath $B$ at temperature $T$) again the equilibrium distribution of the form of eqn.(3) is obtained. The reason for this inconsistency can be traced back to the improper overdamped limit of the original Langevin equation (eqn.(1)). For example in the absence of thermal bath A, Sancho et al. [11] have shown that the correct overdamped Langevin equation should be

$$\Gamma_B f(Q) \dot{Q} = -U'(Q) - \frac{T}{\Gamma_B \sqrt{f(Q)}} \left[ \sqrt{f(Q)} \right]' + \sqrt{f(Q)} \xi_B(t). \quad (5)$$

The above equation leads to the correct equilibrium distribution as mentioned above. The error in the Millonas treatment [9] follows from the incorrect overdamped limit, where he ignores a term like the second term on the right hand side of eqn.(5).

In this brief report, we construct the correct Fokker-Planck equation in the overdamped limit. We use this equation to study fluctuation-induced transport in a system where the function $U(Q)$ and $f(Q)$ are periodic under translation $Q \rightarrow Q + \lambda$, ($U(Q + \lambda) = U(Q)$ and $f(Q + \lambda) = f(Q)$). We obtain the correct expression for the mean velocity $\langle \dot{Q} \rangle$ and study several special cases of physical interest.

Following ref.[11], after a straightforward algebra one can readily obtain Fokker-Planck equation for the variable $Q$ (i.e, the evolution equation for the probability density $P(Q,t)$), in the overdamped limit and is given by
\[
\frac{\partial P}{\partial t} = \frac{\partial}{\partial Q} U'(Q) \Gamma(Q) P + TT_A \frac{\partial}{\partial Q} \frac{1}{\Gamma(Q)} \frac{\partial}{\partial Q} \frac{1}{\Gamma(Q)} P.
\]
\[
+ \frac{\sqrt{f(Q)}}{\Gamma(Q)} \frac{\partial}{\partial Q} \frac{\sqrt{f(Q)}}{\Gamma(Q)} P + TT_B \frac{\partial}{\partial Q} \left[\frac{\sqrt{f(Q)'}}{\Gamma(Q)'}\frac{\sqrt{f(Q)}}{\Gamma(Q)}\right] P.
\] (6)

This is the correct Fokker-Planck equation in the overdamped limit and represents the Smoluchowski approximation to the original eqn.(1). When the potential \( U(Q) \) is unbounded and positive, i.e, \( U(Q) \to \infty \) as \( Q \to \pm \infty \), the system evolves towards the stationary distribution \( P_s(Q) \). This stationary distribution is characterized by no net current flow and is given by

\[
P_s(Q) = Ne^{-\Psi(Q)},
\] (7)

where \( N \) is normalization constant and

\[
\Psi(Q) = \int^Q \left\{ \frac{U'(x)\Gamma(x)}{(TT_A + TT_B f(x))} + \frac{(T - T)}{\Gamma(x)} \frac{\Gamma_A \Gamma_B f'(x)}{(TT_A + TT_B f(x))} \right\} dx.
\] (8)

One can readily notice that in the equilibrium situation, i.e., when \( T = T \), \( P_s(Q) \) reduces to the correct equilibrium distribution as given in eqn.(4).

To study the case of fluctuation-induced transport, we take a simple case where both \( U(Q) \) and \( f(Q) \) are periodic functions and are invariant under the same transformation \( Q \to Q + \lambda \). Now, the basic problem reduces to finding the mean velocity \( \langle \dot{Q} \rangle \) of the subsystem given the shape of \( U(Q) \) and \( f(Q) \). Following the procedure of refs.[9,12,13] closely, one can get the exact expression for the averaged velocity

\[
\langle \dot{Q} \rangle = \frac{\int^\lambda dy \exp[-\Psi(y)] \int_y^{y+\lambda} \frac{[1 - \exp(-\delta)]}{(TT_A + TT_B f(x))} \frac{[f'(x)]^2}{\Gamma(x)'} \exp[\Psi(x)] dx}{\int^\lambda dy \exp[-\Psi(y)] \int_y^{y+\lambda} \frac{[f'(x)]^2}{(TT_A + TT_B f(x))} \exp[\Psi(x)] dx},
\] (9)

where

\[
\delta = \Psi(x) - \Psi(x + \lambda),
\] (10)
and $\Psi$ is given by eqn.(8). It is easy to see from eqns.(9) and (10), that in the equilibrium case, when the temperature difference between the baths is zero ($T = \overline{T}$), the current vanishes indentically (since $\delta = 0$). Also, one can easily verify that when the subsystem is coupled to a single bath, i.e., when either $\Gamma_A$ or $\Gamma_B$ is zero, no net current is possible. It should be noted that the bath $B$ which gives rise to space dependent friction coefficient $\Gamma_B f(Q)$ plays a special role. This can be noticed from the fact that if $f(Q)$ is independent of $Q$ the induced current is zero. In the extreme case of high friction limit ($\Gamma_A \rightarrow \infty$ or $\Gamma_B \rightarrow \infty$) no net current is possible because the particle cannot execute the Brownion motion.

There are two interesting special cases, one being the case of $U(Q) = 0$. It follows from eqn.(9) that even in the absence of external potential fluctuation-induced currents are possible. In this case direction of the current depends on the details of the function $f(Q)$. We see that the current will flow in one direction if $T < \overline{T}$ and in the opposite direction if $T > \overline{T}$. However, their magnitudes are different. Thus, the system acts like a Carnot engine, which extracts work by making use of two thermal baths at different temperatures. In the other case where amplitude modulations in $f(Q)$ and $f'(Q)$ are small compared to the amplitude modulation of the potential $U(Q)$, the second term in the eqn.(8) can be neglected. In this particular limit the problem becomes equivalent to a particle moving in a spatially varying temperature - field, namely, $T'(Q) = (TG_A + \overline{T}\Gamma_B f(Q))/\Gamma(Q)$. It is well-known in earlier literature [12-14] that such a spatial modulation of temperature-field can give induced currents. Moreover, the problem of evolution of a particle in a spatially varying temperature field has a fundamental consequence in relation to local versus global stability criterion in statistical mechanics [15-16]. In a thermal equilibrium state the Boltzmann factor gives a relative occupation probability of states at different local stable points without invoking the behaviour
of the potential profile between the states. However, in the presence of spatially varying temperature-field, the relative stability (or occupation probability) between different states depend sensitively on the intervening potential and more importantly one can control the relative stability among two different state by modifying the kinetics in the sparsely occupied intervening state [14,16].

In conclusion, we have reinvestigated the recently proposed self-consistent microscopic theory of fluctuation-induced transport. We have pointed out errors in the earlier theory. We have obtained an analytical expression for fluctuation-induced current in a non-equilibrium situation and have discussed various cases of physical interest. Finally, we would like to mention that our expression for the stationary distribution (or steady state) $P_s(Q)$ (eqn.(7)) is not a local function of $U(Q)$ and $f(Q)$. In such a situation as discussed above the relative stability between two different local states in $U(Q)$ depends sensitively on the intervening behaviour of $U(Q)$ and $f(Q)$. This can lead to interesting physics. For example, for given external potential $U(Q)$, as one varies physical parameters (in the parameter space of $T, \overline{T}, \Gamma_A$ and $\Gamma_B$) we expect additional maxima and minima to appear in $P_s(Q)$. Thus we can modify the stability properties of the subsystem. The qualitative changes in the stationary state of the subsystem is reflected in change in the behaviour of the extrema of the $P_s(Q)$. Moreover, extrema in $P_s(Q)$ may have little or no relationship to the extrema in the original potential $U(Q)$. Each new structure in $P_s(Q)$ may correspond to an entirely new state of a subsystem. In the spirit of the well known noise-induced phase transitions this is equivalent to having hierarchy of phase transitions, in a non-equilibrium system [17].

Acknowledgement

The author thanks Mangal C. Mahato for several useful discussions on this subject.
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