Asymptotic Behavior of Thermal Non-Equilibrium Steady States for a Driven Chain of Anharmonic Oscillators

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Abstract

We consider a model of heat conduction introduced in [6], which consists of a finite nonlinear chain coupled to two heat reservoirs at different temperatures. We study the low temperature asymptotic behavior of the invariant measure. We show that, in this limit, the invariant measure is characterized by a variational principle. We relate the heat flow to the variational principle. The main technical ingredient is an extension of Freidlin-Wentzell theory to a class of degenerate diffusions.

1 Introduction

We consider a model of heat conduction introduced in [6]. In this model a finite non-linear chain of n d-dimensional oscillators is coupled to two Hamiltonian heat reservoirs initially at different temperatures T_L,T_R, and each of which is is described by a d-dimensional wave equation. A natural goal is to obtain a usable expression for the invariant (marginal) state of the chain analogous to the Boltzmann-Gibbs prescription $\mu = Z^{-1}\exp(-H/T)$ which one has in equilibrium statistical mechanics. What we show here is that the invariant state μ describing steady state energy flow through the chain is asymptotic to the expression $\exp(-W^{(\eta)}/T)$ to leading order in the mean temperature T, $T \to 0$, where the action $W^{(\eta)}$, defined on phase space, is obtained from an explicit variational principle. The action $W^{(\eta)}$ depends on the temperatures only through the parameter $\eta = (T_L - T_R)(T_L + T_R)$. As one might anticipate, in the limit $\eta \to 0$, $W^{(\eta)}$ reduces

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to the chain Hamiltonian plus a residual term from the bath interaction, i.e., $\exp(-W^{(\eta)}/T)$ becomes the Boltzmann-Gibbs expression. We remark that the variational principle for $W^{(\eta)}$ here certainly has analogues in more complicated arrays of oscillators, plates with multiple thermo-coupled baths, etc. The validity of this variational principle in more complex systems, as well as the physical phenomena to be deduced from $W^{(\eta)}$ are questions which remain to be explored.

Turning to the physical model at hand, we assume that the Hamiltonian $H(p,q)$ of the isolated chain is assumed to be of the form

$$\begin{aligned} H(p,q) &= \sum_{i=1}^{n} \frac{p_i^2}{2} + \sum_{i=1}^{n} U^{(1)}(q_i) + \sum_{i=1}^{n-1} U^{(2)}(q_i - q_{i+1}), \\ &\equiv \sum_{i=1}^{n} \frac{p_i^2}{2} + V(q), \end{aligned} \tag{1}$$

where q_i and p_i are the coordinate and momentum of the i-th particle, and where $U^{(1)}$ and $U^{(2)}$ are $\mathcal{C}^\infty$ confining potentials, i.e. $\lim_{|q|\to\infty} V(q) = +\infty$.

The coupling between the reservoirs and the chain is assumed to be of dipole approximation type and it occurs at the boundary only: the first particle of the chain is coupled to one reservoir and the n-th particle to the other heat reservoir. At time $t = 0$ each reservoir is assumed to be in thermal equilibrium, i.e., the initial conditions of the reservoirs are distributed according to (Gaussian) Gibbs measure with temperature $T_1 = T_L$ and $T_n = T_R$ respectively. Projecting the dynamics onto the phase space of the chain results in a set of integro-differential equations which differ from the Hamiltonian equations of motion by additional force terms in the equations for p_1 and p_n. Each of these terms consists of a deterministic integral part independent of temperature and a Gaussian random part with covariance proportional to the temperature. Due to the integral (memory) terms, the study of the long-time limit is a difficult mathematical problem (see [14] for the study of such systems in the case of a single reservoir). But by a further appropriate choice of couplings, the integral parts can be treated as auxiliary variables r_1 and r_n, the random parts become Markovian. Thus we obtain (see [6] for details) the following system of Markovian stochastic differential equations on the extended phase space $\mathbf{R}^{2dn+2d}$: For $x = (p,q,r)$

$$\begin{aligned} \dot{q}_1 &= p_1, \\ \dot{p}_1 &= -\nabla_{q_1} V(q) + r_1, \\ \dot{q}_j &= p_j, \end{aligned}$$

$$
\begin{aligned}
\dot{q}_j &= -\nabla_{q_j} V(q)\,, \quad j = 2, \ldots, n-1\,, \\
\dot{q}_n &= p_n\,, \\
\dot{q}_n &= -\nabla_{q_n} V(q) + r_n\,, \\
dr_1 &= -\gamma(r_1 - \lambda^2 q_1)dt + (2\gamma\lambda^2 T_1)^{1/2} dw_1\,, \\
dr_n &= -\gamma(r_n - \lambda^2 q_1)dt + (2\gamma\lambda^2 T_n)^{1/2} dw_n\,,
\end{aligned}
\tag{2}
$$

In Eq. (2), $w_1(t)$ and $w_n(t)$ are independent d-dimensional Wiener processes, and λ^2 and γ are constants describing the couplings.

It will be useful to introduce a generalized Hamiltonian $G(p, q, r)$ on the extended phase space, given by

$$
G(p, q, r) \;=\; \sum_{i=1,n} \left(\frac{r_i^2}{2\lambda^2} - r_i q_i \right) + H(p, q)\,,
\tag{3}
$$

where $H(p, q)$ is the Hamiltonian of the isolated systems of oscillators given by (1). We also introduce the parameters ε (the mean temperature of the reservoirs) and η (the relative temperature difference):

$$
\varepsilon \;=\; \frac{T_1 + T_n}{2}\,, \quad \eta \;=\; \frac{T_1 - T_n}{T_1 + T_n}\,.
\tag{4}
$$

Then Eq. (2) takes the form

$$
\begin{aligned}
\dot{q} &= \nabla_p G\,, \\
\dot{p} &= -\nabla_q G\,, \\
dr &= -\gamma\lambda^2 \nabla_r G dt + \varepsilon^{1/2}(2\gamma\lambda^2 D)^{1/2} dw\,,
\end{aligned}
\tag{5}
$$

where $p = (p_1, \ldots, p_n)$, $q = (q_1, \ldots, q_n)$, $r = (r_1, r_n)$ and where D is the $2d \times 2d$ matrix given by

$$
D \;=\; \begin{pmatrix} 1+\eta & 0 \\ 0 & 1-\eta \end{pmatrix}.
\tag{6}
$$

The function G is a Liapunov function, non-increasing in time, for the deterministic part of the flow (5). If the system is in equilibrium, i.e, if $T_1 = T_n = \varepsilon$ and $\eta = 0$, it is not difficult to check that the generalized Gibbs measure

$$
\mu_\varepsilon = Z^{-1} \exp\left(-G(p, q, r)/\varepsilon\right),
\tag{7}
$$

is an invariant measure for the Markov process solving Eq. (5).

If the temperature of the reservoirs are not identical, no explicit formula for the invariant measure μ_{T_1,T_n} can be given, in general. It is the goal of this paper to provide a variational principle for the leading asymptotic form for μ_{T_1,T_n}, at low temperature, $\varepsilon \to 0$. To suggest what μ_{T_1,T_n} looks like, we observe that a typical configuration of a reservoir has infinite energy, therefore the reservoir does not only acts as a sink of energy but true fluctuations can take place. The physical picture is as follows: the system spends most of the time very close to the critical set of G (in fact close to a stable equilibrium) and very rarely (typically after an exponential time) an excursion far away from the equilibria occurs. This picture brings us into the framework of rare events, hence into the theory of large deviations and more specifically the Freidlin-Wentzell theory [8] of small random perturbations of dynamical systems.

In the following we employ notation which is essentially that of [8]. Let $\mathcal{C}([0,T])$ denote the Banach space of continuous functions (paths) with values in $\mathbf{R}^{2d(n+1)}$ equipped with the uniform topology. We introduce the following functional $I^{(\eta)}_{x,T}$ on the set of paths $\mathcal{C}([0,T])$: If $\phi(t) = (p(t), q(t), r(t))$ has one L^2-derivative with respect to time and satisfies $\phi(0) = x$ we set

$$I^{(\eta)}_{x,T}(\phi) \;=\; \frac{1}{4\gamma\lambda^2}\int_0^T (\dot r + \gamma\lambda^2 \nabla_r G) D^{-1} (\dot r + \gamma\lambda^2 \nabla_r G) dt \,, \tag{8}$$

if

$$\dot q(t) = \nabla_p G(\phi(t)) \,, \quad \dot p(t) = -\nabla_q G(\phi(t)) \,, \tag{9}$$

and $I^{(\eta)}_{x,T}(\phi) = +\infty$ otherwise. Notice that $I^{(\eta)}_{x,T}(\phi) = 0$ if and only if $\phi(t)$ is a solution of Eq. (5) with the temperature ε set equal to zero. The functional $I^{(\eta)}_{x,T}$ is called a rate function and it describe, in the sense of large deviation, the probability of the path ϕ: roughly speaking, as $\varepsilon \to 0$, the asymptotic probability of the path ϕ is given by

$$\exp\left(-I^{(\eta)}_{x,T}(\phi)/\varepsilon\right) . \tag{10}$$

For $x, y \in \mathbf{R}^{2d(n+1)}$ we define $V^{(\eta)}(x,y)$ as

$$V^{(\eta)}(x,y) \;=\; \inf_{T>0} \inf_{\phi:\phi(T)=y} I^{(\eta)}_{x,T}(\phi) \,, \tag{11}$$

and for any sets B, $C \in \mathbf{R}^{2d(n+1)}$ we set

$$V^{(\eta)}(B,C) \;=\; \inf_{x\in B; y\in C} V^{(\eta)}(x,y) \,. \tag{12}$$

The function $V^{(\eta)}(x,y)$ represents, roughly speaking, the cost to bring the system from x to y (in an arbitrary amount of time). We introduce an equivalence relation on the phase space $\mathbf{R}^{2d(n+1)}$: we say $x \sim y$ if $V^{(\eta)}(x,y) = V^{(\eta)}(y,x) = 0$. We divide the critical set $K = \{x\,;\, \nabla G(x) = 0\}$ (about which the invariant measure concentrates) according to this equivalence relation: we have $K = \cup_i K_i$ with $x \sim y$ if $x \in K_i, y \in K_i$ and $x \not\sim y$ if $x \in K_i, y \in K_j$, $i \neq j$.

Our first assumption is on the existence of an invariant measure, the structure of the set K and the dynamics near temperature zero. Let $\rho > 0$ be arbitrary and denote $B(\rho)$ the ρ-neighborhood of K and let τ_ρ be the first time the Markov process $x(t)$ which solves (5) hits $B(\rho)$.

- **K1** The process $x(t)$ has an invariant measure. The critical set A of the generalized Hamiltonian G can be decomposed into a finite number of inequivalent compact sets K_i. Finally, for any $\varepsilon_0 > 0$, the expected hitting time $E_x(\tau_\rho)$ of the diffusion with initial condition x is bounded uniformly for $0 \leq \varepsilon \leq \varepsilon_0$.

Remark 1.1 The assumption **K1** ensures that the dynamics is sufficiently confining in order to apply large deviations techniques to study the invariant measure.

Remark 1.2 The assumptions used in [6, 5] to prove the existence of an invariant measure imply the assumption made on the structure of the critical set A. But it is not clear that they imply the assumptions made on the hitting time. We will merely assume the validity of condition **K1** in this paper. Its validity can be established by constructing Liapunov-like functions for the model. Such methods allow as well to prove a fairly general theorem on the existence of invariant measures for Hamiltonian coupled to heat reservoirs (under more general conditions that in [6, 5]) and will be the subject of a separate publication [21].

Our second condition is identical to condition **H2** of [6, 5].

- **K2** The 2-body potential $U^{(2)}(q)$ is strictly convex.

Remark 1.3 The condition **K2** will be important to establish various regularity properties of $V^{(\eta)}(x,y)$. It will allow to imply several controllability properties of the control system associated with the stochastic differential equations (5).

Following [8], we consider graphs on the set $\{1, \ldots, L\}$. A graph consisting of arrows $m \to n$, $(m \in \{1, \ldots, L\} \setminus \{i\}$, $m \in \{1, \ldots, L\})$, is called a $\{i\}$-graph if

1. Every point j, $j \neq i$ is the initial point of exactly one arrow.
2. There are no closed cycles in the graph.

We denote $G\{i\}$ the set of $\{i\}$-graphs. The weight of the set K_i is defined by

$$W^{(\eta)}(K_i) \;=\; \min_{g \in G(\{i\})} \sum_{m \to n \in g} V^{(\eta)}(K_m, K_n)\,. \tag{13}$$

Our main result is the following:

Theorem 1.4 *Under the conditions* **K1** *and* **K2** *the invariant measure* $\mu_{T_1,T_n} = \mu_{\varepsilon,\eta}$ *of the Markov process (5) has the following asymptotic behavior: For any open set* D *with compact closure and sufficiently regular boundary*

$$\lim_{\varepsilon \to 0} \varepsilon \log \mu_{\varepsilon,\eta}(D) \;=\; \inf_{x \in D} W^{(\eta)}(x)\,, \tag{14}$$

where

$$W^{(\eta)}(x) \;=\; \min_i \Big(W^{(\eta)}(K_i) + V^{(\eta)}(K_i, x) \Big) - \min_j W^{(\eta)}(K_j)\,. \tag{15}$$

In particular, if $\eta = 0$*, then*

$$W^{(0)}(x) \;=\; G(x) - \min_x G(x)\,. \tag{16}$$

The function $W^{(\eta)}(x)$ *satisfies the bound, for* $\eta \geq 0$*,*

$$(1+\eta)^{-1}\Big(G(x) - \min_x G(x)\Big) \;\leq\; W^{(\eta)}(x) \;\leq\; (1-\eta)^{-1}\Big(G(x) - \min_x G(x)\Big)\,. \tag{17}$$

and a similar bound for $\eta \leq 0$*.*

Remark 1.5 Eqs. (16) and (17) imply that $\mu_{\varepsilon,\eta}$ reduces to the Boltzmann-Gibbs expression $\mu_\varepsilon \sim \exp\left(-G/\varepsilon\right)$ for $\eta \to 0$ in the low temperature limit. Of course, at $\eta = 0$, they are actually equal at all temperatures ε. Moreover these equations imply that the relative probability $\mu_{\varepsilon,\eta}(x)/\mu_{\varepsilon,\eta}(y)$ is (asymptotically) bounded above and below by

$$\exp - \left[\frac{G(x)}{\varepsilon(1 \pm \eta)} - \frac{G(y)}{\varepsilon(1 \mp \eta)} \right], \tag{18}$$

so that no especially hot or cold spots develop for $\eta \neq 0$.

Remark 1.6 The theorem draws heavily from the large deviations theory of Freidlin-Wentzell [8]. But the theory was developed for stochastic differential equations with a non-degenerate (elliptic) generator, but for Eq. (5) this is not the case since the random force acts only on $2d$ of the $2d(n+1)$ variables. A large part of this paper is devoted to simply extending Freidlin-Wentzell theory to a class of Markov processes containing our model. Degenerate diffusions have been considered in [3] but under too stringent conditions and also in [2] but with conditions quite different from ours. We also note that the use of Freidlin-Wentzell theory in non-equilibrium statistical mechanics has been advocated in particular by Graham (see [10] and references therein). In these applications to non-equilibrium statistical mechanics, as in [10], the models are mostly taken as mesoscopic: the variables of the system describe some suitably coarse-grained quantities, which fluctuate slightly around their average values. In contrast to these models, ours is entirely microscopic and derived from first principles and the small-noise limit is seen as a low-temperature limit.

Finally we relate the large deviation functional to a kind of entropy production. As in [7] we define this entropy production Σ by

$$\Sigma = -\frac{F_1}{T_1} - \frac{F_n}{T_n}, \tag{19}$$

where

$$\begin{aligned} F_1(p,q,r) &= p_1(r_1 - \lambda^2 q_1) = \lambda^2 p_1 \nabla_{r_1} G(p,q,r), \\ F_n(p,q,r) &= p_n(r_n - \lambda^2 q_n) = \lambda^2 p_n \nabla_{r_n} G(p,q,r), \end{aligned} \tag{20}$$

are the energy flows from the chain to the respective reservoirs. In [6] it is shown that $\mu_{T_1,T_n}(\Sigma) \geq 0$ and $\mu_{T_1,T_n}(\Sigma) = 0$ if and only if $T_1 = T_n$. This implies that, in the stationary state, energy is flowing from the hotter reservoir bath to the colder one. With the parameters ε and η as defined in (4) we define Θ by

$$\frac{1}{\varepsilon}\Theta = \Sigma = \frac{1}{\varepsilon}\left(-\frac{F_1}{1+\eta} - \frac{F_n}{1-\eta}\right). \tag{21}$$

In order to show the relation between the rate function $I_{x,T}$ and the entropy production Σ, we introduce the time-reversal J, which is the involution on the phase space $\mathbf{R}^{2d(n+1)}$ given by $J(p,q,r) = (-p,q,r)$. The following shows that the value of the rate function of a path ϕ between x and y and is equal (up to a boundary term) to the value of the rate function of the the time reversed path $\tilde{\phi}$ between Jy and Jx minus the entropy produced along this path.

Proposition 1.7 *Let $\phi(t) \in \mathcal{C}([0,T])$ with $\phi(0) = x$ and $\phi(T) = y$. Either $I^{(\eta)}_{x,T}(\phi) = +\infty$ or we have*

$$\begin{aligned} I^{(0)}_{x,T}(\phi) &= I^{(0)}_{Jy,T}(\widetilde{\phi}) + G(y) - G(x)\,, \qquad \text{if } \eta = 0\,, \\ I^{(\eta)}_{x,T}(\phi) &= I^{(\eta)}_{Jy,T}(\widetilde{\phi}) + R(y) - R(x) - \int_0^T \Theta(\phi(s))ds\,, \quad \text{if } \eta \neq 0\,, \end{aligned} \tag{22}$$

where Θ is defined in Eq. (21) and $R(x) = (1+\eta)^{-1}(\lambda^{-1}r_1 - \lambda q_1)^2 + (1-\eta)^{-1}(\lambda^{-1}r_n - \lambda q_n)^2$.

The identities given in Proposition 1.7 are an asymptotic version of identities which appear in various forms in the literature. These identities are the basic ingredient needed for the proof of the Gallavotti-Cohen fluctuation theorem [4, 9] for stochastic dynamics [17, 18, 20] and appear as well in the Jarsynski non-equilibrium work relation [13].

The paper is organized as follows: In Section 2 we recall the large deviation principle for the paths of Markovian stochastic differential equation and using methods from control theory we prove the required regularities properties of the function $V^{(\eta)}(x,y)$ defined in Eq. (11). Section 3 is devoted to an extension of Freidlin-Wentzell results to a certain class of diffusions with hypoelliptic generators (Theorem 3.3): we give a set of conditions under which the asymptotic behavior of the invariant measure is proved. The result of Section 2 implies that our model, under Assumptions **K1** and **K2**, satisfies the conditions of Theorem 3.3. In Section 4 we prove the equality (16) and the bound (17) which depend on the particular properties of our model.

2 Large deviations and Control Theory

In this section we first recall a certain numbers of concepts and theorems which will be central in our analysis: The large deviation principle for the sample path of diffusions introduced by Schilder for the Brownian motion [22] and generalized to arbitrary diffusion by [8, 1, 25] (see also [3]), and the relationship between diffusion processes and control theory, exemplified by the Support Theorem of Stroock and Varadhan [24]. With these tools we then prove several properties of the dynamics for our model. We prove that "at zero temperature" the (deterministic) dynamics given by is dissipative: the ω-limit set is the set of the critical point of $G(p,q,r)$. We also prove several properties of the control system associated to Eq. (5): a local control property around the critical points of $G(p,q,r)$ and roughly speaking a global "smoothness" property of the weight of the paths between x and y, when x and y vary. The central hypothesis in this analysis is condition **K2**: this condition implies the hypoellipticity, [12], of the generator of the Markov semigroup associated to Eq. (5), but it implies in fact a kind of global hypoellipticity which will be used here to prove the aforementioned properties of the dynamics.

2.1 Sample Paths Large Deviation and Control Theory

Let us consider the stochastic differential equation

$$dx(t) \,=\, Y(x)dt + \varepsilon^{1/2}\sigma(x)dw(t)\,, \tag{23}$$

where $x \in X = \mathbf{R}^n$, $Y(x)$ is a $\mathcal{C}^\infty$ vector field, $w(t)$ is an m-dimensional Wiener process and $\sigma(x)$ is a $\mathcal{C}^\infty$ map from $\mathbf{R}^m$ to $\mathbf{R}^n$. Let $\mathcal{C}([0,T])$ denote the Banach space of continuous functions with values in $\mathbf{R}^n$ equipped with the uniform topology. Let $L^2([0,T])$ denote the set of square integrable functions with values in $\mathbf{R}^m$ and $H_1([0,T])$ denote the space of absolutely continuous functions with values in $\mathbf{R}^m$ with square integrable derivatives. Let $x_\varepsilon(t)$ denote the solution of (23) with initial condition $x_\varepsilon(0) = x$. We assume that $Y(x)$ and $\sigma(x)$ are such that, for arbitrary T, the paths of the diffusion process $x_\varepsilon(t)$ belong to $\mathcal{C}([0,T])$. We let P_x^ε denote the probability measure on $\mathcal{C}([0,T])$ induced by $x_\varepsilon(t)$, $0 \le t \le T$ and denote E_x^ε the corresponding expectation.

We introduce the rate function $I_{x,T}(f)$ on $\mathcal{C}([0,T])$ given by

$$I_{x,T}(f) \,=\, \inf_{\{g\in H_1 : f(t)=x+\int_0^T Y(f(s))ds+\int_0^T \sigma(f(s))\dot{g}(s)ds\}} \frac{1}{2}\int_0^T |\dot{g}(t)|^2 dt\,, \tag{24}$$

where, by definition, the infimum over an empty set is taken as $+\infty$. The rate function has a particularly convenient form for us since it accommodates degenerate situations where $\operatorname{rank}\sigma < n$.

In [3], Corollary 5.6.15 (see also [1]) the following large deviation principle for the sample paths of the solution of (23) is proven. It gives a version of the large deviation principle which is uniform in the initial condition of the diffusion.

Theorem 2.1 *Let $x^\varepsilon(t)$ denote the solution of Eq. (23) with initial condition x. Then, for any $x \in \mathbf{R}^n$ and for any $T < \infty$, the rate function $I_{x,T}(f)$ is a lower semicontinuous function on $\mathcal{C}([0,T])$ with compact level sets (i.e. $\{f\,;\, I_{x,T}(f) \le \alpha\}$ is compact for any $\alpha \in \mathbf{R}$). Furthermore the* *family of measures P_x^ε satisfy the large deviation principle on $\mathcal{C}([0,T])$ with rate function $I_{x,T}(f)$:*

1. *For any compact $K \subset X$ and any closed $F \subset \mathcal{C}([0,T])$,*

$$\limsup_{\varepsilon\to 0} \log \sup_{x\in K} P_x(x_\varepsilon \in F) \,\le\, -\inf_{x\in K}\inf_{\phi\in F} I_{x,T}(\phi). \tag{25}$$

2. *For any compact $K \subset X$ and any open $G \subset \mathcal{C}([0,T])$,*

$$\liminf_{\varepsilon\to 0} \log \inf_{x\in K} P_x(x_\varepsilon \in G) \,\ge\, -\sup_{x\in K}\inf_{\phi\in G} I_{x,T}(\phi). \tag{26}$$

Recall that for our model given by Eq. (5), the rate function takes the form given in Eqs. (8) and (9). We introduce further the cost function $V_T(x,y)$ given by

$$V_T(x,y) \,=\, \inf_{\phi\in\mathcal{C}([0,T])\,:\,\phi(T)=y} I_{x,T}(\phi)\,. \tag{27}$$

Heuristically $V_T(x,y)$ describes the cost of forcing the system to be at y at time T starting from x at time 0. The function $V(x,y)$ defined in the introduction, Eq. (11) is equal to

$$V(x,y) \,=\, \inf_{T>0} V_T(x,y)\,, \tag{28}$$

and describes the minimal cost of forcing the system from x to y in an arbitrary amount of time.

The form of the rate function suggest a connection between large deviations and control theory. In Eq. (24), the infimum is taken over functions $g \in H_1([0,T])$ which are more regular than a path of the Wiener process. If we do the corresponding substitution in Eq. (23), we obtain an ordinary differential equation

$$\dot{x}(t) \quad=\quad Y(x(t)) + \sigma(x(t))u(t)\,, \tag{29}$$

where we have set $u(t) = \varepsilon^{1/2}\dot{g}(t) \in L^2([0,T])$. The map u is called a control and the equation (29) a control system. We fix an arbitrary time $T > 0$. We denote by $\varphi_x^u : [0,T] \to \mathbf{R}^n$ the solution of the differential equations (29) with control u and initial condition x. The correspondence between the stochastic system Eq. (23) and the deterministic system Eq. (29) is exemplified by the Support Theorem of Stroock and Varadhan [24]. The support of the diffusion process $x(t)$ with initial condition x on $[0,T]$, is, by definition, the smallest closed subset $\mathcal{S}_x$ of $\mathcal{C}([0,T])$ such that

$$P_x[x(t) \in \mathcal{S}_x] \;=\; 1 \;. \tag{30}$$

The Support Theorem asserts that the support of the diffusion is equal to the set of solutions of Eq. (29) as the control u is varied:

$$\mathcal{S}_x \;=\; \overline{\{\varphi_x^u \;:\; u \in L^2([0,T])\;\}} \;, \tag{31}$$

for all $x \in \mathbf{R}^k$. The control system (29) is said to be *strongly completely controllable*, if for any $T > 0$, and any pair of points x, y, there exist a control u such that $\varphi_x^u(0) = x$ and $\varphi_x^u(T) = x$. In [7] it is shown that, under condition **K2**, the control system associated with the equation (5) is strongly completely controllable. This is an ergodic property and this implies, [7], uniqueness of the invariant measure (provided it exists). In terms of the cost function $V_T(x,y)$ defined in (27), strong complete controllability simply means that $V_T(x,y) < \infty$, for any $T > 0$ and any x, y. The large deviation principle, Theorem 2.1, gives more quantitative information on the actual weight of paths between x and y in time T, in particular that the weight is $\sim \exp(-\frac{1}{\varepsilon}V_T(x,y))$. As we will see below, these weights will determine completely the leading (exponential) behavior of the invariant measure for $x_\varepsilon(t)$, $\varepsilon \downarrow 0$.

2.2 Dissipative properties of the dynamics

We first investigate the ω-limit set of the dynamics "at temperature zero", i.e, when both temperatures T_1, T_n are set equal to zero in the equations of motion. In this case the dynamics is deterministic and, as the following result shows, dissipative.

Lemma 2.2 *Assume condition* **K2**. *Consider the system of differential equations given by*

$$\begin{aligned} \dot{q}_i &= \nabla_{p_i} G \qquad i = 1, \cdots, n\,, \\ \dot{p}_i &= -\nabla_{q_i} G \qquad i = 1, \cdots, n\,, \\ \dot{r}_i &= -\gamma\lambda^2 \nabla_{r_i} G \qquad i = 1, n\,. \end{aligned} \tag{32}$$

Then the ω-limit set of the flow given by Eq.(32) is the set of critical points of the generalized Hamiltonian $G(p,q,r) = \sum_{j=1,n}(\lambda^{-2}r_j^2/2 - r_j q_j) + H(p,q)$, i.e.,

$$A \;=\; \left\{ x \in \mathbf{R}^{2d(n+1)} \;:\; \nabla G(x) = 0 \right\} \;. \tag{33}$$

Proof: As noted in the introduction $G(x)$ is a Liapunov function for the flow given by (32). A simple computation shows that

$$\begin{aligned}\frac{d}{dt}G(x(t)) &= -\gamma\lambda^2 \sum_{i=1,n} (\lambda^{-2} r_i(t) - q_i(t))^2 \\ &= -\gamma\lambda^2 \sum_{i=1,n} |\nabla_{r_i} G(x(t))|^2 \le 0 \,. \end{aligned} \tag{34}$$

Therefore it is enough to show that the flow does not get "stuck" at some point of the hyper-surfaces $(\lambda^{-2} r_i(t) - q_i(t))^2 = 0, i = 1, n$ which does not belong to the set A.

Let us assume the contrary, i.e., that, for some trajectory and some times $T_1 < T_2$ we have

$$G(x(t)) = G(x(T_1)) \text{ for } t \in [T_1, T_2] \,. \tag{35}$$

We show that this implies that $x(t) \in A$, for $t \in [T_1, T_2]$. From Eqs. (34) and (35) we have, for $t \in [T_1, T_2]$, the identity

$$\lambda^{-2} r_1(t) - q_1(t) = \nabla_{r_1} G(x(t)) = 0 \,. \tag{36}$$

Further, using Eq.(32), we obtain

$$0 = \frac{d}{dt}(\lambda^{-2} r_1(t) - q_1(t)) = -\gamma(\lambda^{-2} r_1(t) - q_1(t)) - p_1(t) = -p_1(t) \,. \tag{37}$$

Thus we get

$$p_1(t) = \nabla_{p_1} G(x(t)) = 0 \,. \tag{38}$$

Since $p_1(t)$ is a constant,

$$0 = -\dot{p}_1(t) = \nabla_{q_1} G(x(t)) = \nabla_{q_1} V(q(t)) - r_1(t) \,, \tag{39}$$

and therefore

$$\nabla_{q_1} G(x(t)) = 0 \,. \tag{40}$$

Using that $\lambda^{-2} r_1(t) - q_1(t) = 0$ we can rewrite Eq. (39) as follows:

$$0 = \nabla_{q_1} U^{(1)}(q_1(t)) - \lambda^2 q_1(t) + \nabla_{q_1} U^{(2)}(q_1(t) - q_2(t)) \,. \tag{41}$$

By the convexity condition on $U^{(2)}$, **K2**, $\nabla U^{(2)} : \mathbf{R}^d \to \mathbf{R}^d$ is a diffeomorphism with an inverse which we denote W. We can therefore solve Eq.(41) in terms of q_2 and we obtain

$$q_2(t) = q_1(t) - W\left(\lambda^2 q_1(t) - \nabla_{q_1} U^{(1)}(q_1(t))\right) \equiv F(q_1(t)) \,. \tag{42}$$

From this we conclude that

$$p_2(t) \;=\; \dot q_2(t) \;=\; \nabla_{q_1} F(q_1(t))\dot q_1(t) \;=\; \nabla_{q_1} F(q_1(t))p_1(t) \;=\; 0\,, \tag{43}$$

and thus

$$p_2(t) \;=\; \nabla_{p_2} G(x(t)) \;=\; 0\,. \tag{44}$$

Proceeding by induction along the chain it is easy to see that if $G(x(t))$ is constant on the interval $[T_1, T_2]$, then one has

$$\nabla G(x(t)) \;=\; 0\,, \tag{45}$$

and therefore $x(t) \in A$. This concludes the proof of Lemma 2.2. ∎

2.3 Continuity properties of $V_T^{(\eta)}(x, y)$

In the analysis of the asymptotic behavior of the invariant measure it will be important to establish certain continuity properties of the cost function $V_T^{(\eta)}(x, y)$. We prove first a global property: we show that for any time T, $V_T^{(\eta)}(x, y)$ as a map from $X \times X \to \mathbf{R}$ is everywhere finite and upper semicontinuous. Furthermore we need a local property of $V_T^{(\eta)}(x, y)$ near the ω-limit set of the zero-temperature dynamics (see Lemma 2.2). We prove that if x and y are sufficiently close to this ω-limit set then $V_T^{(\eta)}(x, y)$ is small. Both results are obtained using control theory and hypoellipticity.

Proposition 2.3 *Assume condition* **K2***. Then the functions $V_T^{(\eta)}$, for all $T > 0$ and $V^{(\eta)}$ are upper semicontinuous maps : $X \times X \to$* **R***.*

Proof: By definition $V_T^{(\eta)}(y, z)$ is given by

$$V_T^{(\eta)}(y, z) \;=\; \inf \frac{1}{2} \int_0^T \sum_{j=1,n} |u_j(t)|^2 dt\,, \tag{46}$$

where the infimum in (46) is taken over all $u = (u_1, u_n) \in L^2([0, T])$ such that

$$\begin{aligned} \dot q &= \nabla_p G\,, \\ \dot p &= -\nabla_q G\,, \\ \dot r &= -\gamma\lambda^2 \nabla_r G + (2\gamma\lambda^2 D)^{1/2} u\,, \end{aligned} \tag{47}$$

with boundary conditions

$$(p(0), q(0), r(0)) = y\,, \qquad (p(T), q(T), r(T)) = z\,. \tag{48}$$

In other words, the infimum in (46) is taken over all controls u which steer y to z. For notational simplicity we let $r_1 = q_0$ and $r_n = q_{n+1}$. Furthermore we set $Q = (q_0, q_1, \ldots q_n, q_{n+1}) \in \mathbf{R}^{d(n+2)}$ and $P = (\dot{q}_1, \ldots, \dot{q}_n) \in \mathbf{R}^{dn}$. The equations (47) take the form

$$\begin{aligned}
\dot{q}_0 &= -\gamma\lambda^2 \nabla_{q_0} G(q_0, q_1) + (2\gamma\lambda^2(1+\eta))^{1/2} u_1\,, \\
\ddot{q}_l &= -\nabla_{q_j} G(q_{l-1}, q_l, q_{l+1}) \quad l = 1, \ldots, n\,, \\
\dot{q}_{n+1} &= -\gamma\lambda^2 \nabla_{q_{n+1}} G(q_n, q_{n+1}) + (2\gamma\lambda^2(1-\eta))^{1/2} u_n\,,
\end{aligned} \tag{49}$$

with boundary conditions

$$(P(0), Q(0)) \;=\; y\,, \quad (P(T), Q(T)) \;=\; z\,. \tag{50}$$

By condition **K2**, $\nabla_q U^{(2)}(q)$ is a diffeomorphism. As a consequence the identity

$$\ddot{q}_l \;=\; -\nabla_{q_l} G(q_{l-1}, q_l, q_{l+1}) \tag{51}$$

can be solved for either q_{l-1} or q_{l+1}: there are smooth functions G_l and H_l such that

$$q_{l-1} \;=\; G_l(q_l, \ddot{q}_l, q_{l+1})\,, \tag{52}$$

$$q_{l+1} \;=\; H_l(q_{l-1}, q_l, \ddot{q}_l)\,. \tag{53}$$

Using this we rewrite now the equations in the following form: We assume for simplicity n is an even number and we set $j = n/2$. (If n is odd, take $j = (n+1)/2$ and up to minor modifications the argument goes as in the even case).

We rewrite Eq. (49) as follows: For the first $j+1$ equations we use Eq. (52) and find

$$\begin{aligned}
u_1 &= \frac{1}{(2\gamma\lambda^2(1+\eta))^{1/2}} (\dot{q}_0 + \gamma\lambda^2 \nabla_{q_0} G(q_0, q_1)) \;\equiv\; G_0(q_0, \dot{q}_0, q_1)\,, \\
q_l &= G_{l+1}(q_{l+1}, \ddot{q}_{l+1}, q_{l+2}) \quad l = 0, 1, \ldots, j-1\,.
\end{aligned} \tag{54}$$

For the remaining $n+1-j = j+1$ equations we use Eq. (53) and obtain the equivalent equations

$$\begin{aligned}
u_n &= \frac{1}{(2\gamma\lambda^2(1-\eta))^{1/2}} (\dot{q}_{n+1} + \gamma\lambda^2 \nabla_{q_{n+1}} G(q_n, q_{n+1})) \\
&\equiv H_{n+1}(q_n, q_{n+1}, \dot{q}_{n+1})\,, \\
q_l &= H_{l-1}(q_{l-2}, q_{l-1}, \ddot{q}_{l-1}) \quad l = j+2, \ldots, n+1\,.
\end{aligned} \tag{55}$$

Obviously both sets of equations (54) and (55) can be solved iteratively to express $u_1, q_0, \ldots, q_{j-1}$ and $q_{j+2}, \ldots, q_{n+1}, u_n$ as functions of only q_j, q_{j+1} and a certain number of their derivatives. We note $q^{[\alpha]} = (q, q^{(1)}, \ldots, q^{(\alpha)})$ where $q^{(k)} = d^k q/dt^k$. From Eq. (54) we obtain, for some smooth functions $I_0, \ldots I_j$, the set of equations

$$
\begin{aligned}
u_1 &= I_0\left(q_j^{[2j+1]}, q_{j+1}^{[2j-1]}\right), && (56)\\
q_k &= I_{k+1}\left(q_j^{[2(j-k)]}, q_{j+1}^{[2(j-1-k)]}\right), \quad k = 0, 1, \ldots, j-1. && (57)
\end{aligned}
$$

Similarly from Eq. (55), we find smooth functions $J_0, \ldots J_j$ such that

$$
\begin{aligned}
q_k &= J_{n+2-k}\left(q_j^{[2(k-j-2)]}, q_{j+1}^{[2(k-j-1)]}\right) \quad k = j+2 \ldots, n+1. && (58)\\
u_n &= J_0\left(q_j^{[2j-1]}, q_{j+1}^{[2j+1]}\right). && (59)
\end{aligned}
$$

So far we have simply rewritten the differential equations of motion in an implicit form. From this we can draw the following conclusions. If $(P(t), Q(t))$ is a solution of Eq. (49) with given control $u = (u_1, u_n)$, then, using Eqs. (56) and (59) u can be written as follows: there is a smooth function B such that

$$
u(t) = B\left(q_j^{[2j+1]}(t), q_{j+1}^{[2j+1]}(t)\right), \tag{60}
$$

i.e., u can be expressed as a function of the functions q_j, q_{j+1} and their first $2j+1$ derivatives. Furthermore if $(P(t), Q(t))$ is a solution of Eq. (49), from Eqs. (57) and (58), we can express (P, Q) as a function of q_j, q_{j+1} and their first $2j$ derivatives. In particular this defines a map $N : \mathbf{R}^{2d(n+1)} \to \mathbf{R}^{2d(n+1)}$, where $(P(t), Q(t)) = N\left(q_j^{[2j+1]}, q_{j+1}^{[2j+1]}\right)$ is given by

$$
\begin{aligned}
q_k &= I_{k+1}\left(q_j^{[2(j-k)]}, q_{j+1}^{[2(j-1-k)]}\right), \quad k = 0, 1, \ldots, j-1,\\
\dot{q}_k &= \dot{I}_{k+1}\left(q_j^{[2(j-k)+1]}, q_{j+1}^{[2(j-1-k)+1]}\right), \quad k = 1, \ldots, j-1,\\
q_k &= q_k, \quad k = j, j+1,\\
\dot{q}_k &= \dot{q}_k, \quad k = j, j+1,\\
q_k &= J_{n+2-k}\left(q_j^{[2(k-j-2)]}, q_{j+1}^{[2(k-j-1)]}\right), \quad k = j+2 \ldots, n+1,\\
\dot{q}_k &= \dot{J}_{n+2-k}\left(q_j^{[2(k-j-2)+1]}, q_{j+1}^{[2(k-j-1)+1]}\right), \quad k = j+2 \ldots, n. && (61)
\end{aligned}
$$

We now show that N is a homeomorphism, by constructing explicitly its inverse. We use the equations of motion (49) to derive equations for $q_j^{[2j]}$ and $q_{j+1}^{[2j]}$. Differentiating repeatedly the equations with respect to time one inductively finds functions smooth functions $K_0, \dots K_{2j}$ and $L_0, \dots L_{2j}$ such that

$$\begin{aligned} q_j^{(k)} &= K_k\left(q_0^{[0]}, q_1^{[1]}, \dots, q_{j-1}^{[1]}, q_j^{[k-2]}, q_{j+1}^{[k-2]}\right), \quad k = 0, \dots, 2j\,, & (62)\\ q_{j+1}^{(k)} &= L_k\left(q_j^{[k-2]}, q_{j+1}^{[k-2]}, q_{j+2}^{[1]}, \dots, q_n^{[1]}, q_{n+1}^{[0]}\right), \quad k = 0, 1, \dots, 2j\,. & (63)\end{aligned}$$

Eqs. (62) and (63) define inductively a smooth map M from $\mathbf{R}^{2d(n+1)}$ to $\mathbf{R}^{2d(n+1)}$ given by

$$\left(q_j^{[2j]}, q_{j+1}^{[2j]}\right) = M(P, Q)\,. \tag{64}$$

We have shown that if $(P(t), Q(t))$ is a solution of Eq. (49), then

$$\left(q_j^{[2j]}(t), q_{j+1}^{[2j]}(t)\right) = M\left(P(t), Q(t)\right)\,. \tag{65}$$

Since the solution of (49) is unique this shows that M is the inverse of the map N given by Eq. (61) and thus N is a homeomorphism (in fact a diffeomorphism).

We have proven the following: The system of equations (49) with boundary data (50) is equivalent to equation (60) with the boundary data

$$\left(q_j^{[2j]}(0), q_{j+1}^{[2j]}(0)\right) = M(y)\,, \quad \left(q_j^{[2j]}(T), q_{j+1}^{[2j]}(T)\right) = M(z)\,. \tag{66}$$

From this the assertion of the theorem follows easily: First we see that $V_T^{(\eta)}(y,z) < \infty$, for all $T > 0$ and for all y, z. Indeed choose any sufficiently smooth curves $q_j(t)$ and $q_{j+1}(t)$ which satisfies the boundary conditions (66) and consider the u given by Eq. (60). Then the function $(P(t), Q(t)) = M\left(q_j^{[2j]}(t), q_{j+1}^{[2j]}(t)\right)$ is a solution of Eq. (49) with boundary data (50) and with a control $u(t)$ given by (60) which steers y to z.

In order to prove the upper semicontinuity of $V_T^{(\eta)}(y,z)$, let us choose some $\epsilon > 0$. By definition of $V_T^{(\eta)}$ there is a control u which steers y to z along a path $\phi = \phi^u$ such that

$$I_{y,T}(\phi^u) \le V_T^{(\eta)}(y,z) + \epsilon/2\,, \tag{67}$$

and

$$u(t) = B\left(q_j^{[2j+1]}(t), q_{j+1}^{[2j+1]}(t)\right)\,, \tag{68}$$

Using the smoothness of B, we choose curves $\tilde{q}_j$ and $\tilde{q}_{j+1}$ such that

$$\sup_{t\in[0,T]} |q_j^{[2j+1]} - \tilde{q}_j^{[2j+1]}| + |q_{j+1}^{[2j+1]} - \tilde{q}_{j+1}^{[2j+1]}| \le \delta\,, \tag{69}$$

and δ is so small that

$$\tilde{u}(t) \;=\; B(\tilde{q}_j^{[2j+1]}, \tilde{q}_{j+1}^{[2j+1]})\,, \tag{70}$$

satisfies

$$\sup_{t\in[0,T]} |u(t) - \tilde{u}(t)| \;\le\; \sqrt{\frac{\epsilon}{T}}\,. \tag{71}$$

We note $\tilde{y} = M(\tilde{q}_j^{[2j]}(0), \tilde{q}_{j+1}^{[2j]}(0))$ and $\tilde{z} = N(\tilde{q}_j^{[2j]}(T), \tilde{q}_{j+1}^{[2j]}(T))$ and ϕ^u the path along which the control u steers the system, one obtains

$$|I_{y,T}(\phi^u) - I_{\tilde{y},T}(\phi^{\tilde{u}})| \;\le\; \frac{\epsilon}{2}\,. \tag{72}$$

By the continuity of the map N, we can choose δ' so small that if $|y - \tilde{y}| + |z - \tilde{z}| \le \delta'$, then

$$\begin{aligned} &|q_j^{[2j]}(0) - \tilde{q}_j^{[2j]}(0)| + |q_{j+1}^{[2j]}(0) - \tilde{q}_{j+1}^{[2j]}(0)| \\ &+|q_j^{[2j]}(T) - \tilde{q}_j^{[2j]}(T)| + |q_{j+1}^{[2j]}(T) - \tilde{q}_{j+1}^{[2j]}(T)| \le \delta\,. \end{aligned}$$

Therefore for all such $\tilde{y}, \tilde{z}$ we have

$$V_T^{(\eta)}(\tilde{y}, \tilde{z}) \;\le\; I_{\tilde{y},T}(\phi^{\tilde{u}}) \;\le\; V_T^{(\eta)}(y, z) + \epsilon\,. \tag{73}$$

This shows the upper semicontinuity of $V_T^{(\eta)}(y, z)$ and the upper semicontinuity of $V^{(\eta)}(y, z)$ follows easily from this. This concludes the proof of Lemma 2.3. ∎

An immediate consequence of this Lemma is a bound on the cost function around critical points of the generalized Hamiltonian G.

Corollary 2.4 *For any $x \in A = \{y : \nabla G(y) = 0\}$ and any $h > 0$ there is $\delta > 0$ such that, if $|y - x| + |z - x| \le \delta$, then one has*

$$V^{(\eta)}(y, z) \;\le\; h\,. \tag{74}$$

Proof: If $x \in A$, x is a stationary point of the equation

$$\begin{aligned} \dot{q} &= \nabla_p G\,, \\ \dot{p} &= -\nabla_q G\,, \\ \dot{r} &= -\gamma\lambda^2 \nabla_r G\,. \end{aligned} \tag{75}$$

As a consequence the control $u \equiv 0$ steers 0 to 0 and hence $V^{(\eta)}(x, x) = 0$. The upper semicontinuity of $V^{(\eta)}(y, z)$ immediately implies the statement of the corollary. ∎

Remark 2.5 This corollary slightly falls short of what is needed to obtain the asymptotics of the invariant measure. More detailed information about the geometry of the control paths around the stationary points is needed and will be proved in the next subsection.

2.4 Geometry of the paths around the stationary points

Let us consider a control system of the form

$$\dot{x} = Y(x) + \sum_{i=1}^{m} X_i(x) u_i \tag{76}$$

where $x \in \mathbf{R}^n$, $Y(x), X_i(x)$ are smooth vector fields. We assume that $Y(x), X_i(x)$ are such that Eq. (76) has a unique solution for all time $t > 0$. We want to investigate properties of the set which can be reached from a given point by allowing only controls with bounded size. The class of controls u we consider is given by

$$\mathcal{U}_M = \{u \text{ piecewise smooth, with } |u_i(t)| \leq M \ , \ 1 \leq i \leq m\} \ . \tag{77}$$

We denote $Y^M_{\leq\tau}(x)$ the set of points which can be reached from x in time less than τ with a control $u \in \mathcal{U}_M$. We say that the control system is *small-time locally controllable* (STLC) at x if $Y^M_{\leq\tau}(x)$ contains a neighborhood of x for every $\tau > 0$.

The following result is standard in control theory, see e.g. [23] or [19] for a proof.

Proposition 2.6 *Consider the control system Eq. (76) with $u \in \mathcal{U}_M$. Let x_0 be an equilibrium point of $Y(x)$, i.e., $Y(x_0) = 0$. If the linear span of the brackets*

$$\mathrm{ad}^k(Y)(X_i)(x) \quad i = 1, \ldots, m, \quad k = 0, 1, 2, \ldots \ , \tag{78}$$

has rank n at x_0 then Eq. (76) is STLC at x_0.

Proof: One proves Lemma 2.6 by linearizing around X_0 and using e.g. the implicit function theorem, see e.g. [19], Chapter 6, Theorem 1. ∎

As a consequence of Lemma 2.6 and results obtained in [6] one gets

Lemma 2.7 *Consider the control system given by Eqs. (47) with $u \in \mathcal{U}_M$. Let x_0 be a critical point of $G(x)$. If condition* **K2** *is satisfied, then the system (47) is STLC at x_0.*

Proof: The property of small time local controllability is expressed as a condition that certain brackets generate the whole tangent space at some point x_0. This property is obviously related to the hypoellipticity of the generator of the Markov process (5) associated to the control system (47). The generator of the Markov process which solves $dy(t) = Y(x) + \sum_i X_i(x)dw_i(t)$, where $w_i(t)$ is a 1-dimensional process is given on sufficiently smooth functions by the differential operator $L = (1/2)\sum_i(\nabla \cdot X_i)(X_i \cdot \nabla) + Y \cdot \nabla$. If $Y(x)$ and $X_i(x)$ are $\mathcal{C}^\infty$, then L is hypoelliptic if the Lie algebra generated by $Y(X)$ and $X_i(x)$ generates the tangent space at each point x [12]. For the system of equations (5), it is proved in [6], that if condition **K2** is satisfied, then the brackets

$$\mathrm{ad}^k(Y)(X_i)(x) \quad i = 1, \ldots, m\,, \quad k = 0, 1, 2, \ldots \tag{79}$$

generates the tangent space at each point x, in particular at every critical point x_0, and therefore by Lemma 2.6, the control system Eq. (47) is STLC at x_0. ∎

With these results we can derive the basic fact on the geometry of the control paths around equilibrium points of $G(x)$.

Proposition 2.8 *Consider the control system given by (47). Let x_0 be a critical point of $G(x)$ and $B(\rho)$ the ball of radius ρ centered at X_0. Then for any $h > 0$, there are $\rho' > 0$ and $\rho > 0$ with $\rho < \rho'/3$ such that the following hold: For any $x, y \in B(\rho)$, there is $T > 0$ and $u \in \mathcal{U}_M$ with*

$$\phi^u(0) = x \qquad \phi^u(T) = y\,, \tag{80}$$

$$\phi^u(t) \in B(2\rho'/3)\,, \qquad t \in [0, T]\,, \tag{81}$$

and

$$I_{x,T}(\phi^u) \,\leq\, h\,. \tag{82}$$

Proof: Together with the control system (47), we consider the time-reversed system

$$\begin{aligned} \dot{\tilde{q}} &= -\nabla_p G\,, \\ \dot{\tilde{p}} &= \nabla_q G\,, \\ \dot{\tilde{r}} &= \gamma\lambda^2\nabla_r G + (2\gamma\lambda^2 D)^{1/2} u\,. \end{aligned} \tag{83}$$

Lemma 2.7 implies the STLC of the control system (47). Furthermore from Lemma 2.6 it is easy to see the control system (83) is STLC if and only if the control system (47) is. We note ϕ^u ($\tilde{\phi}^u$) the solution of Eq. (47) (Eq. (83)) and $Y_T^M(x)$ ($\tilde{Y}_T^M(x)$) the set of reachable points for the control system (47) ((83)). Using the convexity of the set of values the control can assume and the continuous dependence of ϕ^u on u, it is easy to see ([23], Prop. 2.3.1) that $Y_T^M(x)$ is a compact set.

We choose now M and T such that $M^2 T \le h$. Since $Y_T^M(x)$ and $\tilde{Y}_T^M(x)$ are compact, there is $\rho' > 0$ such that

$$Y_T^M(x), \tilde{Y}_T^M(x) \subset B(2\rho'/3) \,. \tag{84}$$

Furthermore we may choose ρ' arbitrarily small by choosing M and/or T sufficiently small. By Lemma 2.7, both systems (47) and (83) are STLC and thus there is $\rho > 0$ with $\rho < \rho'/3$ and

$$B(\rho) \subset Y_T^M(x), \tilde{Y}_T^M(x) \,. \tag{85}$$

Therefore there are controls $u_1, u_2 \in \mathcal{U}_M$ such that

$$\phi^{u_1}(0) \,=\, x_0 \,, \qquad \phi^{u_1}(T) \,=\, y \,, \tag{86}$$

$$\widetilde{\phi}^{u_2}(0) \,=\, x_0 \,, \qquad \widetilde{\phi}^{u_2}(T) \,=\, x \,. \tag{87}$$

By reversing the time, the trajectory $\widetilde{\phi}^{u_2}(t)$ yields a trajectory $\phi^{u_2}(t)$ with $\phi^{u_2}(0) = x$ and $\phi^{u_2}(T) = x_0$. Concatenating the trajectories $\phi^{u_2}(t)$ and $\phi^{u_1}(t)$ yields a path ϕ from x to y which does not leave the ball $B(2\rho'/3)$ and for which we have the estimate

$$I_{x,2T}(\phi) \,=\, \frac{1}{2}\int_0^{2T} dt|u(t)|^2 \,\le\, M^2 T \,\le\, h \,, \tag{88}$$

and this concludes the proof of Corollary 2.8. ∎

3 Asymptotics of the invariant measure

In this section we prove an extension of Freidlin-Wentzell theory [8] for a certain class of diffusion processes with hypoelliptic generators concerning the invariant measure. Such extensions, for the problem of the exit from a domain, exist, see [2], where a strong hypoellipticity condition is assumed which is not satisfied in our model and see also [3], where their assumption of small-time local controllability on the boundary of the domain is too strong for our purposes. Once the control theory estimates have been established, our proof follows rather closely the proof of Freidlin-Wentzell [8] and the presentation of it given in [3] with a number of technical modifications.

We consider a stochastic differential equation of the form

$$dx_\varepsilon \;=\; Y(x_\varepsilon) + \varepsilon^{1/2}\sigma(x_\varepsilon)dw\,, \tag{89}$$

where $x \in X = \mathbf{R}^n$, $Y(x)$ is a $\mathcal{C}^\infty$ vector field, $\sigma(x)$ a $\mathcal{C}^\infty$ map from $\mathbf{R}^m$ to $\mathbf{R}^n$ and $w(t)$ a standard m-dimensional Wiener process. We view the stochastic process given by Eq. (89) as a small perturbation of the dynamical system

$$\dot{x} \;=\; Y(x)\,. \tag{90}$$

We denote $I_{x,T}(\cdot)$ the large deviation functional associated to Eq. (89) (see Eq. (24)) and denote $V_T(x,y)$ and $V(x,y)$ the cost functions given by (27) and (28). As in [8] we introduce an equivalence relation $\sim$ on X defined as follows: $x \sim y$ if $V(x,y) = V(y,x) = 0$.

Our assumptions on the diffusion process $x_\varepsilon(t)$ are the following

- **L0** The process $x_\varepsilon(t)$ has an invariant measure μ_ε.
- **L1** There is a finite number of compact sets $K_1, K_2, \dots K_L$ such that
  1. For any two points x, y belonging to the same K_i we have $x \sim y$.
  2. If $x \in K_i$, $y \in K_j$, with $i \neq j$, then $x \not\sim y$.
  3. Every ω-limit set of the dynamical system (90) is contained in K_i.

  We let $B(\rho)$ denote the ρ neighborhood of $\cup_i K_i$ and τ_ρ the first time the diffusion $x_\varepsilon(t)$ hits the set $B(\rho)$. We assume that for any $\varepsilon_0 > 0$ the expected hitting time $E_x(\tau_\rho)$ of the diffusion with initial condition x is bounded uniformly for $0 \leq \varepsilon \leq \varepsilon_0$.
- **L2** The diffusion process $x_\varepsilon(t)$ has an hypoelliptic generator. Moreover, for any $x \in K_i$ the control system associated to Eq. (89) is small-time locally controllable.
- **L3** The diffusion process is strongly completely controllable, i.e., for all $T > 0$, $V_T(x,y) < \infty$ and, moreover, $V_T(x,y)$ is upper semicontinuous as a map from $X \times X$ to $\mathbf{R}$.

Remark 3.1 For the model we consider, condition which ensures that **L0** holds are given in [6, 5]. For condition **L1** we assume that the set of critical points of $G(p,q,r)$ is a compact set and item (iii) follows from Lemma 2.2. The bound on the expected hitting time will be proved in a separate publication [21]. For condition **L2**, the hypoellipticity of the generator and the small-time local controllability follows from **K2**, see Lemmas 2.6, 2.7 and 2.8. Condition **L3** is a consequence of condition **K2**, see Proposition 2.3.

Remark 3.2 Condition **L2** is a *local* property of the dynamics and as such sufficient conditions can be given in terms of adequate Lie algebra. A simple sufficient condition for small-time local controllability was quoted and used in Section 2.4. More general sufficient conditions have been proved, see [23] and references therein. condition **L3** is a *global* condition on the dynamics and we are not aware of any general condition which would imply **L3** (except of course ellipticity of the generator).

To describe the asymptotic behavior of the invariant measure μ_ε we will need the following quantities. We let

$$\begin{aligned} V(K_i, K_j) &= \inf_{y\in K_i, z\in K_j} V(y,z)\,, \quad i,j = 1,\ldots,L\,, &(91)\\ V(K_i, z) &= \inf_{y\in K_i} V(y,z)\,, \quad i = 1,\ldots,L\,. &(92)\end{aligned}$$

We set

$$W(K_i) \,=\, \min_{g\in G\{i\}} \sum_{(m\to n)\in g} V(K_m, K_n)\,, \tag{93}$$

where the set of $\{i\}$-graphs $G\{i\}$ is defined in the paragraph above Theorem 1.4. The asymptotics of the invariant measure is given by the function $W(x)$ given by

$$W(x) \,=\, \min_i \left(W(K_i) + V(K_i, x)\right) - \min_j W(K_j)\,. \tag{94}$$

We call a domain $D \subset X$ regular, if the boundary of D, ∂D is a piecewise smooth manifold. Our main result is the following:

Theorem 3.3 *Assume conditions* **L0-L3***. Let D be a regular domain with compact closure such that* $\mathrm{dist}(D, \cup_i K_i) > 0$*. Then the (unique) invariant measure μ_ε of the process $x_\varepsilon(t)$ satisfies*

$$\lim_{\varepsilon\to 0} \varepsilon \ln \mu_\varepsilon(D) \,=\, -\inf_{z\in D} W(z)\,. \tag{95}$$

In particular if there is a single critical set K one has

$$\lim_{\varepsilon\to 0} \varepsilon \ln \mu_\varepsilon(D) \;=\; -\inf_{z\in D} V(K,z)\,. \tag{96}$$

We first recall some general results on hypoelliptic diffusions obtained in [15], in particular a very useful representation of the invariant measure μ_ϵ in terms of embedded Markov chains, see Proposition 3.4 below. Then we prove the large deviations estimates. Let U and V be open subset of X with compact closure with $\overline{U} \subset V$. Below, U and V will be the disjoint union of small neighborhoods of the sets K_i. We introduce an increasing sequence of Markov times $\tau_0, \sigma_0, \tau_1, \ldots$ defined as follows. We set $\tau_0 = 0$ and

$$\sigma_n \;=\; \inf\{t > \tau_n \,:\, x_\varepsilon(t) \in \partial V\} \tag{97}$$

$$\tau_n \;=\; \inf\{t > \sigma_{n-1} \,:\, x_\varepsilon(t) \in \partial U\} \tag{98}$$

As a consequence of hypoellipticity and the strong complete controllability of the control problem associated to the diffusion $x_\varepsilon(t)$ (condition **L2** and **L3**) we have the following result proven in [15] which extends to diffusions with hypoelliptic generators the characterization of invariant measures in terms of recurrence properties of the process $x_\varepsilon(t)$ and which is standard for diffusions with elliptic generators.

We recall that the diffusion $x_\varepsilon(t)$ is positive recurrent if

1. It is recurrent, i.e., for all $x \in X$ for all open set $U \subset X$ one has

$$P_x^\varepsilon(\mathcal{R}_U) \;=\; 1 \tag{99}$$

   where $\mathcal{R}_U$ is the event given by

$$\mathcal{R}_U = \{x_\varepsilon(t_n) \in U \text{ for an increasing sequence } t_n \to \infty\}\,. \tag{100}$$

2. For all $x \in X$ and for all open sets $U \subset X$, one has

$$E_x^\varepsilon(\sigma_U) \;<\; \infty \tag{101}$$

   where $\sigma_U = \inf\{t, x_\varepsilon(t) \in U\}$.

It is proven in [15], Theorem 4.1, that if the diffusion $x_\varepsilon(t)$ is hypoelliptic and strongly completely controllable then the diffusion admits a (unique) invariant measure μ_ε if and only if $x_\varepsilon(t)$ is positive recurrent. Clearly it follows from this result that, almost surely, the Markov times τ_j and σ_j defined in Eqs. (97) and (98) are finite.

An important ingredient in the proof of the results in [15] is the following representation of the invariant measure μ_ε: Suppose $x_\varepsilon(0) = x \in \partial U$. Then $\{x_\varepsilon(\tau_j)\}$ is a Markov chain with a (compact) state space given by ∂U and which admits an invariant measure $l_\varepsilon(dx)$. The following result relates the measure l_ε to the invariant measure μ_ε, see e.g. [11], Chap. IV, Lemma 4.2. for a proof.

Proposition 3.4 *Let the measure ν_ε be defined as*

$$\nu_\varepsilon(D) \,=\, \int_{\partial U} l_\varepsilon(dx) E_x^\varepsilon \int_0^{\tau_1} \mathbf{1}_D(x_\varepsilon(t))dt \,, \tag{102}$$

where D is a Borel set and $\mathbf{1}_D$ is the characteristic function of the set D. Then one has

$$\mu_\varepsilon(D) \,=\, \frac{\nu_\varepsilon(D)}{\nu_\varepsilon(X)} \,. \tag{103}$$

Up to the normalization, the invariant measure μ_ε assigns to a set D a measure equals to the time spent by the process in D between two consecutive hits on ∂U.

The proof of Theorem 3.3 is quite long and will be split into a sequence of Lemmas. The proof is based on the following ideas: As $\varepsilon \to 0$ the invariant measure is more and more concentrated on a small neighborhood of the critical set $\cup_i K_i$. To estimate the measure of a set D one uses the representation of the invariant measure given in Proposition 3.4 where the sets U and V are neighborhoods of the sets $\{K_i\}$. Let $\rho > 0$ and denote $B(i,\rho)$ the ρ-neighborhood of K_i and $B(\rho) = \cup_i B(i,\rho)$. Let D be a regular open set such that $\mathrm{dist}(\cup_i K_i, D) > 0$. We choose ρ' so small that $\mathrm{dist}(B(i,\rho'), B(j,\rho')) > 0$, for $i \neq j$ and $\mathrm{dist}(B(i,\rho'), D) > 0$, for $i = 1, \ldots, L$, and we choose $\rho > 0$ such that $0 < \rho < \rho'$. We set $U = B(\rho)$ and $V = B(\rho')$. We let σ_0 and τ_1 be the Markov times defined in Eqs. (97) and (98) and let τ_D be the Markov time defined as follows:

$$\tau_D \,=\, \inf\{t \,:\, x_\varepsilon(t) \in D\} \,. \tag{104}$$

The first two Lemmas will yield an upper bound on $\nu_\varepsilon(D)$, the unnormalized measure given by Eq. (102). The first Lemma shows that, for ε sufficiently small, the probability that the diffusion wanders around without hitting $B(\rho)$ or D is negligible.

Lemma 3.5 *For any compact set K one has*

$$\lim_{T\to\infty} \limsup_{\varepsilon\to 0} \varepsilon \log \sup_{x\in K} P_x^\varepsilon(\min\{\tau_D \wedge \tau_1\} > T) \,=\, -\infty \tag{105}$$

Proof: If $x \in D \cup B(\rho)$, $\tau_D \wedge \tau_1 = 0$ and there is nothing to prove. Otherwise consider the closed sets

$$F_T \;=\; \{\phi \in \mathcal{C}([0,T]) \,:\, \phi(s) \notin D \cup B(\rho),\ \text{for all } s \in [0,T]\}\,. \qquad (106)$$

Clearly the event $\{\tau > T\}$ is contained in $\{x_\varepsilon \in F_T\}$. By Theorem 2.1, we have for all $T < \infty$,

$$\limsup_{\varepsilon \to 0} \varepsilon \log \sup_{x \in K} P_x^\varepsilon(x_\varepsilon \in F_T) \;\leq\; -\inf_{x \in K} \inf_{\phi \in F_T} I_{x,T}(\phi)\,. \qquad (107)$$

In order to complete the proof of the Lemma it is enough to show that

$$\lim_{T \to \infty} \inf_{x \in K} \inf_{\phi \in F_T} I_{x,T}(\phi) \;=\; \infty\,. \qquad (108)$$

Let ϕ^x be the trajectory of (90) starting at $x \in K$. By condition **L1**, ϕ^x hits $B(\rho/3)$ in a finite time t^x. By the continuous dependence of ϕ^x on its initial condition, there is an open set W^x such that for all $y \in W^x$, ϕ^y hits the set $B(2\rho/3)$ before t^x. Since K is compact, there is T such that, for all $x \in K$, ϕ^x hits $B(2\rho/3)$ before T. Assume now that the identity (108) does not hold. Then, for some $M < \infty$, and every integer n, there is $\psi_n \in F_{nT}$ such that $I_{nT}(\psi_n) \leq M$. Consequently, for some $\psi_{n,k} \in F_T$, we have

$$M \;\geq\; I_{nT}(\psi_n) \;=\; \sum_{k=1}^{n} I_T(\psi_{n,k}) \;\geq\; n \min_{k=1}^{n} I_T(\psi_{n,k})\,. \qquad (109)$$

Therefore there is a sequence $\phi_n \in F_T$ such that $\lim_{n\to\infty} I_T(\phi_n) = 0$. Since the set $\{\phi \,:\, I_{x,T}(\phi) \leq 1, \phi(0) \in K\}$ is compact, ϕ^n has a limit point $\phi \in F_T$. Since I_T is lower semicontinuous, we have $I_T(\phi) = 0$ and therefore ϕ is trajectory of (90). Since $\phi \in F_T$, ϕ remains outside of $B(2\rho/3)$ and this is a contradiction with the definition of T. This concludes the proof of Lemma 3.5. ■

Instead of the quantities $V(K_i, K_j)$ and $V(K_i, z)$ defined in Eqs. (91) and (92), it is useful to introduce the following quantities:

$$\begin{aligned} \tilde{V}(K_i, K_j) &= \inf_{T>0} \inf\{I_{x,T}(\phi),\ \phi(0) \in K_i, \phi(T) \in K_j, \phi(t) \notin \cup_{l \neq i,j} K_l\}\,, \\ \tilde{V}(K_i, z) &= \inf_{T>0} \inf\{I_{x,T}(\phi),\ \phi(0) \in K_i, \phi(T) = x, \phi(t) \notin \cup_{l \neq i} K_l\} \end{aligned} \qquad (110)$$

The following Lemma will yield an upper bound on the on $\nu_\varepsilon(D)$, where ν_ε is the (unnormalized) measure given by Eq. (102).

Lemma 3.6 *Given $h > 0$, for $0 < \rho < \rho'$ sufficiently small one has*

$$(i) \qquad \limsup_{\varepsilon\to 0} \varepsilon \log \sup_{y\in\partial B(i,\rho')} P^\varepsilon_y(\tau_D < \tau_1) \;\le\; -(\inf_{z\in D} \tilde V(K_i,z) - h)\,, \tag{111}$$

$$(ii) \qquad \limsup_{\varepsilon\to 0} \varepsilon \log \sup_{y\in\partial B(i,\rho')} P^\varepsilon_y(x_\varepsilon(\tau_1) \in \partial B(j,\rho)) \;\le\; -(\tilde V(K_i,K_j) - h)\,. \tag{112}$$

Proof: We first prove item (i). If $\inf_{z\in D} \tilde V(K_i,z) = +\infty$ there is no curve connecting K_i to $z \in D$ without touching the other K_j, $j \neq i$.. Therefore $P^\varepsilon_y(\tau_D < \tau_1) = 0$ and there is nothing to prove. Otherwise, for $h > 0$ we set $\tilde V_h = \inf_{z\in D} \tilde V(K_i,z) - h$. Since $V(y,z)$ satisfies the triangle inequality, we have, by condition **L2**, that, for ρ small enough

$$\inf_{y\in\partial B(i,\rho')} \inf_{z\in D} \tilde V(y,z) \;\ge\; \inf_{y\in\partial B(i,\rho')} \inf_{z\in D} \tilde V(K_i,z) - \sup_{y\in\partial B(i,\rho')} \tilde V(K_i,y) \;\ge\; \tilde V_h\,. \tag{113}$$

where

$$\tilde V(y,z) \;=\; \inf_{T>0} \inf \left\{ I_{x,T}(\phi),\, \phi(0) = y, \phi(T) = z, \phi(t) \notin \cup_{l\neq i} K_l \right\}\,. \tag{114}$$

By Lemma 3.5, there is $T < \infty$ such that

$$\limsup_{\varepsilon\to 0} \varepsilon \log \sup_{y\in\partial B(i,\rho')} P^\varepsilon_y(\tau_D \wedge \tau_1 > T) \;<\; -V_h\,. \tag{115}$$

Let G_T denote the subset of $\mathcal{C}([0,T])$ which consists of functions $\phi(t)$ such that $\phi(t) \in \overline{D}$ for some $t \in [0,T]$ and $\phi(t) \notin B(\rho)$ if $t \le \inf\{s\,, \phi(s) \notin D\}$. The set G_T is closed as is seen by considering its complement.

We have

$$\inf_{y\in\partial B(i,\rho')} \inf_{\phi\in G_T} I_{y,T}(\phi) \;\ge\; \inf_{y\in\partial B(i,\rho')} \inf_{z\in\overline{D}} \tilde V(y,z) \;\ge\; V_h\,, \tag{116}$$

and thus by Theorem 2.1, we have

$$\limsup_{\varepsilon\to 0} \varepsilon \log \sup_{y\in\partial B(i,\rho')} P^\varepsilon_y(x_\varepsilon \in G_T) \;\le\; -\inf_{y\in\partial B(i,\rho')} \inf_{\phi\in G_T} I_{y,T}(\phi) \;\le\; -V_h\,. \tag{117}$$

We have the inequality

$$P^\varepsilon_y(\tau_D < \tau_1) \le P^\varepsilon_y(\tau_D \wedge \tau_1 > T) + P^\varepsilon_y(x_\varepsilon \in G_T)\,, \tag{118}$$

and combining the estimates (115) and (117) yields

$$\limsup_{\varepsilon\to 0} \varepsilon \log \sup_{y\in\partial B(i,\rho')} P^\varepsilon_y(\tau_D \wedge \tau_1) \;\le\; -V_h\,. \tag{119}$$

This completes the proof of item (i) of Lemma 3.6.

The proof of part (ii) of the Lemma is very similar to the first part and follows closely the corresponding estimates in [8], Chapter 6, Lemma 2.1. The details are left to the reader. ∎

The following Lemma will yield a lower bound on $\nu_\varepsilon(D)$. It makes full use of the information contained in Lemmas 2.3 and 2.8.

Lemma 3.7 *Given $h > 0$, for $0 < \rho' < \rho$ sufficiently small one has*

$$(i) \qquad \liminf_{\varepsilon \to 0} \varepsilon \log \inf_{x \in \partial B(i,\rho)} P_x^\varepsilon(\tau_D < \tau_1) \;\geq\; -(\inf_{z \in D} \tilde{V}(K_i, z) + h)\,. \tag{120}$$

$$(ii) \qquad \liminf_{\varepsilon \to 0} \varepsilon \log \inf_{x \in \partial B(i,\rho)} P_x^\varepsilon(x_\varepsilon(\tau_1) \in \partial B(j,\rho)) \;\geq\; -(\tilde{V}(K_i, K_j) + h)\,. \tag{121}$$

Proof: We start with the proof of item (i). If $\inf_{z \in D} \tilde{V}(K_i, z) = +\infty$ there is nothing to prove. Otherwise let $h > 0$ be given. By condition **L2**, (see Corollary 2.8), there are ρ and $\rho' > 0$ with $\rho < \rho'/3$ and $T_0 < \infty$ such that, for all $x \in \partial B(i, \rho)$, there is a path $\psi^x \in \mathcal{C}([0, T_0])$ which satisfies $I_{x,T_0}(\psi^x) \leq h/3$ with $\psi^x(0) = x$ and $\psi^x(T_0) = x_0 \in K_i$ and $\psi^x(t) \in B(2\rho'/3)$, $0 \leq t \leq T_0$.

By condition **L3**, there are $z \in D$, $T_1 < \infty$ and $\phi_1 \in \mathcal{C}([0, T_1])$ such that $I_{x_0,T_1}(\phi_1) \leq \inf_{z \in D} \tilde{V}(K_i, z) + h/3$ and $\phi_1(0) = x_0 \in K_i$ and $\phi_1(T_1) = z$ and ϕ_1 does not touch K_j, with $j \neq i$. We may and will assume that ρ and ρ' are chosen such that $2\rho' \leq \mathrm{dist}(\phi_1(t), \cup_{j \neq i} K_j$. We note $\Delta = \mathrm{dist}(z, \partial D)$. Let x_1 be the point of last intersection of ϕ_1 with $\partial B(i, \rho)$ and let t_1 such that $\phi_1(t_1) = x_1$. We note $\phi_2 \in \mathcal{C}([0, T_2])$, with $T_2 = T_1 - t_1$, the path obtained from ϕ_1 by deleting up to time t_1 and translating in time. Notice that the path ϕ_2 may hit several times $\partial B(i, \rho')$, but hits $\partial B(i, \rho)$ only one time (at time 0). Denote as

$$\sigma = \inf\{t : \phi_2(t) \in \partial B(i, \rho')\} \tag{122}$$

the first time $\phi_2(t)$ hits $\partial B(i, \rho')$. We choose Δ' so small that if $\psi \in \mathcal{C}([0, T_2])$ belongs to the Δ'-neighborhood of ϕ_2, then $\psi(t)$ does not intersect $\partial B(i, \rho)\}$ and $\partial B(i, \rho')\}$ for $0 < t < \sigma$ and and does not intersect $\partial B(i, \rho)\}$ for $t > \sigma$.

By condition **L2**, there are $T_3 < \infty$ and $\phi_3 \in \mathcal{C}([0, T_3])$ such that $\phi_3(0) = x_0$, $\phi_3(T_3) = x_1$, $\phi_3(t) \in B(2\rho'/3)$, $0 \leq t \leq T_3$, and $I_{x_0,T_3}(\phi_3) \leq h/3$. Concatenating ψ^x, ϕ_3 and ϕ_2, we obtain a path $\phi^x \in \mathcal{C}([0, T])$ with $T = T_0 + T_3 + T_2$ and $I_{x,T}(\phi^x) \leq \inf_{z \in D} \tilde{V}(K_i, z) + h$. By construction the path ϕ^x avoids $\partial B(i, \rho)\}$ after the time $T_0 + T_3 + \sigma$ where σ defined in Eq. (122).

We consider the open set

$$U_T \;=\; \bigcup_{x\in\partial B(\rho)} \left\{ \psi \in \mathcal{C}([0,T]) \,:\, \|\psi - \phi_x\| \leq \min\{\frac{\rho}{3}, \frac{\Delta}{2}, \frac{\Delta'}{2}\} \right\} . \tag{123}$$

By construction the event $\{x_\varepsilon(t) \in U_T\}$ is contained in the event $\{\tau_D \leq \tau_1\}$. By Theorem 2.1 we have

$$\begin{aligned}
\liminf_{\varepsilon\to 0} \varepsilon \log \inf_{x\in\partial B(\rho)} P_x^\varepsilon(\tau_D < \tau_1) \;&\geq\; \liminf_{\varepsilon\to 0} \varepsilon \log \inf_{x\in\partial B(\rho)} P_x^\varepsilon(x_\varepsilon \in U_T) \\
&\geq\; - \sup_{x\in\partial B(\rho)} \inf_{\psi\in U_T} I_{x,T}(\psi) \\
&\geq\; - \sup_{x\in\partial B(\rho)} I_{x,T}(\phi^x) \\
&\geq\; -(\inf_{z\in D} \tilde{V}(K_i, z) + h) \,.
\end{aligned} \tag{124}$$

This concludes the proof of item (i).

The proof of (ii) follows very closely the corresponding estimate in [8], Chapter 6, Lemma 2.1., which considers the case where the generator of the diffusion is elliptic: for any $h > 0$ one construct paths $\phi^{xy} \in \mathcal{C}([0,T])$ from $x \in \partial B(i,\rho)$ to $y \in \partial B(j,\rho)$ such that $I_{x,T}(\phi^{xy}) \leq \tilde{V}(K_i, K_j) + h/2$ and such that if $x_\varepsilon(t)$ is in a small neighborhood of ϕ^{xy}, then $x_\varepsilon(\tau_1) \in \partial B(j,\rho)$. As in part (i) of the Lemma, the key element to construct the paths ϕ^{xy} is the condition **L2** of small-time controllability around the sets K_i. The details are left to the reader.

This concludes the proof of lemma 3.7. ∎

The following two Lemmas give upper and lower bounds on the normalization constant $\nu_\varepsilon(X)$, where ν_ε is defined in Eq. (102).

Lemma 3.8 *For any $h > 0$, we have*

$$\liminf_{\varepsilon\to 0} \varepsilon \log \nu_\varepsilon(X) \;\geq\; -h \,. \tag{125}$$

Proof: We choose an arbitrary $h > 0$. For any $\rho' > 0$ we have the inequality:

$$\begin{aligned}
\nu_\varepsilon(X) \;&\geq\; \nu_\varepsilon(B(\rho')) \\
&=\; \int_{\partial B(\rho)} l_\varepsilon(dx) E_x^\varepsilon \int_0^{\tau_1} \mathbf{1}_{B(\rho')}(x_\varepsilon(t)) dt \\
&\geq\; \int_{\partial B(\rho)} l_\varepsilon(dx) E_x^\varepsilon \int_0^{\sigma_0} \mathbf{1}_{B(\rho')}(x_\varepsilon(t)) dt \\
&=\; \int_{\partial B(\rho)} l_\varepsilon(dx) E_x^\varepsilon(\sigma_0) \,.
\end{aligned}$$

We use a construction similar as that used in Lemma 3.7. Using condition **L2**, there are ρ and $\rho' > 0$ with $\rho < \rho'/3$ such that such that for all $x \in \partial B(\rho)$, there are $T_1 < \infty$ and $\psi^x \in \mathcal{C}([0,T_1])$ such that $\psi^x(0) = x$, $\psi^x(T_1) = x_0 \in \cup_i K_i$, $\psi^x(t) \in B(2\rho/3)$, $0 \le t \le T_1$ and $I_{x,T_1}(\psi^x) \le h/4$. Furthermore, using Corollary 2.4, for ρ' small enough, there are $z \in \partial B(\rho')$, $T_2 < \infty$, and $\psi \in \mathcal{C}([0,T_2])$ such that $\psi(0) = x_0$, $\psi(T_2) = z$, $\psi(t) \in B(\rho')$ for $0 \le t \le T_2$, and $I_{x_0,T_2}(\psi) \le h/4$. We denote $\phi^x \in \mathcal{C}([0,T])$, with $T = T_1 + T_2$, the path obtained by concatenating ψ^x and ψ. It satisfies $I_{x,T}(\psi) \le h/2$. We consider the open set

$$V_T \;=\; \bigcup_{x\in\partial B(\rho)} \left\{\psi \in \mathcal{C}([0,T]) \;:\; \|\psi - \phi_x\| < \frac{\rho}{3}\right\}. \tag{126}$$

Applying Theorem 2.1, one obtains

$$\liminf_{\varepsilon\to 0} \varepsilon \log \inf_{x\in\partial B(\rho)} P_x^\varepsilon(x_\varepsilon \in V_T) \;\ge\; -\frac{h}{2}. \tag{127}$$

There is $T^* > 0$, such that for any $\phi \in V_T$ the time spent in $B(\rho')$ is at least T^*. Therefore, for ε small enough we obtain the bound

$$\int_{\partial B(\rho)} l_\varepsilon(dx) E_x^\varepsilon(\sigma_0) \;\ge T^* \exp\left(-\frac{h}{2\varepsilon}\right) \;\ge\; \exp\left(-\frac{h}{\varepsilon}\right), \tag{128}$$

and this completes the proof of Lemma 3.8. ∎

To get an upper bound on the normalization constant $\nu_\varepsilon(X)$ we will need an upper bound on the escape time out of the ball $B(\rho')$ around $\cup_i K_i$, starting from $x \in \partial B(\rho)$.

Lemma 3.9 *Given $h > 0$, for $0 < \rho < \rho'$ sufficiently small,*

$$\limsup_{\varepsilon\to 0} \varepsilon \log \sup_{x\in\partial B(\rho)} E_x^\varepsilon(\sigma_0) \le h. \tag{129}$$

Proof: Fix $h > 0$ arbitrary. As in Lemma 3.8, we see that, for $0 < \rho < \rho'$ sufficiently small and for all $x \in \partial B(\rho)$, there are $T_1, T_2 \le \infty$, $z \notin B(\rho')$ and $\phi^x \in \mathcal{C}([0, T_1+T_2])$ such that $\phi^x(0) = x$, $\phi^x(T_1) \in \cup_i K_i$, and $\phi^x(T_1+T_2) = z$, and $I_{x,T_1+T_2}(\phi^x) \le h/2$. We set $T_0 = T_1 + T_2$ and $\Delta = \mathrm{dist}(z, B(\rho'))$ and consider the open set

$$W_{T_0} \;=\; \bigcup_{x\in\partial B(\rho)} \left\{\psi \in \mathcal{C}([0,T_0]) \;:\; \|\psi - \phi_x\| < \frac{\Delta}{2}\right\}, \tag{130}$$

so that if $\psi \in W_{T_0}$ it escapes from $B(\rho')$ in a time less than T_0, i.e., the event$\{x_\varepsilon \in W_{T_0}\}$ is contained in the event $\{\sigma_0 < T_0\}$. Using Theorem 2.1, we see that for sufficiently small ε, one has the bound

$$q \,\equiv\, \inf_{x\in\partial B(\rho)} P_x^\varepsilon(\sigma_0 < T_0) \,\geq\, \exp\left(-\frac{h}{2\varepsilon}\right). \tag{131}$$

Consider the events $\sigma_0 > kT_0$, $k = 1, 2, \ldots$. Using the Markov property one obtains the bound

$$\begin{aligned} P_x^\varepsilon(\sigma_0 > (k+1)T_0) \quad &\leq \quad [1 - P_x^\varepsilon(kT_0 < \sigma_0 \leq (k+1)T_0)]\, P_x^\varepsilon(\sigma_0 > kT_0) \\ &\leq \quad (1-q)P_x^\varepsilon(\sigma_0 > kT_0). \end{aligned} \tag{132}$$

Iterating over k yields

$$\sup_{x\in\partial B(\rho)} P_x^\varepsilon(\sigma_0 > kT_0) \,\leq\, (1-q)^k\,. \tag{133}$$

Therefore

$$\begin{aligned} \sup_{x\in\partial B(\rho)} E_x^\varepsilon(\sigma_0) \quad &\leq \quad T_0\left[1 + \sum_{k=1}^\infty \sup_{x\in\partial B(\rho)} P_x^\varepsilon(\sigma_0 > kT_0)\right] \\ &\leq \quad T_0 \sum_{k=0}^\infty (1-q)^k \,=\, \frac{T_0}{q}\,. \end{aligned} \tag{134}$$

Since $q \geq \exp\left(-\frac{h}{2\varepsilon}\right)$ one obtains, for sufficiently small ε

$$\sup_{x\in\partial B(\rho)} E_x^\varepsilon(\sigma_0) \,\leq\, T_0 \exp\left(\frac{h}{2\varepsilon}\right) \,\leq\, \exp\left(\frac{h}{\varepsilon}\right). \tag{135}$$

This concludes the proof of Lemma 3.9. ∎

With this Lemma we have proved all large deviations estimates needed in the proof of Theorem 3.3. We will need upper and lower estimates on $l_\varepsilon(\partial B(i,\rho))$ where l_ε is the invariant measure of the Markov chain $x_\varepsilon(\tau_j)$. These estimates are proved in [8], Chapter 6, Section 3 and 4 and are purely combinatorial and rely on the representation of the invariant measure of a Markov chain with a finite state space via graphs on the state space. By Lemma 3.6, (ii) and 3.7, (ii) we have the following estimates on the probability transition $q(x,y)$, $x, y \in \partial B(\rho)$ of the Markov chain $x_\varepsilon(\tau_j)$: Given $h > 0$, for $0 < \rho < \rho'$ sufficiently small

$$\exp -\frac{1}{\varepsilon}(\tilde{V}(K_i, K_j) + h) \,\leq\, q(x, \partial B(j,\rho)) \,\leq\, \exp -\frac{1}{\varepsilon}(\tilde{V}(K_i, K_j) - h)\,, \tag{136}$$

for all $x \in \partial B(i,\rho)$ and sufficiently small ε. It is shown in [8], Chapter 6, Lemmas 3.1 and 3.2 that the bound (136) implies a bound on $l_\varepsilon(\partial B(i,\rho))$. One obtains

$$\exp\left(-\frac{1}{\varepsilon}(\tilde{W}(K_i) - \min_j \tilde{W}(K_j) + h)\right) \le l_\varepsilon(\partial B(i,\rho)) \le \\ \le \exp\left(-\frac{1}{\varepsilon}(\tilde{W}(K_i) - \min_j \tilde{W}(K_j) - h)\right) \qquad (137)$$

for sufficiently small ε, where

$$\tilde{W}(K_i) = \min_{g\in G\{i\}} \sum_{(m\to n)\in g} \tilde{V}(K_m, K_n)\,. \qquad (138)$$

Also in [8], Chapter 6, Lemma 4.1, $\tilde{W}(K_i)$ is shown to be in fact equal to $W(K_i)$ defined in Eq. (93):

$$\begin{aligned} \tilde{W}(K_i) &= \min_{g\in G\{i\}} \sum_{(m\to n)\in g} V(K_m, K_n) \\ &= W(K_i)\,. \end{aligned} \qquad (139)$$

Furthermore it is shown Lemma 4.2 there that the function $W(x)$, defined by Eq. (94), satisfies the identity

$$\begin{aligned} W(x) &= \min_i (W(K_i) + V(K_i, x)) - \min_j W(K_j) \\ &= \min_i (\tilde{W}(K_i) + \tilde{V}(K_i, x)) - \min_j \tilde{W}(K_j) \end{aligned} \qquad (140)$$

We can turn to the proof of Theorem 3.3.
Proof of Theorem 3.3:

In order to prove Eq. (95), it is enough to show that, for any $h > 0$, there is $\varepsilon_0 > 0$ such that, for $\varepsilon < \varepsilon_0$ we have the inequalities:

$$\mu_\varepsilon(D) \ge \exp\left(-\frac{1}{\varepsilon}(\inf_{z\in D} W(z) + h)\right), \qquad (141)$$

$$\mu_\varepsilon(D) \le \exp\left(-\frac{1}{\varepsilon}(\inf_{z\in D} W(z) - h)\right). \qquad (142)$$

We let $\rho' > 0$ such that $\rho' < \mathrm{dist}(x_{\min}, D)$. Recall that $\tau_D = \inf\{t : x_\varepsilon(t) \in D\}$ is the first hitting time of the set D. we have the following bound on the $\nu_\varepsilon(D)$

$$\begin{aligned} \nu_\varepsilon(D) &\le \sum_i l_\varepsilon(\partial B(i,\rho)) \sup_{x\in\partial B(i,\rho)} E^\varepsilon_x \int_0^{\tau_1} \mathbf{1}_D(x_\varepsilon(t))dt \\ &\le L \max_i l_\varepsilon(\partial B(i,\rho)) \sup_{x\in\partial B(i,\rho)} P^\varepsilon_x(\tau_D \le \tau_1) \sup_{y\in\partial D} E^\varepsilon_y(\tau_1)\,. \end{aligned} \qquad (143)$$

By **L1**, there exist a constant C independent of ε such that

$$\sup_{y\in\partial D} E_y^\varepsilon(\tau_1) \,\leq\, C\,, \tag{144}$$

for $\varepsilon \leq \varepsilon_0$. From Lemma 3.6, (i), given $h > 0$, for sufficiently small $0 < \rho < \rho'$, we have the bound

$$P_x^\varepsilon(\tau_D < \tau_1) \,\leq\, \exp\left(-\frac{1}{\varepsilon}(\inf_{z\in D}\tilde{V}(K_i,z) - h/4)\right), \tag{145}$$

for sufficiently small ε. From Eq. (137), given $h > 0$, for sufficiently small $0 < \rho < \rho'$, we have the bound

$$l_\varepsilon(\partial B(i,\rho)) \,\leq\, \exp\left(-\frac{1}{\varepsilon}(\tilde{W}(K_i) - \min_j \tilde{W}(K_j) - h/4)\right) \tag{146}$$

From the estimates (143)-(146), and the identity (140) we obtain the bound

$$\nu_\varepsilon(D) \,\leq\, \exp\left(-\frac{1}{\varepsilon}(\min_{z\in D} W(z) + h/2)\right), \tag{147}$$

for sufficiently small ε. From Lemma 3.8, given $h > 0$, for sufficiently small $0 < \rho < \rho'$, we have the bound

$$\nu_\varepsilon(X) \,\geq\, \exp\left(-\frac{h}{2\varepsilon}\right), \tag{148}$$

for sufficiently small ε. Combining estimates (147) and (148), we obtain that

$$\mu_\varepsilon(D) \,\leq\, \exp\left(-\frac{1}{\varepsilon}(\inf_{z\in D} W(z) - h)\right), \tag{149}$$

for sufficiently small ε and this gives the bound (142).

In order to prove (141), we consider the set $D_\delta = \{x \in D \,:\, \mathrm{dist}(x, \partial D) \geq \delta\}$. For δ sufficiently small, $D_\delta \neq \emptyset$. By **L3**, $\tilde{V}(K_i, z)$ is upper semicontinuous in z so that $\tilde{V}(K_i, z') \leq \tilde{V}(K_i, z) + h/4$, for $z' - z \leq \delta$. Therefore

$$\inf_{z\in D_\delta} \tilde{V}(K_i,z) \leq \inf_{z\in D} \tilde{V}(K_i,z) + h/4\,. \tag{150}$$

We have the bound

$$\nu_\varepsilon(D) \,\geq\, \max_i l_\varepsilon(\partial B(i,\rho)) \inf_{x\in\partial B(i,\rho)} P_x^\varepsilon(\tau_{D_\delta} < \tau_1) \inf_{x\in\partial D_\delta} E_x^\varepsilon \int_0^{\tau_1} \mathbf{1}_D(x_\varepsilon(t))dt\,. \tag{151}$$

There is $\varepsilon_0 > 0$ and a constant $\overline{C} > 0$ such that we have the bound

$$\inf_{x \in D_\delta} E_x^\varepsilon \int_0^{\tau_1} \mathbf{1}_D(x_\varepsilon(t))dt \, \geq \, \overline{C} \, > \, 0 \, , \tag{152}$$

uniformly in $\varepsilon \leq \varepsilon_0$. From Eq. (137), given $h > 0$, for sufficiently small $0 < \rho < \rho'$, we have the bound

$$l_\varepsilon(\partial B(i, \rho)) \, \geq \, \exp\left(-\frac{1}{\varepsilon}(\tilde{W}(K_i) - \min_j \tilde{W}(K_j) + h/4)\right) , \tag{153}$$

for sufficiently small ε. Furthermore, by Lemma 3.7 and inequality (150), given $h > 0$, for $0 < \rho < \rho'$ sufficiently small, we have

$$\inf_{x \in \partial B(i,\rho)} P_x^\varepsilon(\tau_{D_\delta} \leq \tau_1) \, \geq \, \exp\left(-\frac{1}{\varepsilon}(\inf_{z \in D} \tilde{V}(K_i, z) + h/4)\right) , \tag{154}$$

for sufficiently small ε. Combining estimates (151)–(154) and identity (140) we find

$$\nu_\varepsilon(D) \, \geq \, \exp\left(-\frac{1}{\varepsilon}(\inf_{z \in D} W(z) + h/2)\right) . \tag{155}$$

In order to give an upper bound on the normalization constant $\nu_\varepsilon(X)$, we use Eq. (102). Using the Markov property, we obtain

$$\begin{aligned} \nu_\varepsilon(X) \quad &= \quad \int_{\partial B(\rho)} l_\varepsilon(dx) E_x^\varepsilon(\tau_1) \\ &= \quad \int_{\partial B(\rho)} l_\varepsilon(dx) \left(E_x^\varepsilon(\sigma_0) + E_x^\varepsilon(E_{x_\varepsilon(\sigma_0)}^\varepsilon(\tau_1)) \right) \\ &\leq \quad \sup_{x \in \partial B(\rho)} E_x^\varepsilon(\sigma_0) + \sup_{y \in \partial B(\rho')} E_y^\varepsilon(\tau_1) \, . \end{aligned} \tag{156}$$

By Lemma 3.9, given $h > 0$, for sufficiently small $0 < \rho < \rho'$ we have the estimate

$$\sup_{x \in \partial B(\rho)} E_x^\varepsilon(\sigma_0) \, \leq \, \exp\left(\frac{h}{2\varepsilon}\right) , \tag{157}$$

for sufficiently small ε. By **L1**, the second term on the right hand side of (156) is bounded by a constant, uniformly in $0 \leq \varepsilon \leq \varepsilon_0$. Therefore for we obtain the estimate

$$\nu_\varepsilon(X) \, \leq \, \exp\left(\frac{h}{2\varepsilon}\right) , \tag{158}$$

for sufficiently small ε. Combining estimates (155) and (158) we obtain the bound

$$\mu_\varepsilon(D) \, \geq \, \exp\left(-\frac{1}{\varepsilon}(\inf_{z \in D} W(z) + h)\right) , \tag{159}$$

and this is the bound (141). This concludes the proof of Theorem 3.3. ∎

4 Properties of the rate function

In this section we prove assertions (16) and (17) of Theorem 1.4 and Proposition 1.7. Recall that for Eq. (5), the rate function, $I_{x,T}^{(\eta)}(\phi)$, takes the following form: For $\phi(t) = (p(t), q(t), r(t))$,

$$I_{x,T}^{(\eta)}(\phi) = \frac{1}{4\gamma\lambda^2}\int_0^T (\dot{r} + \gamma\lambda^2\nabla_r G)D^{-1}(\dot{r} + \gamma\lambda^2\nabla_r G) \tag{160}$$

if

$$\dot{q} = \nabla_p G\,, \quad \dot{p} = -\nabla_q G\,, \tag{161}$$

and is $+\infty$ otherwise. Recall that for a path $\phi \in \mathcal{C}([0,T])$ with $\phi(0) = x$ and $\phi(T) = y$ we denote $\tilde{\phi}$ the time reversed path which satisfy $\tilde{\phi}(0) = Jy$ and $\tilde{\phi}(T) = Jx$.

Proof of Proposition 1.7: We rewrite the rate function $I_{x,T}^{(\eta)}(\phi)$ as

$$\begin{aligned} I_{x,T}^{(\eta)}(\phi) &= \\ &= \frac{1}{4\gamma\lambda^2}\int_0^T (\dot{r} + \gamma\lambda^2\nabla_r G)D^{-1}(\dot{r} + \gamma\lambda^2\nabla_r G)dt \\ &= \frac{1}{4\gamma\lambda^2}\int_0^T (\dot{r} - \gamma\lambda^2\nabla_r G)D^{-1}(\dot{r} - \gamma\lambda^2\nabla_r G)dt + \int_0^T (\nabla_r G)D^{-1}\dot{r}dt \\ &\equiv K_1(\phi) + K_2(\phi) \end{aligned} \tag{162}$$

The term $K_1(\phi)$ has the following interpretation: It is the rate function corresponding to the the set of stochastic differential equations

$$\begin{aligned} dq &= \nabla_p G dt\,, \\ dp &= -\nabla_q G dt\,, \\ dr &= +\gamma\lambda^2\nabla_r G dt + \varepsilon^{1/2}(2\gamma\lambda^2 D)^{1/2}dw\,. \end{aligned} \tag{163}$$

In particular there is $u \in L^2([0,T])$ such that for $\phi(t) = (p(t), q(t), r(t))$, with $\phi(0) = x$ and $\phi(T) = y$ we have

$$\begin{aligned} \dot{q} &= \nabla_p G\,, \\ \dot{p} &= -\nabla_q G\,, \\ \dot{r} &= +\gamma\lambda^2\nabla_r G + (2\gamma\lambda^2 D)^{1/2}u\,. \end{aligned} \tag{164}$$

Consider now the transformation $(p, q, r) \to J(p, q, r)$ and $t \to -t$. This transformation maps the solution of Eq. (164) into $\tilde{\phi}(t) = (\tilde{p}(t), \tilde{q}(t), \tilde{r}(t))$

which is the solution to

$$\begin{aligned}
\dot{\tilde{q}} &= \nabla_p G\,, \\
\dot{\tilde{p}} &= -\nabla_q G\,, \\
\dot{\tilde{r}} &= -\gamma\lambda^2\nabla_r G + (2\gamma\lambda^2 D)^{1/2}\tilde{u}(t)\,,
\end{aligned} \tag{165}$$

with $\tilde{\phi}(0) = Jy$, $\tilde{\phi}(T) = Jx$. This implies the equality

$$\begin{aligned}
K_1(\phi) &= \frac{1}{4\gamma\lambda^2}\int_0^T (\dot{r} - \gamma\lambda^2\nabla_r G)D^{-1}(\dot{r} - \gamma\lambda^2\nabla_r G) \\
&= \frac{1}{4\lambda^2\gamma}\int_0^T (\dot{\tilde{r}} + \gamma\lambda^2\nabla_r G)D^{-1}(\dot{\tilde{r}} + \gamma\lambda^2\nabla_r G)dt \\
&= I^{(\eta)}_{Jy,T}(\tilde{\phi})\,.
\end{aligned} \tag{166}$$

This means that $K_1(\phi)$ is nothing but the weight of the time reversed path, i.e. the path starting at time 0 from Jy and leading to Jx at time T.

We now consider the second term $K_2(\phi)$ in Eq. (162). We consider separately the equilibrium case (i.e., $\eta = 0$) and the non-equilibrium case (i.e. $\eta \neq 0$). For $\eta = 0$ the matrix D is the identity and we find

$$K_2(\phi) = \int_0^T \nabla_r G\dot{r}dt \tag{167}$$

Using the constraints $\dot{q} = \nabla_p G$ and $\dot{p} = -\nabla_q G$ we obtain the identity $\nabla_p G\dot{p} + \nabla_q G\dot{q} = 0$ and therefore we get

$$\begin{aligned}
\int_0^T \nabla_r G\dot{r}dt &= \int_0^T (\nabla_r G\dot{r} + \nabla_p G\dot{p} + \nabla_q G\dot{q})\,dt \\
&= \int_0^T \frac{d}{dt}Gdt \,=\, G(y) - G(x)\,,
\end{aligned} \tag{168}$$

and this proves Eq. (22) in the case $\eta = 0$.

To prove Eq. (22) in the case $\eta \neq 0$ observe that we have the identity,

$$\frac{d}{dt}\frac{1}{2}(\lambda^{-1}r_i - \lambda q_i)^2 \,=\, (\lambda^{-1}r_i - \lambda q_i)(\lambda^{-1}\dot{r}_i - \lambda\dot{q}_i) \,=\, \lambda\nabla_{r_i}G(\lambda^{-1}\dot{r}_i - \lambda p_i)\,, \tag{169}$$

for $i = 1, n$, and therefore

$$\nabla_{r_i}G\dot{r}_i = \lambda^2\nabla_{r_i}Gp_i + \frac{d}{dt}\frac{1}{2}(\lambda^{-1}r_i - \lambda q_i)^2\,. \tag{170}$$

Hence, using the definition (21), we obtain

$$K_2(\phi) \;=\; \int_0^T \nabla_r D^{-1} G\dot{r} dt \;=\; R(\phi(T)) - R(\phi(0)) - \int_0^T \Theta(\phi(t))dt \quad (171)$$

This completes the proof of Proposition 1.7. ■

With generalized detailed balance we show the following

Proposition 4.1 *If* $\eta = 0$ *then* $W^{(0)}(x) = G(x) - \min_x G(x)$.

Proof: The function $W^{(0)}(x)$ is given by

$$W^{(0)}(x) \;=\; \min_i \Big(W^{(0)}(K_i) + V^{(0)}(K_i, x) \Big) - \min_j W^{(0}(K_j)\,. \quad (172)$$

where the minimum is taken over all compact sets K_i. In Eq. (172), $W^{(0)}(K_i)$ is given by

$$W^{(0)}(K_i) \;=\; \min_{g \in G\{i\}} \sum_{(m \to n) \in g} V^{(0)} K_m, K_n)\,. \quad (173)$$

The sets K_j are the critical sets of the generalized Hamiltonian $G(p, q, r)$, therefore G is constant on K_j and we set $G(x) = G_j$ for all $x \in K_j$. Furthermore if $(p, q, r) \in K_j$, then $p = 0$ and therefore the sets K_j are invariant under time reversal: $JK_j = K_j$. Using the generalized detailed balance, we see that for any path $\phi \in \mathcal{C}([0, T])$ with $\phi(0) = x \in K_m$ and $\phi(t) = y \in K_n$ we have

$$I^{(0)}_{x,T}(\phi) \;=\; I^{(0)}_{Jy,T}(\tilde{\phi}) + G(y) - G(x) \;=\; I^{(0)}_{y,T}(\tilde{\phi}) + G_n - G_m\,. \quad (174)$$

Taking the infimum over all paths ϕ and all time T, we obtain the identity

$$V^{(0)}(K_m, K_n) \;=\; V^{(0)}(K_n, K_m) + G_m - G_n\,. \quad (175)$$

In Eq. (173) the minimum is taken over all $\{i\}$-graphs (see the paragraph above Theorem 1.4 in the introduction). Given an $\{i\}$-graph and a j with $j \neq i$, there is a sequence of arrows leading from j to i. Consider now the graph obtained by reversing all the arrows leading from j to i; in this way we obtain a $\{j\}$-graph. Using the identity (175) the weight of this graph is equal to the weight of the original graph plus $G_j - G_i$. Taking the infimum over all graphs we obtain the identity

$$W^{(0)}(K_i) \;=\; W^{(0)}(K_j) + G_j - G_i\,, \quad (176)$$

and therefore we have

$$W^{(0)}(K_i) \;=\; G_i + \mathrm{const}\,, \tag{177}$$

and so

$$W^{(0)}(x) \;=\; \min_i (G_i + V^{(0)}(K_i, x)) - \min_j G_j\,. \tag{178}$$

The second term in Eq. (178) is equal to $\min_x G(x)$, since $G(x)$ is bounded below.

We now derive upper and lower bounds on the first term in Eq. (178). A lower bound follows easily from Proposition 1.7: For any path $\phi \in \mathcal{C}([0,T])$ with $\phi(0) = z \in K_i$ and $\phi(T) = x$ we obtain the inequality

$$I^{(0)}_{z,T}(\phi) \;=\; I^{(0)}_{Jx,T}(\tilde{\phi}) + G(x) - G_i \;\geq\; G(x) - G_i\,, \tag{179}$$

since the rate function is nonnegative. Taking infimum over all paths ϕ and time T we obtain

$$W^{(0)}(x) \;\geq\; G(x) - \min_x G(x)\,. \tag{180}$$

To prove the lower bound we consider the trajectory $\tilde{\phi}$ starting at Jx at time 0 which is the solution of the equation

$$\begin{aligned} \dot{q}_i &= \nabla_{p_i} G \qquad i = 1, \cdots, n\,, \\ \dot{p}_i &= -\nabla_{q_i} G \qquad i = 1, \cdots, n\,, \\ \dot{r}_i &= -\gamma\lambda^2 \nabla_{r_i} G \qquad i = 1, n\,. \end{aligned} \tag{181}$$

By Lemma 2.2, there is some K_j such that $\lim_{t\to\infty} \tilde{\phi}(t) \in K_j$. Furthermore, since $\tilde{\phi}$ is a solution of Eq. (181), the rate function of this path vanishes $I^{(0)}_{Jx,T}(\tilde{\phi}) = 0$, for any $T > 0$. Note that an infinite amount of time is needed to reach K_j in general. Now consider the time reversed path $\phi(t)$. It starts at $t = -T$ with $T \leq \infty$ at K_i and reaches x at time 0. For such a path we have

$$\lim_{T\to\infty} I^{(0)}_{z,T}(\phi) \;=\; \lim_{T\to\infty} I^{(0)}_{Jx}(\tilde{\phi}) + G(x) - G_i \;=\; G(x) - G_i\,, \tag{182}$$

and therefore

$$V^{(0)}(K_i, x) \;\leq\; G(x) - G_i\,. \tag{183}$$

We finally obtain

$$W^{(0)}(x) \;\leq\; G_i + V^{(0)}(K_i, x) - \min_x G(x) \;\leq\; G(x) - \min_x G(x) \tag{184}$$

and this concludes the proof of Proposition 4.1. ∎

We have the following bound on the rate function:

Lemma 4.2 *If $\eta \geq 0$ then for any $\phi \in \mathcal{C}([0,T])$,*

$$(1+\eta)^{-1} I_{x,T}^{(0)}(\phi) \;\leq\; I_{x,T}^{(\eta)}(\phi) \;\leq\; (1-\eta)^{-1} I_{x,T}^{(0)}(\phi)\,, \tag{185}$$

and a similar bound for $\eta \leq 0$.

Proof: The proof follows from the fact that the subset of $\mathcal{C}([0,T])$ on which $I_{x,T}^{(\eta)}(\phi) < \infty$ is independent of η. This is seen from the definition of rate function (24). Inspection of Eq. (160) implies the bound (185). ∎

From this we obtain immediately

Corollary 4.3 *If $\eta \geq 0$ then*

$$(1+\eta)^{-1}(G(x) - \min_x G(x)) \;\leq\; W^{(\eta)}(x) \;\leq\; (1-\eta)^{-1}(G(x) - \min_x G(x))\,. \tag{186}$$

and a similar bound for $\eta \leq 0$.

This concludes the proof of Theorem 1.4.

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References

[1] R. Azencott, Grandes deviations et applications. In *Ecole d'été de probabilités de Saint-Flour VIII-1978*, Lectures notes in mathematics 778, 2–176, Springer (1980).

[2] G. Ben Arous and R. Léandre, Décroissance exponentielle du noyau de la chaleur sur la diagonale. I and II. Probab. Theory Related Fields, **90**, 175–202, and 377–402 (1991).

[3] A. Dembo and O. Zeitouni, *Large deviations techniques and applications.* Applications of mathematics, Vol 38, Springer (1998).

[4] D. J. Evans, E. G. D. Cohen, and G. P. Morris, Probability of second law violations in shearing steady states. Phys. Rev. Lett. **71**, 2401–2404 (1993)

[5] M. Hairer and J.-P. Eckmann, Non-equilibrium statistical mechanics of strongly anharmonic chains of oscillators. Preprint, University of Geneva (1999).

[6] J.-P. Eckmann, C.-A. Pillet and L. Rey-Bellet, Non-equilibrium statistical mechanics of anharmonic chains coupled to two heat baths at different temperatures. Commun. Math. Phys., **201**, 657–697 (1999).

[7] J.-P. Eckmann, C.-A. Pillet and L. Rey-Bellet, Entropy production in non-linear, thermally driven Hamiltonian systems. J. Stat. Phys., **95**, 305–331 (1999).

[8] M.I. Freidlin and A.D. Wentzell, *Random perturbations of dynamical systems*. Grundlehren der mathematischen Wissenschaft 260, Springer (1984).

[9] G. Gallavotti and E. G. D. Cohen, Dynamical ensembles in stationary states. J. Stat. Phys. **80**, 931–970 (1995).

[10] R. Graham, Weak noise limit and nonequilibrium potentials of dissipative dynamical systems. In *Instabilities and nonequilibrium structures*, 271–290, Math. Appl., 33, Reidel (1987).

[11] R.Z. Has'minskii, *Stochastic stability of differential equations*. Sijthoff and Noordhoff (1980).

[12] L Hörmander, *The Analysis of linear partial differential operators*. Vol III, Springer (1985).

[13] C. Jarzynski, Hamiltonian derivation of a detailed fluctuation theorem. To appear in J. Stat. Phys.

[14] V. Jakšić and C.-A. Pillet, Ergodic properties of classical dissipative systems. I. Acta Math. **181** 245–282 (1998).

[15] W. Kliemann, Recurrence and invariant measures for degenerate diffusions. Ann. of Prob., **15**, 690–702 (1987).

[16] A. Komech, H. Spohn, and M. Kunze, Long-time asymptotics for a classical particle interacting with a scalar wave field. Comm. Partial Differential Equations **22** 307–335 (1997).

[17] J. Kurchan, Fluctuation theorem for stochastic dynamics. J. Phys. A **31**, 3719–3729 (1998).

[18] J. L. Lebowitz and H. Spohn, A Gallavotti-Cohen-type symmetry in the large deviation functional for stochastic dynamics. J. Stat. Phys., **95**, 333–365 (1999).

[19] E. B. Lee and L. Markus, *Foundations of optimal control theory.* The SIAM ser. in Appl. Math., Wiley (1967).

[20] C. Maes, The fluctuation theorem as a Gibbs property. J. Stat. Phys., **95**, 367–392 (1999).

[21] L. Rey-Bellet and L. E. Thomas, Energy decay estimates for Hamiltonian systems coupled to heat reservoirs. In preparation.

[22] M. Schilder, Some asymptotic formulae for Wiener integrals. Trans. Amer. Math. Soc. **125**, 63–85 (1966).

[23] H. J. Sussmann, Lie brackets, real analyticity and geometric control. In *Differential Geometric Control Theory, Proc. conf. Michigan*, 1–116 Birkäuser, (1983).

[24] D.W. Stroock and S.R.S. Varadhan, On the support of diffusion processes with applications to the strong maximum principle. In *Proc. 6-th Berkeley Symp. Math. Stat. Prob.*, vol III, 333–368 (1972).

[25] S.R.S. Varadhan, *Large Deviations and Applications.* SIAM, Philadelphia, (1984).