Communications in Mathematical Physics manuscript No.
(will be inserted by the editor)

Brownian Motion with Restoring Drift: Micro-canonical Ensemble and the Thermodynamic Limit

B. Rider

Mathematics Department, Duke University Durham, NC 27708. rider@math.duke.edu

The date of receipt and acceptance will be inserted by the editor

Abstract: We take up the old problem of micro-canonical conditioning in the context of diffusion. Starting with a potential $F : \mathbb{R}^d \to \mathbb{R}$, the Schrödinger operator $-\mathfrak{G}_0 = (1/2)\triangle - F$ with ground state ψ is carried by a conjugation into the diffusion generator $\mathfrak{G} = (1/2)\triangle + (\nabla\psi/\psi)\cdot\nabla$ with invariant density ψ^2. The latter motion $t \to X(t)$ is made micro-canonical by first conditioning the path to be periodic, $X(0) = X(L)$, and then further conditioning on the empirical mean-square or "particle number" $(1/L)\int_0^L |X(t)|^2 dt \simeq D$. The thermodynamics are then studied by taking $L \uparrow \infty$ while D remains fixed. The problem in this form owes its inception to McKean-Vaninsky [8] who obtained the following result. For $F(x)/|x|^2 \uparrow \infty$ with $|x| \uparrow \infty$, they showed the same type of diffusion appears in the thermodynamic limit, but with drift arising from the shifted potential $F + c|x|^2$, c being such that the limiting mean-square equals D. Their method of proof predicts the same outcome for $F(x)/|x|^2 \downarrow 0$, so long as D is smaller than the canonical mean-square $D_0 = \int_{\mathbb{R}^d} |x|^2\psi^2(x)dx$, while if $D > D_0$, the matter was unresolved. The purpose of this note is to show a type of phase transition takes place in this case: the conditioning is overcome in the limit and one sees the original (stationary) diffusion on the line. The proof employs an entropy inequality due to Csiszár [1].

1. Introduction

Consider the diffusion $t \to X(t) \in \mathbb{R}^d$ with infinitesimal operator

$$\mathfrak{G} = \frac{1}{2}\Big(\frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}\Big) + \frac{\nabla\psi(x)}{\psi(x)} \cdot \Big(\frac{\partial}{\partial x_1}, \cdots, \frac{\partial}{\partial x_d}\Big) = \frac{1}{2}\triangle + \frac{\nabla\psi}{\psi}\cdot\nabla \qquad (1)$$

where ψ is smooth and satisfies $\int_{\mathbb{R}^d} \psi^2(x)dx = 1$; it is the Brownian Motion plus restoring drift of the title. The corresponding Markovian measure on paths starting from $\bullet \in \mathbb{R}^d$ is denoted by $P_\bullet$. We are concerned with the *micro-canonical ensemble* obtained by first conditioning this motion to be periodic with periodicity L and then further conditioning it to remain near the sphere $\int_0^L |X(t)|^2 dt = LD$ with fixed positive D. The objective is to understand the *thermodynamic limit*, that is, what are the limiting processes on the line as $L \uparrow \infty$. The problem as stated was introduced by McKean-Vaninsky [8] in connection with the study of statistical mechanics for non-linear wave equations (see [7], [9], and also [6]).

To define the various ensembles, we first bring in the Schrödinger operator $\mathfrak{G}_0 = -(1/2)\Delta + F$ with $F = (1/2)\psi^{-1}\Delta\psi$ and ground state ψ. We assume throughout that $F(x) \uparrow \infty$ with $|x|$ so that $\mathfrak{G}_0$ has pure point spectrum: $\Lambda_0(\mathfrak{G}_0) < \Lambda_1(\mathfrak{G}_0) <$ etc $\uparrow \infty$. It is connected to $\mathfrak{G}$ through the conjugation $\psi\mathfrak{G}\psi^{-1} = -\mathfrak{G}_0 + \Lambda_0(\mathfrak{G}_0)$; this is one way to see that $P_\bullet$ is reversible with respect to $\psi^2(x)dx$, its stationary measure. Note that the growth rate of F at ∞ reflects the strength of the restoring drift.

Next, with $p(t,x,x')$ being the transition density for $P_\bullet$, the periodic ensemble $\mathbb{P}_L$ is defined by first conditioning on $X(0) = X(L)$ and then distributing this common starting/ending point according to the (finite) measure $p(L,x,x)dx$. In symbols this is[1]

$$E^{\mathbb{P}_L}[\phi(X)] = Z_L^{-1} \int_{\mathbb{R}^d} E_x\Big[\phi(X), X(L) = x\Big] dx$$

with the normalizer Z_L. By reversibility and our assumption on F the latter can be expressed as

$$Z_L = \int_{\mathbb{R}^d} p(L,x,x)\ dx = \sum_{n=0}^{\infty} e^{L\Lambda_n(\mathfrak{G})} = \sum_{n=0}^{\infty} e^{-L(\Lambda_n(\mathfrak{G}_0)-\Lambda_0(\mathfrak{G}_0))},$$

so that, not only is Z_L finite, but in fact $Z_L \simeq 1$ for $L \uparrow \infty$. The advantage of enforcing the periodicity in this way is that $\mathbb{P}_L$ is invariant under rotations of the circle as may be easily checked.

As to the micro-canonical ensemble, denoted by $\mathbb{M}_L$, we pick a fixed $\delta > 0$ and take $\mathbb{M}_L$ to be the measure on paths with partition function

$$\mathfrak{Z}_L = \int_{\mathbb{R}^d} E_x\Big[\int_0^L |X(t)|^2 dt \in L[D, D+\delta], X(L) = x\Big] dx, \tag{2}$$

from which you see what was meant by *near* the sphere $\int_0^L |X|^2 = LD$. We note that while [8] took the conditioning point-wise ($\delta = 0$), our method requires opening the ensemble up a bit, letting $\delta \downarrow 0$ after $L \uparrow \infty$.[2]

Now, $\mathbb{M}_L$ clearly inherits the rotation invariance of $\mathbb{P}_L$, and so to understand the thermodynamic limit it is enough to examine a rich enough class of short test functions of the path. That is, for some ϕ depending on $X(t')$ for $0 \le t' \le t < L$

[1] Throughout we use the useful notion $P[f(X) = x]$ and the like to indicate densities: $P[f(X) = x] = \partial/\partial z P[f(X) \le z]|_{z=x}$.

[2] One may even take $\delta \downarrow 0$ *with* $L \uparrow \infty$, but that changes nothing in the nature of the result.

only, the problem is to compute the micro-canonical mean value

$$\begin{aligned}\mathbb{M}_L[\phi] &= \mathfrak{Z}_L^{-1}\int_{\mathbb{R}^d} E_x\Big[\phi(X),\int_0^L |X(s)|^2 ds \in L[D,D+\delta], X(L)=x\Big]dx\\ &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_0^\infty dx dx' dI\ E_x\Big[\phi(X),\ \int_0^t |X(s)|^2 ds = I, X(t)=x'\Big]\\ &\quad\times \mathfrak{Z}_L^{-1} P_{x'}\Big[\int_0^{L-t}|X(s)|^2 ds \in L[D,D+\delta]-I, X(L-t)=x\Big] \quad (3)\end{aligned}$$

for $L\uparrow\infty$.

In their investigation, McKean-Vaninsky treated the case $d=1$ and developed a method best suited to "strong" potentials, $F(x)/|x|^2\uparrow\infty$ with $|x|$. Under that condition they showed that the limiting mean-value $\mathbb{M}_\infty[\phi]$ equals that for new (stationary) diffusion with generator $\mathfrak{G}^* = (1/2)\partial^2 + (\log\psi^*)'\partial$. Here ψ^* is the ground state for the Schrödinger operator with potential $F^*(x) = F(x) + c|x|^2$; the number c is adjusted so that $\mathbb{M}_\infty[|X|^2(0)] = \int_{-\infty}^{\infty}|x|^2[\psi^*(x)]^2 dx = D$. This shift from F to F^* is as predicted by *Gibbs' Principle of Equivalence of Ensembles.*

The key to their approach was that the growth condition on F permits the assumption that the conditioned value of D and the canonical mean-square $\int |x|^2\psi^2(x)dx$ are actually the same. Indeed, in that case the factor $e^{c\int_0^L X^2(t)dt}$ is integrable with respect to $P_\bullet$ for any c, and, if incorporated into the $P_\bullet$ mean as a density, allows one to arbitrarily raise/lower the mean-square by raising/lowering the constant c. Further, if $\delta=0$, that factor may be added above and below in (3) without any change to the overall $\mathbb{M}_L$ mean. Led by this observation McKean-Vaninsky proceeded in the spirit of Doeblin [3] to establish the local limit theorem

$$P_\bullet\Big[\int_0^L X^2(t)dt = LD,\ X(L)=x\Big]\sim L^{-1/2}\psi^2(x)\times[1+\mathrm{o}(1)] \quad \text{for} \quad L\uparrow\infty.$$

Formal substitution of this estimate in (3) explains their result.

But what happens when the shift to the "correct" mean-square cannot be made ahead of time? This is the case when, for example, the potential is "weak", $F(x)/|x|^2\to 0$, and $D > \int |x|^2\psi^2(x)dx$. Whatever the outcome, it *cannot* be described by a Gibbsian shift. Increasing the mean-square requires that $c>0$, but, as one may check, $E_\bullet[\exp(c\int_0^L |X(t)|^2 dt)] = +\infty$ for such F's. The answer is that there is a type of phase transition: the conditioning is overcome in the limit and you see the original (stationary) diffusion on the line. We will prove the following.

Theorem 1. *Let $\mathfrak{G}$ and $\mathfrak{G}_0$ be as above and set $D_0 = \int_{\mathbb{R}^d}|x|^2\psi^2(x)dx$. Our method is partial to potentials satisfying* $\limsup_{|x|\uparrow\infty} F(x)/|x|^2 < \infty$ *- otherwise [8] applies. There are two cases.*

(1) If either $\liminf_{|x|\uparrow\infty} F(x)/|x|^2 > 0$ *or $D < D_0$ then* $\lim_{\delta\downarrow 0}\lim_{L\uparrow\infty}\mathbb{M}_L = P^*_{[\psi^*]^2}$*, the stationary diffusion with generator $\mathfrak{G}^* = (1/2)\triangle + (\nabla\psi^*/\psi^*)\cdot\nabla$. Here ψ^* is the ground state for $\mathfrak{G}_0^* = \mathfrak{G}_0 + c|x|^2$ and is such that $E^*_{[\psi^*]^2}[|X|^2(0)] = D$.*

(2) If on the other hand $F(x) = o(|x|^2)$ in any cone tending to infinity and $D > D_0$ then $\lim_{\delta \downarrow 0} \lim_{L \uparrow \infty} \mathbb{M}_L = P_{\psi^2}$, the original motion taken stationary on the line.

In both cases the convergence takes place in entropy, and so in total variation, over short fields.

We will see that this transition is a consequence of heavy-tailed behavior: it occurs when the micro-canonical fiat is not a rare enough event to produce a shift, Gibbsian or otherwise, in the limit. Note the subtle dependence on the shape of F; the potential need only be "weak" along a given direction to result in a breaking between micro-canonically raising/lowering the mean-square.

The proof of Theorem 1 is anchored by an entropy inequality due to Csiszár [1], and we begin in Section 2 by describing his work on conditioned (micro-canonical) sequences of independent identically distributed variables. Here we also prepare the notion of relative entropy between a stationary process and a diffusion and prove various properties thereof. The bulk is contained in Section 3. There, the important Lemma 4 identifies the thermodynamic limit and is a version of Csiszár's inequality for diffusions. Along with this the proof of Theorem 1 is completed, the phase transition demonstrated through Lemma 5 which analyzes a variational problem stemming from the free energy of the $\mathbb{M}_L$ ensemble. Section 4 explains the connection to non-linear waves. As a final remark, Section 5 recasts the current work in terms of a parabolic Martin Boundary problem.

Remark 1. The choice of the mean-square is natural and keeps things concrete. The result of Theorem 1 is easily extended to $\mathbb{M}_L$ obtained by conditioning on other "energies."

2. Preliminaries

2.1. Csiszâr's Original Inequality. Conditional limit theorems of the type we are interested in have been widely studied for independent identically distributed variables. Probably the most far reaching results are those of Csiszár [1] whose ideas we borrow freely.

For any two probability measures μ and λ on a nice space X, let $H(\mu|\lambda)$ be the relative entropy of μ given λ: with $C(X)$ denoting the space of bounded continuous functions,

$$H(\mu|\lambda) = \inf\Big\{c : \int \phi(x)\mu(dx) \le c + \log \int e^{\phi(x)}\lambda(dx) \text{ for all } \phi \in C(X)\Big\}.$$

$H(\mu|\lambda)$ is nonnegative and convex as a function of μ. It is finite if and only if μ is absolutely continuous with respect to λ and $d\mu/d\lambda = f(x)$ satisfies $\int f(x)\log f(x)\lambda(dx) < \infty$, in which case $H(\mu|\lambda) = \int \log f(x)\mu(dx)$. Important here is the fact that relative entropy bounds total variation distance.

Next let $X_1, X_2, \dots$ be a sequence of say real valued independent random variables with common distribution P_X, and introduce the empirical distribution $L_n = \frac{1}{n}\sum_1^n \delta_{X_i}$. For a set $\Pi \subset M_1(\mathbb{R})$ – the space of probability measures on the real line – let $P_{X^n|\Pi}$ be the distribution of the sequence $X_k : k \le n$ conditional on $L_n \in \Pi$. The remarkable observation of Csiszár is the following.[3]

[3] This is but an instance Csiszár's Theorem 1 [1] – his technical setup is more elaborate.

Let Π be a convex subset of $M_1(\mathbb{R})$ with $P(L_n \in \Pi) > 0$. Also let P_* be the minimizer: $\inf_{P\in\Pi} H(P|P_X) = H(P_*|P_X)$ *which may be shown to exist. Then*

$$\frac{1}{n}H(P_{X^n|\Pi}|P_*^n) \leq -\frac{1}{n}\log P(L_n \in \Pi) - H(P^*|P_X).$$

Now for any $\mu \in M_1(\mathbb{R}^n)$ and $\lambda \in M_1(\mathbb{R})$, one has $\sum_{i=1}^n H(\mu_i|\lambda) \leq H(\mu|\lambda^n)$, in which μ_i denotes the marginal of μ on the i-th co-ordinate. Using the exchangeable nature of the conditioned variables, Csiszár concludes that

$$H(P_{X^1|\Pi}|P_*) \leq -\frac{1}{n}\log P(L_n \in \Pi) - H(P_*|P_X). \tag{4}$$

The point being that the distance between the conditioned distribution and the entropy minimizer is controlled by an object to which Large Deviation theory - in particular Sanov's Theorem - applies. Indeed, convergence of the free energy to its anticipated value implies convergence of the conditional distribution of X_1 to P_* in entropy and so also in total variation.

The proof of Csiszár's inequality (4) is based on a "triangle inequality" for relative entropies, also proved in [1]: if P^* minimizes $H(\cdot|P)$ over the convex set Π, then

$$H(Q|P) \geq H(Q|P_*) + H(P_*|P) \quad \text{for all } Q \in \Pi; \tag{5}$$

the geometric picture being that if $H(\cdot|\cdot)$ tries to be a squared distance, then the angle between the lines connecting Q to P and Q to P^* is acute.

Csiszár's setup has been extended to discrete parameter Markov Chains by Schroeder [14] and Dembo-Zeitouni [2].

2.2. Technicalities. For us the the chain of iid variables above is replaced by the diffusion X with generator $\mathfrak{G} = (1/2)\Delta + (\nabla\psi/\psi)\cdot\nabla$ conditional on $X(0) = X(L)$ and $\int_0^L |X|^2(t)dt \in L[D, D+\delta]$. It is a point of good fortune that the joint motion $t \to [X(t), I(t) = \int_0^t |X(s)|^2 ds]$ is also a diffusion with generator $\mathfrak{G}_+ = \mathfrak{G} + |x|^2\partial/\partial I$. While the latter is degenerate in that $\partial^2/\partial I^2$ is missing from the top, a theorem of Hörmander shows that $\mathfrak{G}_+$ is "hypo-elliptic," *i.e.*, the joint density $P_x[X(t) = x', \int_0^t |X(s)|^2 ds = I]$ is smooth in all its variables and also positive, provided only that $t, I > 0$.[4] Thus, we also have a smooth positive density function for the micro-canonical marginal $\mathbb{M}_L[X(\cdot) \in dx] = m_L(x)dx$:

$$m_L(x) = \mathfrak{Z}_L^{-1}\int_{L[D,D+\delta]} P_x\Big[X(L) = x, \int_0^L |X(t)|^2 dt = N\Big]dN,$$

a small technical point that will be useful in what follows.

Next, in the diffusion format, the Donsker-Varadhan I-function will play the role of relative entropy; we review a few definitions. For our reversible operator $\mathfrak{G}$, the I-function takes the particularly nice form: with $\mu(dx) = f^2(x)dx$ a probability measure on $\mathbb{R}^d$,

$$I(\mu : \mathfrak{G}) = \frac{1}{2}\int_{\mathbb{R}^d} |\nabla f|^2 dx + \int_{\mathbb{R}^d} \frac{\Delta\psi}{2\psi} f^2 dx.$$

---

[4] Krylov [5] explains such matters. Replacing $|x|^2$ with a more general energy $U(x)$ is amenable to the same theory provided U has no zero of infinite order.

The importance of the I-function lies in that it controls the large deviations of $\mathfrak{L}(t,X)(dx) = (1/t)\int_0^t 1_{X(s)\in dx} ds$, the occupation measure of the process. To wit, Donsker and Varadhan [4] have proved that:

$$\liminf_{L\to\infty} \frac{1}{L} \log P_\bullet(\mathfrak{L}(L,X) \in G) \geq -\inf_{\mu\in G} I(\mu : \mathfrak{G}) \quad \text{for open sets } G \subset M_1(\mathbb{R}^d)$$

and

$$\limsup_{L\to\infty} \frac{1}{x} \log P_\bullet(\mathfrak{L}(L,X) \in F) \leq -\inf_{\mu\in F} I(\mu : \mathfrak{G}) \quad \text{for closed sets } F \subset M_1(\mathbb{R}^d),$$

with $I(\mu : \mathfrak{G}) = 0$ if and only if μ is the invariant measure of the process. The relevance here, of course, is that our micro-canonical event $\int_0^L |X(t)|^2 dt \simeq LD$ may be written $\int_{\mathbb{R}^d} |x|^2 \mathfrak{L}(L,X)(dx) \simeq D$.

Finally, as the convergence of the micro-canonical ensemble will be shown to hold in entropy, properties of the relative entropy between a diffusion P and a stationary process M are now described. In these computations, the initial point of the diffusion is distributed according to the marginal of M. Lemma 1 shows that entropy defined in this manner is super-additive; Lemma 2 relates it the I-function. In both $t \to \omega(t)$ denotes the generic path.

Lemma 1. *If M is a stationary processes with marginal $M[\omega(0) \in dx] = m(dx)$ and $P_\bullet$ is a diffusion, then the relative entropy $H_{\mathfrak{F}_0^t}(M|P_m)$ is super-additive in t: for $0 \leq t' \leq t$,*

$$H_{\mathfrak{F}_0^{t'}}(M|P_m) + H_{\mathfrak{F}_0^{t-t'}}(M|P_m) \leq H_{\mathfrak{F}_0^t}(M|P_m).$$

Proof. It is well known that entropy increases over fields, that is, we have the identity

$$H_{\mathfrak{F}_0^t}(M|P_m) = H_{\mathfrak{F}_0^{t'}}(M|P_m) + E^M\left[H_{\mathfrak{F}_0^t}(M_{(\omega,t')}|P_{m,(\omega,t')})\right].$$

Here $M_{(\omega,t')}$ is the regular conditional probability distribution of M given $\mathfrak{F}_0^{t'}$ and likewise for P_m. The paths of $M_{(\omega,t')}$, $P_{m,(\omega,t')}$ agree on $\mathfrak{F}_0^{t'}$. This, together with the stationarity of M and the Markov property of P, imply

$$H_{\mathfrak{F}_0^t}(M_{(\omega,t')}|M_{m,(\omega,t')}) = H_{\mathfrak{F}_{t'}^t}(M_{(\omega,t')}|P_{\omega(t')}) = \sup_\phi\left\{E^{M_{(\omega,t')}}[\phi] - \log E^{P_{\omega(t')}}[e^\phi]\right\},$$

the supremum being taken over all continuous functions $\phi : \omega \to R$ which are measurable over the field $\mathfrak{F}_{t'}^t$. However, for any such ϕ,

$$E^M[\phi] = E^M\left[E^{M_{(\omega,t')}}[\phi]\right] \leq E^M\left[H_{\mathfrak{F}_{t'}^t}(M_{(\omega,x)}|P_{m,(\omega,t')}) + \log E^{P_{\omega(t')}}[e^\phi]\right],$$

and so

$$\begin{aligned} E^M\left[H_{\mathfrak{F}_0^t}(M_{(\omega,t')}|P_{m,(\omega,t')})\right] &\geq \sup_\phi\left\{E^M[\phi] - E^M\left[\log E^{P_{\omega(t')}}[e^\phi]\right]\right\} \\ &\geq \sup_\phi\left\{E^M[\phi] - \log E^{P_m}[e^\phi]\right\} = H_{\mathfrak{F}_0^{t-t'}}(M|P_m). \end{aligned}$$

Jensen's inequality and the stationarity of M are used in the second line. The proof is finished.

Lemma 2. *Now let M be a stationary process whose marginal distribution has positive C^1 density function with respect to Lebesgue measure, $M\big[\omega(t) \in dx\big] = m(x)dx$. Further, let $\hat{P}_\bullet$ be the diffusion process generated by $\hat{\mathfrak{G}} = (1/2)\triangle + (\nabla\sqrt{m}/\sqrt{m}) \cdot \nabla$. If, as before, $P_\bullet$ corresponds to the generator $\mathfrak{G} = (1/2)\triangle + (\nabla\psi/\psi) \cdot \nabla$, then*

$$tI(m : \mathfrak{G}) = H_{\mathcal{F}_0^t}(M|P_m) - H_{\mathcal{F}_0^t}(M|\hat{P}_m).$$

Proof. $P_\bullet$ and $\hat{P}_\bullet$ are mutually absolutely continuous over short fields, and P_m and $\hat{P}_m$ inherit this feature. It follows that

$$H_{\mathcal{F}_0^t}(M|P_m) = H_{\mathcal{F}_0^t}(M|\hat{P}_m) + E^M\Big[\log\Big\{\frac{d\hat{P}_m}{dP_m}\Big|_{\mathcal{F}_0^t}\Big\}\Big].$$

Now the claim will follow from evaluating the second term on the right as $tI(m : \mathfrak{G})$. To see this, take Brownian Motion ($BM_\bullet$) as reference measure and use the Cameron-Martin formula to express

$$\frac{d\hat{P}_m}{dP_m}\Big|_{\mathcal{F}_0^t} = \frac{\frac{d\hat{P}_m}{dBM_\bullet}}{\frac{dP_m}{dBM_\bullet}}\Big|_{\mathcal{F}_0^t} = \frac{\exp\Big[\int_0^t \frac{\nabla\sqrt{m}}{\sqrt{m}}(\omega(t')) \cdot d\omega(t') - \frac{1}{2}\int_0^t\Big|\frac{\nabla\sqrt{m}}{\sqrt{m}}\Big|^2(\omega(t'))dt'\Big]}{\exp\Big[\int_0^t \frac{\nabla\psi}{\psi}(\omega(t')) \cdot d\omega(t') - \frac{1}{2}\int_0^t\Big|\frac{\nabla\psi}{\psi}\Big|^2(\omega(t'))dt'\Big]}.$$

An application of Itô's Lemma yields

$$\begin{aligned}\frac{d\hat{P}_m}{dP_m}\Big|_{\mathcal{F}_0^t} = \exp\Big[&\log\frac{m(\omega(t))}{m(\omega(0))} - \log\frac{\psi(\omega(t))}{\psi(\omega(0))} \\ &+\frac{1}{2}\int_0^t \frac{\triangle\psi}{\psi}(\omega(t'))dt' - \frac{1}{2}\int_0^t \frac{\triangle\sqrt{m}}{\sqrt{m}}(\omega(t'))dt'\Big].\end{aligned}$$

After taking logarithms and then expectation under the M-measure of the right hand side, you will see that the first two terms in the exponent vanish by the stationarity of M. What remains is

$$\begin{aligned}E^M\left[\log\Big\{\frac{d\hat{P}_m}{dP_m}\Big|_{\mathcal{F}_0^t}\Big\}\right] &= E^M\left[\frac{1}{2}\int_0^t\Big\{\frac{\triangle\psi}{\psi}(\omega(t')) - \frac{\triangle\sqrt{m}}{\sqrt{m}}(\omega(t'))\Big\}dt'\right] \\ &= t\int_{\mathbb{R}^d}\Big\{\frac{\triangle\psi}{2\psi}(x) - \frac{\triangle\sqrt{m}}{2\sqrt{m}}(x)\Big\}m(x)dx \\ &= t\Big\{\frac{1}{2}\int_{\mathbb{R}^d}|\nabla\sqrt{m}|^2dx + \int_{\mathbb{R}^d}\frac{\triangle\psi}{2\psi}m(x)dx\Big\} = tI(m : \mathfrak{G}),\end{aligned}$$

where the second line is justified by Fubini and another application of the stationarity of M. The proof is finished.

Remark 2. In the applications to follow, the stationary process M will be our periodic or micro-canonical diffusion. The statements of Lemmas 1 and 2 remain valid in this case so long as the periodicity L exceeds t.

3. The Thermodynamic Limit

The intuition is as follows. We know at least that $\mathbb{M}_\infty$ is stationary. Supposing it is also Markovian there is an obvious program before you. Minimizing the I-function over the micro-canonical set produces some measure $\mu^*(dx) = [\psi^*(x)]^2 dx$ which should serve as the marginal for the limiting $P_\bullet^*$. To pin down the full limit, one notes that as it must be absolutely continuous to $P_\bullet$ over short fields (their relative entropy being finite), its generator takes the form $\mathfrak{G}^* = (1/2)\triangle + b \cdot \nabla$. For $d = 1$, $P_\bullet^*$ would now be determined. The scale and speed measures, which uniquely characterize the process, satisfy:

$$\frac{scale(dx)}{dx} = \exp\left\{-2\int_0^x b(x')dx'\right\} \quad \text{and} \quad \frac{speed(dx)}{dx} = \exp\left\{2\int_0^x b(x')dx'\right\},$$

the latter being $[\psi^*]^2$ up to a normalizer, *i.e.*, $b = (\log \psi^*)'$. For $d > 1$, one may only say $0 = (\mathfrak{G}^*)^\dagger [\psi^*]^2 = (1/2)\triangle[\psi^*]^2 - \nabla(b[\psi^*]^2)$, and, while $b = \nabla \log \psi^*$ is a solution, there is no uniqueness. However, as one would expect, this is the limit identified below.

3.1. The entropy bound. To carry out the above, we develop a version of Csiszár's Inequality (4) for (reversible) diffusions - Lemma 4 below. This in turn relies on Lemma 3, the "triangle inequality" for I-functions; compare (5).

Now, as these are both rather generic tools, we state them in a slightly broader context than needed in the present. An entire class of micro-canonical ensembles may be derived by restricting $\mathbb{P}_L$ to the those paths satisfying $\mathfrak{L}(L, X) \in \Pi \subset M_1(\mathbb{R}^d)$ - our choice of $\int_0^L |X(t)|^2 dt \in L[D, D+\delta]$ is but an example. Lemmas 3 and 4 require only that (1) Π is convex and (2) that $\mathbb{P}_L(\mathfrak{L}(L, X) \in \Pi) > 0$.

Lemma 3. *Given the generator $\mathfrak{G} = (1/2)\triangle + (\nabla\psi/\psi)\cdot\nabla$ with smooth invariant density ψ^2, let μ^* minimize $I(\nu : \mathfrak{G})$ over the convex set Π:*

$$I(\Pi : \mathfrak{G}) = \inf_{\nu \in \Pi} I(\nu : \mathfrak{G}) = I(\mu^* : \mathfrak{G}).$$

This is useless if $I(\mu^* : \mathfrak{G}) = +\infty$. If $I(\mu^* : \mathfrak{G}) < \infty$, then μ^* has a density $[\psi^*]^2$ such that $\psi^* \in W^{1,2}(\mathbb{R}^d)$ (see [4]), and one may define the generator $\mathfrak{G}^* = (1/2)\triangle + (\nabla\psi^*/\psi^*)\cdot\nabla$ with invariant measure μ^*. The processes corresponding to $\mathfrak{G}$ and $\mathfrak{G}^*$ are mutually absolutely continuous over short fields, and for any $\nu \in \Pi$,

$$I(\nu : \mathfrak{G}) \geq I(\nu : \mathfrak{G}^*) + I(\mu^* : \mathfrak{G}).$$

Proof. Let $\nu \in \Pi$ satisfy $I(\nu : \mathfrak{G}) < \infty$. This implies that ν is absolutely continuous with respect to μ and has density φ^2 with $\varphi \in W^{1,2}(\mathbb{R}^d)$. Consider

$$H(\varepsilon) = I(\varepsilon\nu + (1-\varepsilon)\mu^* : \mathfrak{G})$$

for $0 \leq \epsilon \leq 1$. By the convexity of the I-function, $H(\varepsilon)$ is a (bounded) convex function of ε. Since

$$I(\mu^* : \mathfrak{G}) \leq I(\varepsilon\nu + (1-\varepsilon)\mu^* : \mathfrak{G}) = I(\varepsilon\varphi^2 + (1-\varepsilon)\psi^2 : \mathfrak{G}),$$

$H(\varepsilon)$ is a non-decreasing function of ϵ. Thus

$$H^{+}(0) = \lim_{\varepsilon \to 0} \frac{d}{d\varepsilon}\, I(\varepsilon\nu + (1-\varepsilon)\mu^{*} : \mathfrak{G}) \geq 0,$$

the existence of the limit being automatic.

The proof of the inequality follows Csiszár quite closely. One starts from the obvious

$$I(\nu : \mathfrak{G}) - I(\mu^{*} : \mathfrak{G}) \geq I(\nu : \mathfrak{G}) - I(\mu^{*} : \mathfrak{G}) - \frac{1}{\varepsilon}\Big[H(\varepsilon) - H(0)\Big], \qquad (6)$$

holding for all $\epsilon > 0$. The limit $\epsilon \downarrow 0$ is then taken, and the lemma is proved by means of the evaluation

$$H^{+}(0) = I(\nu : \mathfrak{G}) - I(\nu : \mathfrak{G}^{*}) - I(\mu^{*} : \mathfrak{G}).$$

It is convenient to introduce the notation $\nu_\varepsilon = \varepsilon\nu + (1-\varepsilon)\mu^{*}$ and

$$f_\varepsilon = \frac{d\nu_\varepsilon}{d\mu} = \epsilon\frac{d\nu}{d\mu} + (1-\varepsilon)\frac{d\mu^{*}}{d\mu} = \varepsilon\frac{\varphi^2}{\psi^2} + (1-\varepsilon)\frac{\psi^{*2}}{\psi^2} \equiv \varepsilon f_1 + (1-\varepsilon) f_0.$$

Note that $\sqrt{f_\varepsilon} \in W^{1,2}$. Then

$$H(\varepsilon) = \int_{\mathbb{R}^d} \sqrt{f_\varepsilon}\, \left(-\mathfrak{G}\sqrt{f_\varepsilon}\right)\, d\mu = \int_{\mathbb{R}^d} |\nabla\sqrt{f_\varepsilon}|^2\, d\mu$$

and so, if the differentiation could be passed inside the last integral, the conclusion would be

$$H^{+}(0) = \frac{1}{8}\int_{\mathbb{R}^d} \frac{d}{d\varepsilon}\left[\frac{|\nabla f_\varepsilon|^2}{f_\varepsilon}\right]_{\varepsilon=0} d\mu = \frac{1}{4}\int_{\mathbb{R}^d}\left[\left(\frac{\nabla f_\varepsilon}{\sqrt{f_\varepsilon}}\right)\frac{d}{d\varepsilon}\left(\frac{\nabla f_\varepsilon}{\sqrt{f_\varepsilon}}\right)\right]_{\varepsilon=0} d\mu. \quad (7)$$

To see that this is the case, consider the limit of $\varepsilon^{-1}\big[H(\varepsilon) - H(0)\big]$ in conjunction with the whole right hand side of (6). Setting $H(\varepsilon) = \int h(\varepsilon, x)d\mu(x)$, we write in which $h(\varepsilon, x) = (1/2)|\nabla\sqrt{f_\varepsilon}(x)|^2$. Then

$$\begin{aligned}
&I(\nu : \mathfrak{G}) - I(\mu^{*} : \mathfrak{G}) - \frac{1}{\varepsilon}\left(H(\varepsilon) - H(0)\right) \\
&= \frac{1}{2}\int_{\mathbb{R}^d} |\nabla\sqrt{f_1}|^2\, d\mu(x) - \frac{1}{2}\int_{\mathbb{R}^d} |\nabla\sqrt{f_0}|^2\, d\mu(x) - \frac{1}{\varepsilon}\big[H(\varepsilon) - H(0)\big] \\
&= \int_{\mathbb{R}^d} \left\{h(1,x) - h(0,x) - \frac{1}{\varepsilon}\Big[h(\varepsilon,x) - h(0,x)\Big]\right\}\, d\mu(x).
\end{aligned}$$

The advantage of this being, of course, that, for each x, $\varepsilon \to h(\varepsilon, x) = (1/2)|\nabla\sqrt{f_\varepsilon}(x)|^2$ is convex on $(0, 1]$. It follows that

$$h(1,x) - h(0,x) - \frac{1}{\varepsilon}\Big[h(\varepsilon,x) - h(0,x)\Big]$$

is monotone non-decreasing, and the manipulation inherent in (7) holds by monotone convergence. Now, since

$$\frac{d}{d\varepsilon}\left[\frac{\nabla f_\varepsilon}{\sqrt{f_\varepsilon}}\right] = \frac{\nabla f_1 - \nabla f_0}{\sqrt{\varepsilon f_1 + (1-\varepsilon) f_0}} - \frac{1}{2}\,\frac{\varepsilon \nabla f_1 + (1-\varepsilon)\nabla f_0}{(\varepsilon f_1 + (1-\varepsilon) f_0)^{3/2}}\,(f_1 - f_0)$$
$$= \frac{\nabla f_1 - \nabla f_0}{\sqrt{f_0}} - \frac{1}{2}\frac{\nabla f_0}{\sqrt{f_0}}\,\left(\frac{f_1 - f_0}{f_0}\right)$$

at $\varepsilon = 0$, we have that

$$\frac{d}{d\varepsilon}\,\left(|\nabla\sqrt{f_\varepsilon}|^2\right)\Big|_{\varepsilon=0} = \frac{1}{2}\nabla\left(\frac{f_1 - f_0}{\sqrt{f_0}}\right)\nabla\sqrt{f_0},$$

and so also,

$$H^+(0) = \int_{\mathbb{R}^d} \frac{f_1 - f_0}{\sqrt{f_0}}(-\mathfrak{G}\sqrt{f_0})\;d\mu = \int_{\mathbb{R}^d}(f_1 - f_0)(-\mathfrak{G}^{\sqrt{f_0}}1)\;d\mu.$$

In the rightmost expression of the last display the $\sqrt{f_0}$ upstairs refers to the conjugate or "h-transform" of $\mathfrak{G}$ defined by

$$\mathfrak{G}^{\sqrt{f_0}} = \frac{1}{\sqrt{f_0}}\mathfrak{G}\sqrt{f_0} = \mathfrak{G} + \frac{\nabla f_0}{f_0}\cdot\nabla + \frac{\mathfrak{G} f_0}{f_0} = \mathfrak{G}^* + \frac{1}{2}\left(\frac{\triangle\psi^*}{\psi^*} - \frac{\triangle\psi}{\psi}\right).$$

The proof is then finished by

$$\begin{aligned}
&I(\nu : \mathfrak{G}) - I(\mu^* : \mathfrak{G}) - H^+(0)\\
&= \int_{\mathbb{R}^d}\sqrt{f_1}(-\mathfrak{G}\sqrt{f_1})\;d\mu - \int_{\mathbb{R}^d}\sqrt{f_0}\,(-\mathfrak{G})\,\sqrt{f_0}\;d\mu\\
&\qquad - \int_{\mathbb{R}^d}(f_1 - f_0)(-\mathfrak{G}^{\sqrt{f_0}}(1))\;d\mu\\
&= \int_{\mathbb{R}^d}\sqrt{f_1 f_0}\left(-\mathfrak{G}^{\sqrt{f_0}}\right)\frac{\sqrt{f_1}}{\sqrt{f_0}}\;d\mu - \int_{\mathbb{R}^d} f_1(-\mathfrak{G}^{\sqrt{f_0}}(1))\;d\mu\\
&= \int_{\mathbb{R}^d}\frac{\sqrt{f_1}}{\sqrt{f_0}}(-\mathfrak{G}^{\sqrt{f_0}})\frac{\sqrt{f_1}}{\sqrt{f_0}}\;d\mu^* - \int_{\mathbb{R}^d}\frac{f_1}{f_0}(-\mathfrak{G}^{\sqrt{f_0}})(1)\;d\mu^*\\
&= \int_{\mathbb{R}^d}\left[\frac{\sqrt{f_1}}{\sqrt{f_0}}(-\mathfrak{G}^*)\frac{\sqrt{f_1}}{\sqrt{f_0}} - \frac{f_1}{f_0}\left(\frac{\mathfrak{G}\sqrt{f_0}}{\sqrt{f_0}}\right)\right]\;d\mu^*\\
&\qquad - \int_{\mathbb{R}^d}\left[\frac{f_1}{f_0}\left((-\mathfrak{G}^*(1))\;-\frac{\mathfrak{G}\sqrt{f_0}}{\sqrt{f_0}}\right)\right]\;d\mu^*\\
&= \int_{\mathbb{R}^d}\frac{\sqrt{f_1}}{\sqrt{f_0}}(-\mathfrak{G}^{\sqrt{f_0}})\frac{\sqrt{f_1}}{\sqrt{f_0}}\;d\mu^* = \int_{\mathbb{R}^d}\sqrt{\frac{\psi}{\varphi}}(-\mathfrak{G}^*)\sqrt{\frac{\psi}{\varphi}}\;d\mu^* = I(\nu : \mathfrak{G}^*),
\end{aligned}$$

as advertised.

Lemma 4. *Assume the convex set Π satisfies $I(\Pi : \mathfrak{G}) = I(\mu^* : \mathfrak{G}) < \infty$ and that μ^* admits a nice (C^1, positive) density. Further assume that the micro-canonical marginal $\mathbb{M}_L[X(\cdot) \in dx] = \mathbb{P}_L[X(\cdot) \in dx | \mathcal{L}(L, X) \in \Pi]$ has a C^1 positive density. Then, for fixed $t < L$,*

$$H_{\mathcal{F}_0^t}(\mathbb{M}_L | P^*_{m_L}) \leq \frac{Lt}{L-1}\left[-\frac{1}{L}\log \mathbb{P}_L(\mathcal{L}(L,X) \in \Pi) - \frac{L-1}{L} I(\mu^* : \mathfrak{G}) \right.$$
$$\left. -\frac{1}{L}\mathbb{M}_L\left[\log\left\{\frac{dP_{m_L}}{d\mathbb{P}_L}\Big|_{\mathcal{F}_0^{L-1}}\right\}\right]\right]. \tag{8}$$

Proof. Since $\mathbb{M}_L(\Gamma) = \mathbb{P}_L(\Gamma \cup \mathcal{L}(L,X) \in \Pi)/\mathbb{P}_L(\mathcal{L}(L,X) \in \Pi)$, it follows that $\mathbb{M}_L$ is absolutely continuous with respect to $\mathbb{P}_L$ and that

$$H_{\mathcal{F}_0^L}(\mathbb{M}_L | \mathbb{P}_L) = -\log \mathbb{P}_L(\mathcal{L}(L,X) \in \Pi) < \infty.$$

As entropy increases with the field,

$$-\log \mathbb{P}_L(\mathcal{L}(L,X) \in \Pi) \geq H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | \mathbb{P}_L)$$
$$= H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | P_{m_L}) + \mathbb{M}_L\left[\log\left\{\frac{dP_{m_L}}{d\mathbb{P}_L}\Big|_{\mathcal{F}_0^{L-1}}\right\}\right]$$

where $m_L(dx) = \mathbb{M}_L\big[X(0) \in dx\big]$, the assumed positivity of the corresponding density makes the last line have a sense.

The rotation invariance of $\mathbb{M}_L$ then allows an application of Lemma 2 for short fields $\mathcal{F}_0^{L'}$ with $L' < L$ and $\hat{P}_\bullet$ the diffusion generated by $\hat{\mathfrak{G}} = (1/2)\triangle + (\nabla m_L / m_L) \cdot \nabla$. The outcome is,

$$H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | P_{m_L}) = H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | \hat{P}_{m_L}) + (L-1)\ I(m_L : \mathfrak{G});$$

in particular, the right hand side is finite as $\mathbb{P}_L(\mathcal{L}(L,X) \in \Pi) > 0$. Thus, you may also write

$$-\log \mathbb{P}_L(\mathcal{L}(L,X) \in \Pi)$$
$$\geq H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | \hat{P}_{m_L}) + (L-1) I(m_L : \mathfrak{G}) + \mathbb{M}_L\left[\log\left\{\frac{dP_{m_L}}{d\mathbb{P}_L}\Big|_{\mathcal{F}_0^{L-1}}\right\}\right]. \tag{9}$$

Next, apply Lemma 2 once more to give

$$H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | P^*_{m_L}) = H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | \hat{P}_{m_L}) + (L-1)\ I(m_L : \mathfrak{G}^*) \tag{10}$$

where both the first and third term may, perhaps, be infinite. To see that is not so, first notice that by the rotation invariance of $\mathbb{M}_L$ the marginal m_L is contained in the (convex) set Π for each $L < \infty$. An application the triangle inequality of Lemma 3,

$$I(m_L : \mathfrak{G}) \geq I(m_L : \mathfrak{G}^*) + I(\mu^* : \mathfrak{G}), \tag{11}$$

then shows that $I(m_L : \mathfrak{G}^*)$ is finite. Substitution of (10) into (9) produces

$$-\log \mathbb{P}_L(\mathcal{L}(L,X) \in \Pi) \geq H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | P^*_{m_L})$$
$$+(L-1)\big[I(m_L : \mathfrak{G}) - I(m_L : \mathfrak{G}^*)\big] + \mathbb{M}_L\left[\log\left\{\frac{dP_{m_L}}{d\mathbb{P}_L}\Big|_{\mathcal{F}_0^{L-1}}\right\}\right],$$

which, together with (11), gives you

$$\frac{1}{L} H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | P^*_{m_L})$$
$$\leq -\frac{1}{L} \log \mathbb{P}_L(\mathcal{L}(L, X) \in \Pi) - \frac{L-1}{L} I(\mu^* : \mathfrak{G}) - \frac{1}{L} \mathbb{M}_L \left[\log \left\{ \frac{dP_{m_L}}{d\mathbb{P}_L} \Big|_{\mathcal{F}_0^{L-1}} \right\} \right].$$

Finally, by the super-additive property established in Lemma 1, $H_{\mathcal{F}_0^{L-1}}(\mathbb{M}_L | P^*_{m_L}) \geq (L-1)/t H_{\mathcal{F}_0^t}(\mathbb{M}_L | P^*_{m_L})$. The proof is finished.

3.2. Identifying the Limit. The proof of Theorem 1 may now be completed; it follows from Lemma 4 and a few quick checks. Note that with the micro-canonical fiat taken $\int_0^L |X(t)|^2 dt \in L[D, D+\delta]$ the assumptions of the lemma (smoothness of the micro-canonical marginal densities etc.) are satisfied due to the discussion of Section 2.2.

The point is that convergence of the right hand side of (8) to zero as $L \uparrow \infty$ implies the desired result of the convergence of the micro-canonical ensemble $\mathbb{M}_L$ in entropy over short fields to the diffusion P^* with generator

$$\mathfrak{G}^* = \frac{1}{2}\triangle + \frac{\nabla \psi^*}{\psi^*} \cdot \nabla \tag{12}$$

in which ψ^* is the square-root of the minimizing density - $\mu^*(dx) = [\psi^*(x)]^2 dx$ - for the variational problem

$$I(\mu^* : \mathfrak{G}) = \lim_{\delta \downarrow 0} \inf_{\int |x|^2 \nu(dx) \in [D, D+\delta]} I(\nu : \mathfrak{G}). \tag{13}$$

There are two limits to be established. The first, which encodes the identification of $M_\infty = P^*$,

$$\lim_{\delta \downarrow 0} \liminf_{L \to \infty} \frac{1}{L} \log \mathbb{P}_L \Big[\int_0^L |X|^2(t) dt \in L[D, D+\delta] \Big] \geq -I(\mu^* : \mathfrak{G}),$$

is an application of the work of Donsker-Varadhan (see, for example, [11]), and we omit the proof. Then there is the "error term": we need

$$\liminf_{L \to \infty} \frac{1}{L} \mathbb{M}_L \left[\log \left\{ \frac{dP_{m_L}}{d\mathbb{P}_L} \Big|_{\mathcal{F}_0^{L-1}} \right\} \right] \geq 0. \tag{14}$$

This is treated in Lemma 6 below. First however, we turn to the particulars of the phase transition. This manifests itself in the limiting drift through the variational problem (13). We have the following.

Lemma 5. *Let $F(x)$ be continuous and tending to ∞ with $|x|$. Define*

$$I_F(f) = \frac{1}{8} \int_{\mathbb{R}^d} \frac{|\nabla f(x)|^2}{f(x)} dx + \int_{\mathbb{R}^d} F(x) f(x) dx.$$

The infimum of $I_F(f)$ for $\int f(x)dx = 1$ is achieved at a unique strictly positive f_0, $\sqrt{f_0}$ being the ground state for $\mathfrak{G}_0 = -(1/2)\triangle + F$.

Next let $D_0 = \int_{\mathbb{R}^d} |x|^2 f_0(x)dx$. *To understand (13) is to examine*

$$\mathfrak{I}_F(D) = \inf\Big\{ I_F(f) : \int_{\mathbb{R}^d} f(x)dx = 1 \int_{\mathbb{R}^d} |x|^2 f(x)dx = D \Big\};$$

there are two cases.

(1) *If either* $D < D_0$ *or if the growth of* F *is fast enough* $(\liminf_{|x|\uparrow\infty} F(x)/|x|^2 > 0)$, *then the infimum* $\mathfrak{I}_F(D)$ *is achieved at a unique nonnegative* f_* *such that* $\int_{\mathbb{R}^d} |x|^2 f_*(x)dx = D$ *and there exists a constant* $c = c(D)$ *such that* $\sqrt{f_*}$ *is ground state for the adjusted operator* $\mathfrak{G}_0^* = -(1/2)\triangle + F(x) + c|x|^2$.

(2) *If, on the other hand,* $D \geq D_0$ *and* $F(x)/|x|^2 \to 0$ *for* $|x| \uparrow \infty$ *in some cone, then* $\mathfrak{I}_F(D) = \mathfrak{I}_F(D_0)$ *with minimizer* $f_* = f_0$.

Remark 3. This describes the limiting drift in (12): $\psi^* = \sqrt{f_*}$.

Proof. (1) Take $F(x)/|x|^2 \uparrow \infty$, this being typical. All that needs be checked is the existence of a constant c such that the ground state for $\mathfrak{G}_0^*$ has second moment D. Now, for $c \uparrow \infty$, the ground state $\sqrt{f_*}$ for $\mathfrak{G}_0^*$ satisfies

$$\begin{aligned} c\int_{\mathbb{R}^d} |x|^2 f_*(x)dx &\leq \frac{1}{2}\int_{\mathbb{R}^d} |\nabla\sqrt{f_*(x)}|^2 dx + \int_{\mathbb{R}^d} F^*(x) f_*(x)dx \\ &\leq \frac{1}{2}\int_{\mathbb{R}^d} |\nabla\sqrt{f(x)}| dx + \int_{\mathbb{R}^d} F(x)f(x)dx + c\int_{\mathbb{R}^d} |x|^2 f(x)dx \end{aligned}$$

for any smooth non-negative f with $\int f = 1$. Thus, $\int |x|^2 f_*$ may be made as small as you want by concentrating f near the origin. Likewise, for $c \downarrow -\infty$, $\int |x|^2 f_*$ can be made large by spreading f out. The uniqueness is obvious.

(2) We show that there exists a sequence of strictly positive functions f_n with $\int f_n = 1, \int |x|^2 f_n = D$ and

$$\liminf_{n\uparrow\infty} I_F(f_n) \leq I_F(f_0) = \inf_{\int f=1} I_F(f).$$

We can assume that we are working in the cone $\{x : x_1 \geq |x|\cos\theta\}$ with $0 < \theta < \pi/2$. Now, f_0 is strictly positive so $\inf\{f_0(x) : |x| \leq 1\} \equiv \delta$ is positive. Next define

$$f_n(x) = f_0(x) + \frac{1}{n^{d+2}}\eta_0\Big(\frac{x - \alpha n e_1}{n}\Big) + \frac{1}{n^2}\rho_0(x) \equiv f_0 + \eta_n + \rho_n$$

where $\eta_0 \in C_0^\infty$ is positive with support in the ball B_r about the origin of radius $r = \alpha\sin\theta$; and ρ_0 is a smooth function supported in the unit ball, such that $\int |x|^2\rho_0(x)dx = 0$ and $\int \rho_0(x)\ dx < 0$ as may be achieved by concentrating the negative part of ρ_0 near the origin.

To show that f_n can be adjusted to satisfy $\int f_n = 1$ and $\int |x|^2 f_n = D$, first note that proper choice of the constant α permits you to make

$$\int_{\mathbb{R}^d} |x|^2\eta_n(x)dx = \frac{1}{n^{d+2}}\int_{\mathbb{R}^d} |x|^2\eta_0\Big(\frac{x - \alpha e_1 n}{n}\Big)dx = \int_{B_r} |x + \alpha e_1|^2\eta_0(x)dx$$

equal to $D - D_0$ and thus to adjust the mean-square for a given η_0. Also, by the evaluation

$$\int_{\mathbb{R}^d} \eta_n(x)dx = \frac{1}{n^{d+2}}\int_{\mathbb{R}^d} \eta_0\Big(\frac{x - \alpha e_1 n}{n}\Big)dx = \frac{1}{n^2}\int_{B_r} \eta_0(x)dx$$

you see that taking $\int \eta_0 = -\int \rho_0$ keeps $\int f_n = 1$. Lastly, for all large n, $||\rho_n||_\infty$ will lie under δ: in short, the f_n are honest probability densities.

To finish, observe that $f \to I_F(f)$ is convex and so sub-additive; this gives you $I_F(f_n) \le I_F(f_0) + a_n + b_n$ with

$$a_n = \frac{1}{n^2}\Big\{\int_{B_1} \frac{|\nabla \rho_0(x)|^2}{\rho_0(x)} dx + \int_{B_1} F(x)\rho_0(x)dx\Big\} \quad \to \quad 0$$

and

$$\begin{aligned} b_n &= \frac{1}{n^{d+4}} \int \frac{|\nabla \eta_0(\frac{x-\alpha e_1 n}{n})|^2}{\eta_0(\frac{x-\alpha e_1 n}{n})} dx + \frac{1}{n^{d+2}} \int F(x)\ \eta_0(\frac{x-\alpha e_1 n}{n}) dx \\ &= \frac{1}{n^4} \int_{B_r} \frac{|\nabla \eta_0(x)|^2}{\eta_0(x)} dx + \frac{1}{n^2} \int_{B_r} |F(n(x+\alpha e_1))|\ \eta_0(x)\ dx \\ &\le \frac{1}{n^4} C_1 + \frac{1}{n^2} C_2 \sup_{x \in B_{rn}+\alpha n e_1} |F(x)| \quad \to \quad 0. \end{aligned}$$

The proof is complete.

Lemma 5 shows that the phase transition - the possibility that the micro-canonical conditioning is overcome and the thermodynamic limit is the original (stationary) diffusion - obtains if in the I-minimization problem (13) the optimizer falls out of micro-canonical set and takes place at the global minimum. The latter is of course the original invariant density ($\psi^* = \psi$) which explains the change of phase as a consequence of heavy-tailed behavior: the event defined by the micro-canonical condition is not exponentially rare and so not felt at $L = \infty$.

Finally we provide the proof of (14) in the case that F is at most quadratic at ∞ - exactly when phase transition may occur. This finishes the proof of Theorem 1.

Lemma 6. *Let again* $\mathfrak{G} = (1/2)\triangle + (\nabla\psi/\psi)\cdot\nabla$ *and* $\mathbb{M}_L$ *our model micro-canonical measure obtained by restricting the mean-square. If* $F(x)$ *grows at most like* $|x|^2$ *at infinity, then*

$$\liminf_{L\uparrow\infty} \frac{1}{L}\mathbb{M}_L\left[\log\Big\{\frac{dP_{m_L}}{d\mathbb{P}_L}\Big|_{\mathfrak{F}_0^{L-1}}\Big\}\right] \ge 0$$

independently of the value of D.

Proof. The Radon-Nikodym derivative over $\mathfrak{F}_0^{L-1}$ of the periodic diffusion $\mathbb{P}_L$ with respect to its stationary counterpart P_{ψ^2} is $Z_L^{-1} p_0(1, X(L-1), X(0))$ where $p_0(t,x,x')$ is the (symmetric) transition density for $P_\bullet$ with respect to $\psi^2(x)dx$. Recall $Z_L \simeq 1$ for large L is the partition function for $\mathbb{P}_L$. You may then write

$$\mathbb{M}_L\left[\log\Big\{\frac{dP_{m_L}}{d\mathbb{P}_L}\Big|_{\mathfrak{F}_0^{L-1}}\Big\}\right] = -\log(Z_L) + \mathbb{M}_L\Big[\log p_0(1, X(0), X(1))\Big] + H(m_L|\psi^2)$$

using the rotation invariance of $\mathbb{M}_L$ to reduce the second summand to its present form.

The first term causes no problem. Neither does $H(m_L|\psi^2)$ which is positive: we are concerned with the possibility that the above is large negative. As for the second term, the potential difficulty lies in rapid decay of $p_0(1,x,x')$ for large $|x|$ or $|x'|$, but, with the present conditions, we just get by.

For $\triangle\psi/\psi \le C(1+|x|^2)$ we may use the Cameron-Martin formula to obtain an easy estimate of $p_0(1,x,x')$ from below: with $g(1,x,x') = (2\pi)^{-d/2}e^{-|x-x'|^2/2}$ and $E_{\bullet\bullet}$ = the Brownian Bridge,

$$\begin{aligned} p_0(1,x,x') &= E_{xx'}\Big[\exp\Big\{\int_0^1 \frac{\nabla\psi}{\psi}(X)\cdot dX - \frac{1}{2}\int_0^1 \Big|\frac{\nabla\psi}{\psi}\Big|^2 (X(t))dt\Big\}\Big]\frac{g(1,x,x')}{\psi^2(x')} \\ &= E_{00}\Big[\exp\Big\{-\int_0^1 \frac{\triangle\psi}{2\psi}(x+t(x'-x)+X(t))dt\Big\}\Big]\frac{g(1,x,x')}{\psi(x)\psi(x')} \\ &\ge c_1 \exp\Big[-c_2(|x|^2+|x'|^2)\Big]. \end{aligned} \tag{15}$$

Here we have used two facts: (1) ψ is positive and decaying so it's reciprocal is bounded below, and (2) the expectation $E_{00}[\exp(-C\int_0^1 |X|^2)]$ is bounded below as well. Finally, (15) implies that

$$\mathbb{M}_L\Big[\log p_0(1,X(0),X(1))\Big] \ge \log c_1 - 2c_2\mathbb{M}_L\Big[|X|^2(0)\Big] \ge \log c_1 - 4c_2 D$$

to finish the proof.

In conclusion, Theorem 1, answers the question left opened in [8] and points out a different phenomenon than encountered there. On the other hand it only complements that paper in terms of the underlying technology. Where [8] treated the case $F(x)/|x|^2 \uparrow \infty$, we require that ratio to be bounded. Now the former condition is intuitively much nicer, corresponding roughly to better recurrence properties, and one expects the present method to work throughout. Closing the gap requires extending the result of Lemma 6: $\lim_{L\uparrow\infty} L^{-1}\mathbb{M}_L[\log p_0(1,X(0),X(1))] = 0$ to a wider class of diffusions. As seen in the proof, the needed limit may be rephrased in terms of a moment condition: it is enough to have $\mathbb{M}_L[|X(0)|^\alpha] = \mathrm{o}(L)$ for some α such that $|F(x)|/|x|^\alpha = \mathrm{o}(1)$ at infinity. That the condition can be written in such a straightforward manner demonstrates the niceties of the diffusion format.

4. Statistical Mechanics for Wave Equations

Consider for a moment the (one-dimensional) non-linear wave equation $\partial^2 Q/\partial t^2 - \partial^2 Q/\partial x^2 + f(Q) = 0$ with periodic boundary conditions on $0 \le x \le L$. Defining $P = \partial Q/\partial t$ this equation can be written in Hamiltonian form $\partial Q/\partial t = \partial H/\partial P$, $\partial P/\partial t = -\partial H/\partial Q$ in which

$$H = \int_0^L F(Q(x))dx + \frac{1}{2}\int_0^L |Q'(x)|^2 dx + \frac{1}{2}\int_0^L P^2(x)dx$$

and $F(Q) = \int^Q f$. The idea of Gibbs' investigated by McKean-Vaninsky et al is that

$$e^{-H}d(\text{volume}) = e^{-\int_0^L F(Q(x))dx} \times \frac{e^{-\frac{1}{2}\int_0^L |Q'(x)|^2 dx}}{(2\pi 0+)^{\infty/2}} d^\infty Q \times \frac{e^{-\frac{1}{2}\int_0^L P^2(x)dx}}{(2\pi/0+)^{\infty/2}}. \tag{16}$$

ought to provide an invariant measure for the flow. This formal object has the following interpretation. The middle factor indicates that Q is a "circular" Brownian Motion (CBM), obtained by conditioning the standard Brownian Motion so that $Q(0) = Q(L) = c$ and then distributing this value over the line according to the infinite measure $(2\pi L)^{-1/2} \times dc$. In suit, the third factor defines the velocity P as a White Noise. The first factor is just a density with respect to the CBM. It is a comforting result [7] that if F tends to infinity at $\pm\infty$ and so acts as restoring force for the wave equation, then this density provides the needed control for the measure (16) to be finite.

To connect with the present work consider again the Schrödinger operator $\mathfrak{G}_0 = -(1/2)\triangle + F(Q)$ and its ground state $\psi(Q)$. Itô's Lemma ($(dQ)^2 = dx$) will show

$$0 = \int_0^L d\log\psi[Q(x)] = \int_0^L \nabla\log\psi(Q)\cdot dQ + \int_0^L \frac{1}{2}\triangle\log\psi(Q)(dQ)^2$$
$$= \int_0^L \frac{\nabla\psi}{\psi}(Q)\cdot dQ - \frac{1}{2}\int_0^L \left|\frac{\nabla\psi}{\psi}\right|^2(Q)dx + \int_0^L F(Q)dx - \Lambda_0(\mathfrak{G}_0)]L,$$

which, if substituted in (16), tells you that the density $\exp[-\int_0^L F(Q)dx]$ is, up to a constant multiple, the Cameron-Martin factor for the diffusion of type $\mathfrak{G}$ used throughout this work. That is, our periodic diffusion $\mathbb{P}_L$ and the Q part of the above Gibbs ensemble are one and the same.

The micro-canonical ensemble/thermodynamic limit for these measures was considered by McKean-Vaninsky to be a model for the harder problem of focussing cubic Schrödinger. There $\sqrt{-1}\partial Q/\partial t = -\partial^2 Q/\partial x^2 + |Q|^2 Q$ with Hamiltonian $H = (1/2)\int_0^L |Q'|^2 - (1/4)\int_0^L |Q|^4$, and the canonical Gibbs measure is

$$e^{-H}d(\text{volume}) = e^{(1/4)\int_0^L |Q|^4(x)dx}\frac{e^{-(1/2)\int_0^L |Q'(x)|^2 dx}}{(2\pi 0+)^\infty}d^\infty(\text{real } Q)d^\infty(\text{imag } Q).$$

Now $\int_0^L |Q|^2$ is a constant of the motion; Lebowitz-Rose-Speer [6] pointed out that conditioning on it being fixed is necessary to make the total mass finite.[5] As to the thermodynamic limit, neither the methods of [8] or this paper apply, but see [10] and [12] for a different approach.

5. The Martin Boundary

As a final remark, we wish to point out the connection between the present work and that of computing the Martin Boundary for the space-time motion $t \to [t, X(t), I(t) = \int^t |X|^2(t')dt']$. The latter is again a diffusion with generator $\mathfrak{L} = \partial_t + \mathfrak{G} + |x|^2\partial_I$; its Martin Boundary is defined as the complete list of (minimal) positive solutions to $\mathfrak{L}h = 0$.[6]

[5] We mention that this ensemble and the one of (16) have solid mechanical meaning: their invariance under the flow is proved in [7] for classical waves and [9] for cubic Schrödinger.

[6] For a spirited introduction to Martin's Boundary, [13] is recommended.

Returning to the the expression (3) for the micro-canonical mean of $\phi[X(t'):0 \le t' \le t]$, one should notice that all that changes in $\mathbb{M}_L[\phi]$ for $L \uparrow \infty$ is the ratio

$$\mathfrak{Z}_L^{-1} P_x \Big[\int_0^{L-t} |X|^2(t')dt' \in L[D, D+\delta] - I, X(L-t) = x' \Big]. \qquad (17)$$

Thus, the thermodynamic limit problem is equivalent to understanding the large L behavior of this last display. The results of Krylov [5] show the family $\mathfrak{Z}_L^{-1}P_x[etc]$ is tight and more. The $L \uparrow \infty$ limit $h(t,x,x',I)$ is unique and, just as one would hope from a glance at (17) satisfies, $0 = \partial_t h + \mathfrak{G}_x h + |x|^2 \partial_I h$. Now the link is plain: our h's make up a "micro-canonical boundary" sitting inside the full Martin Boundary.

It is a simple matter to identify the $h's$. The preceding comments indicate that the thermodynamic limit may be expressed through $\mathbb{M}_\infty[\phi] =$

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_0^\infty E_{x'}\Big[\phi(X), X(t) = x, \int_0^t |X(s)|^2 ds = I\Big] h(t,x,x',I)dx'dxdI. \quad (18)$$

The results of [8] and the present work show that this is also

$$\int_{\mathbb{R}^d} E^*_{x'}[\phi(X)][\psi^*(x')]^2 dx' = \int_{\mathbb{R}^d} E_{x'}\Big[\phi(X(t'):0 \le t' \le t), \frac{dP^*}{dP}\Big][\psi^*(x')]^2 dx'; \qquad (19)$$

the mean value for either a new stationary diffusion with adjusted potential $F^* = F + c|x|^2$, or just the original stationary mean. In the former case, bring in once more ψ^* as well as Λ_0^*, the corresponding eigenvalue. Next, one computes that over $0 \le t' \le t$ the density (dP^*/dP) equals

$$\frac{\exp[\int_0^t \frac{\nabla\psi^*}{\psi^*}\cdot dX - (1/2)\int_0^t |\frac{\nabla\psi^*}{\psi^*}|^2]}{\exp[\int_0^t \frac{\nabla\psi}{\psi}\cdot dX - (1/2)\int_0^t |\frac{\nabla\psi}{\psi}|^2]} = \frac{\psi(X(0))}{\psi(X(t))}\frac{\psi^*(X(t))}{\psi^*(X(0))}\exp\Big[c\int_0^t |X|^2 + \Lambda_0^* t\Big],$$

which, by comparing (18) to (19), implies

$$h(t,x,x',I) = \psi^*(x')\psi(x')\frac{\psi^*(x)}{\psi(x)}\exp\Big[cI + \Lambda_0^* t\Big]. \qquad (20)$$

In the latter case, the case of phase transition, $dP^*/dP = 1$ and $h(t,x,x',I) = \psi^2(x')$.

For a concrete example take X an Ornstein-Uhlenbeck process of mass m $(\psi^2(x) = \exp[-m|x|^2])$. In this case the complete list of minimal space-time functions (the full Martin Boundary) may be worked out:

$$h(t,x,\bullet,I) = \exp\Big[\alpha t e^{m't} - \frac{\alpha^2}{2}\frac{e^{2m't}-1}{2m'} - \beta t + \beta\gamma^2 - \gamma I/2\Big]$$

for $\gamma \ge -m^2$, $2\beta = m \pm \sqrt{\gamma + m^2}$ either for $\alpha = 0$ or $m' = \mp(1/2)\sqrt{\gamma+m^2}$. That is, the Martin Boundary is a topological plane, and, you note by comparison with (20), the micro-canonical boundary is just the line corresponding to $\alpha = 0$. As was natural, it was conjectured in [8] that the general case is similar. However, the phase transition described in the present paper shows that is not so: in that case all points of the expected micro-canonical line are identified for $D \ge D_0 = \int |x|^2\psi^2(x)dx$. The effect of this truncation on the full boundary is an interesting problem for the future.

Acknowledgements. This research was supported in part by NSF grant DMS-9802310. It is a pleasure to thank my advisor, H.P. McKean, for suggesting the problem and his ongoing support. Thanks as well to Ofer Zeitouni for pointing me to the work of Csiszár. Finally, sincere appreciation goes out to the referee whose comments greatly improved the prose.

References

1. Csiszár, I.: Sanov property, generalized I-projection and a conditional limit theorem. Ann. Probab. **12**, 768-793 (1984)
2. Dembo, A. and Zeitouni,).: Refinements of the Gibbs conditioning principle. Prob. Theory and Related Fields **104**, 1, 1-14 (1996)
3. Doeblin, W,: Sur les propriétés asymptotiques de mouvement régis par certains types de chaines simples. Bull. Math. Roum. Sci **39**, No. 1, 57-115, No 2. 3-61 (1937)
4. Donsker, M.D. and Varadhan, S.R.S.: Asymptotic evaluation of certain Markov process expectations for large time - II. Comm. Pure Appl. Math. **29**, 389-461 (1976)
5. Krylov, N.V.: *Nonlinear elliptic and parabolic equations of second order*, Dodrecht, Boston, Lancaster, Tokyo: Reidel 1987
6. Lebowitz, J.L., Rose, H. and Speer, E.: Statistical mechanics of nonlinear Schrödinger Equation. Journal of Stat. Phys. **50**, 657-687 (1988)
7. McKean, H.P. and Vaninsky, K.: Statistical mechanics of nonlinear wave equations, *Trends and Perspectives in Appl. Math*, ed. L. Sirovich, Springer, 1994
8. McKean, H.P. and Vaninsky, K.: Brownian motion with restoring drift: The petit and micro-canonical ensembles. Comm. Math. Phys. **160**, 615-630 (1994)
9. McKean, H.P.: Statistical mechanics of nonlinear wave equations (IV): cubic Schrödinger. Comm. Math. Phys. **168**, 479-491 (1995)
10. McKean, H.P.: A Martin boundary connected with the ∞-volume limit of focussing cubic Schrödinger, *Itô's Stochastic Calculus and Probability Theory*, 251–259, Springer, 1996.
11. Ney, P. and Nummelin, E.: Markov Additive Processes I, II. Ann. Probab. **15**, 2, 561-592, 593-604. (1987)
12. Rider, B.: On the ∞-volume limit of focussing cubic Schrödinger, to appear Comm. Pure Appl. Math.
13. Rogers, L.C.G. and Williams, D.: *Diffusions, Markov Processes, and Martingales Vol 1*, Wiley Chichester, 1994.
14. Schroeder, C.: I-projection and conditional limit theorems for discrete parameter Markov processes, Ann. Probab. **21**, 721-758 (1993)