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Diffusion in a Periodic Potential with a Local Perturbation

K. Golden,[1,2] **S. Goldstein,**[1] **and J. L. Lebowitz**[1,3]

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We consider the diffusion of a particle at $\mathbf{X}_t$ in a drift field derived from a smooth potential of the form $V+B$, where V is periodic and B is a bump of compact support. With no bump, $B=0$, the mean squared displacement $E(t) \equiv E\,|\mathbf{X}_t - \mathbf{X}_0|^2 = D(V)t + C + O(e^{-\lambda t})$, $\lambda > 0$, in any dimension. When $B \neq 0$, we establish in one dimension the asymptotic expansion $E(t) = D(V)t + \alpha\sqrt{t} + C + (1/\sqrt{t}) \sum_{n=0}^{\infty} \alpha_n / t^n$, $\alpha \neq 0$, as $t \to \infty$. Our analysis relies on the Nash estimates developed in previous work for the transition density of the process and their consequences for the analytic structure of the Laplace transform $\tilde{E}(s)$ of $E(t)$.

KEY WORDS: Diffusion; periodic potential; local perturbation; Nash estimates; mean squared displacement; velocity autocorrelation function.

1. INTRODUCTION

In order to analyze the structure of the mean squared displacement (MSD) $E(t) = E\,|\mathbf{X}_t - \mathbf{X}_0|^2$ (where E denotes expectation) of a particle at $\mathbf{X}_t$ at time t diffusing in the gradient of a smooth, bounded potential, we developed in Ref. 1 upper and lower Gaussian bounds on the transition density $u(\mathbf{x}, t)$, i.e., Nash-type *a priori* estimates on u. Here we use these estimates to study diffusion in $V+B$ for $d=1$, where V is periodic and B, the "bump," is a *local* potential with compact support.

For stationary random ergodic potentials (a class which includes periodic and quasiperiodic potentials) the diffusion on a macroscopic scale behaves like Brownian motion with some effective diffusion tensor

[1] Department of Mathematics, Rutgers University, New Brunswick, New Jersey 08903.
[2] Present address: Department of Mathematics, Princeton University, Princeton, New Jersey 08544.
[3] Department of Physics, Rutgers University, New Brunswick, New Jersey 08903.

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$\mathsf{D}(V)$.[2-4] Then $E(t)$ behaves like Dt, $D=\mathrm{tr}(\mathsf{D})$, for large t. In Ref. 1 we proved, using the Nash estimates, that adding a bump B to a stationary random ergodic V leaves this limiting behavior unchanged. This general result, however, gives no information on the effect of the bump on the correction $C(t)$ to the dominant behavior of $E(t)=D(V)t+C(t)$. The correction $C(t)$ is of physical interest due to its relation to the "velocity" autocorrelation function[5-8] of the system, which, through Fourier transform, is related to the frequency (ν)-dependent properties of the system, such as diffusivity $\mathsf{D}(\nu)$.

Using spectral theory, we easily show here for any d that for V periodic, $E(t)=D(V)t+C+O(e^{-\lambda t})$, $\lambda>0$. However, when a bump is added, we prove for $d=1$ that

$$E(t)=D(V)t+\alpha\sqrt{t}+C+\frac{1}{\sqrt{t}}\sum_{n=0}^{\infty}\frac{\alpha_n}{t^n}$$

which is an asymptotic series as $t\to\infty$, with α typically unequal to zero. The latter result is based on a Floquet analysis of the periodic Schrödinger operator associated with the generator of the unperturbed process. When this analysis is combined with the Nash estimates for large t, we show that the Laplace transform $\tilde{E}(s)$ of $E(t)$ is holomorphic and single-valued in a punctured neighborood of the origin of a two-sheeted Riemann surface with parameter $\sqrt{s}$, and has a fourth-order pole at $\sqrt{s}=0$. Then, using the general fact that $\tilde{E}(s)\to 0$ as $s\to\infty$ away from the negative real axis, which we proved in Ref. 1 using the Nash estimates, we invert the transform to give the above asymptotic series in t.

The present paper is one of several[1,9-11] containing results on the structure of the MSD. We remark that the locally perturbed potentials considered here and in Ref. 1 give the same power law decay of the second derivative of the MSD as one expects for "truly" random media.[7,8] In particular, in Ref. 1 we prove that for a rapidly decaying potential, $E(t)=t+O(\sqrt{t})$ for $d=1$, $E(t)=2t+O(\log t)$ for $d=2$, and $E(t)=dt+O(1/t^{d/2-1})$ for $d\geqslant 3$. However, in Ref. 11 we find simple quasiperiodic potentials for which there is *no* law of decay, i.e., correlations fall off more slowly than any function decreasing to zero that can be *explicitly* written down.

2. FORMULATION

Let $V(\mathbf{x})$, $\mathbf{x}\in\mathbb{R}^d$, be uniformly bounded and smooth, i.e., having uniformly bounded first, second, and third derivatives. Given $V(\mathbf{x})$, we consider on a probability space (S, G, P) the $\mathbb{R}^d$-valued process $\mathbf{X}_t$, $t \in \mathbb{R}$, governed by the stochastic differential equation

$$d\mathbf{X}_t = -\nabla V(\mathbf{X}_t)\, dt + d\mathbf{W}_t \tag{2.1}$$

with $\mathbf{X}_0 = \mathbf{x}_0$, where $\mathbf{W}_t$ is standard d-dimensional Brownian motion with mean 0 and covariance matrix tI, where I is the identity. [In general the equation governing the diffusion $\mathbf{X}_t$ is $d\mathbf{X}_t = -\sigma_0 \nabla V(\mathbf{X}_t)\, dt + (2D_0)^{1/2}\, d\mathbf{W}_t$, where σ_0 and D_0 are the "bare" mobility and diffusion constants. In (2.1) we have chosen units in which $\sigma_0 = 2D_0 = 1$ for simplicity.] Associated with (2.1) is the transition probability $p[A, t, \mathbf{y}, t'] = P[\mathbf{X}_t \in A \mid \mathbf{X}_{t'} = \mathbf{y}]$, where $t, t' \in \mathbb{R}$, $t' < t$, $\mathbf{y} \in \mathbb{R}^d$, and A is a Borel subset of $\mathbb{R}^d$. Under the above smoothness conditions, $p[A, t, \mathbf{y}, t']$ has a density $u(\mathbf{x}, t, \mathbf{y}, t')$, which is a fundamental solution of both the backward equation

$$\frac{\partial u}{\partial t'} + Lu = 0, \qquad \lim_{t' \uparrow t} u(\mathbf{x}, t, \mathbf{y}, t') = \delta_{\mathbf{x}}(\mathbf{y}) \tag{2.2}$$

and the forward equation

$$\frac{\partial u}{\partial t} - L^* u = 0, \qquad \lim_{t \downarrow t'} u(\mathbf{x}, t, \mathbf{y}, t') = \delta_{\mathbf{y}}(\mathbf{x}) \tag{2.3}$$

where L is the backward generator

$$L = \tfrac{1}{2}\Delta - \nabla V \cdot \nabla \tag{2.4}$$

which acts in the $\mathbf{y}$ variable, and L^* is the forward generator

$$L^* = \tfrac{1}{2}\Delta + \nabla \cdot \nabla V \tag{2.5}$$

which acts in the $\mathbf{x}$ variable, and is the (formal) adjoint of L.

We shall be interested in the MSD (mean squared displacement) of the diffusing particle,

$$E[|\mathbf{X}_t - \mathbf{x}_0|^2] = \int_S |\mathbf{X}_t - \mathbf{x}_0|^2\, dP \tag{2.6}$$

$$= \int_{\mathbb{R}^d} |\mathbf{x} - \mathbf{x}_0|^2\, u(\mathbf{x}, t, \mathbf{x}_0, 0)\, dx \tag{2.7}$$

So far we have not assumed that V is macroscopically homogeneous, which is important for well-defined, large-scale behavior. When such homogeneity is present, i.e., for periodic, quasiperiodic, or stationary random potentials, there is a useful representation of the "equilibrium" averaged MSD $E_e\,|\mathbf{X}_t-\mathbf{x}_0|^2$. For V periodic, the equilibrium averaged expectation E_e is defined by following the usual averaging in (2.6) by an average of the starting point $\mathbf{x}_0$ over a period cell with weight proportional to $\exp[-2V(\mathbf{x}_0)]$. (For a general stationary random potential, E_e involves an average over an abstract space of potentials.[1,3]) It may be shown that E_e is invariant under time reversal. Now write (2.1) as

$$(\mathbf{X}_t-\mathbf{x}_0)+\int_0^t \nabla V(\mathbf{X}_s)\,ds=\mathbf{W}_t \tag{2.8}$$

The first term on the left is antisymmetric under time reversal (about $t/2$), while the second term is symmetric. Squaring both sides and taking equilibrium expectation E_e gives the "velocity" autocorrelation representation[12,13,2]

$$E_e\,|\mathbf{X}_t-\mathbf{x}_0|^2=td-2\int_0^t (t-s)\,E_e[\nabla V(\mathbf{x}_0)\cdot\nabla V(\mathbf{X}_s)]\,ds \tag{2.9}$$

since the cross term in the square of the left-hand side of (2.8) vanishes due to antisymmetry and the time-reversal invariance of E_e.

3. MSD FOR A PERIODIC POTENTIAL

In this section we give the structure of the MSD for diffusion in a smooth, periodic potential $V(\mathbf{x})$ with

$$V(\mathbf{x}+\mathbf{e}_j)=V(\mathbf{x}),\qquad j=1,\dots,d \tag{3.1}$$

where the $\mathbf{e}_j$ are the standard unit vectors in $\mathbb{R}^d$. We first study the equilibrium averaged MSD given by (2.9), and then the MSD for fixed $\mathbf{x}_0$, for which (2.9) does not hold.

By the periodicity of V, the process $\mathbf{X}_t$ can be replaced on the right side of (2.9) by the torus process $\hat{\mathbf{X}}_t=\mathbf{X}_t \bmod A$, where $A=\{\mathbf{x}: 0\leqslant x_i\leqslant 1,\ i=1,\dots,d\}$ is the period cell of V, which can be identified with the unit d-torus T^d. The (L^2) generator $\hat{L}$ of the torus process is given by $\hat{L}=\frac{1}{2}\Delta-\nabla V\cdot\nabla$ acting on $\mathscr{H}=L^2(T^d,d\mu)$, where

$$\mu=[\exp(-2V)]\Big/\int_{T^d}\exp[-2V(\mathbf{y})]\,d\mathbf{y}$$

In terms of $\hat{L}$, (2.9) can be written as

$$E[|\mathbf{X}_t-\mathbf{x}_0|^2]=td-2\int_0^t (t-s)\langle\nabla V\,[\exp(\hat{L}s)]\,\nabla V\rangle\,ds \tag{3.2}$$

where $\langle\cdot\rangle$ denotes inner product in $L^2(T^d, d\mu)$. The time integral in (3.2) can be carried out by employing the spectral theorem in $L^2(T^d, d\mu)$, where $\hat{L}$ is a negative self-adjoint operator, to obtain

$$E_e[|\mathbf{X}_t-\mathbf{x}_0|^2]=Dt-2\langle\nabla V\cdot\hat{L}^{-2}[\exp(\hat{L}t)-1]\,\nabla V\rangle \tag{3.3}$$

In (3.3)

$$D=d+2\langle\nabla V\cdot\hat{L}^{-1}\,\nabla V\rangle \tag{3.4}$$

is the diffusion constant, which is the trace of the diffusion matrix

$$D_{ij}=\delta_{ij}+2\left\langle\frac{\partial V}{\partial x_i}\hat{L}^{-1}\frac{\partial V}{\partial x_j}\right\rangle, \qquad i,j=1,\dots,d$$

[We remark that ∇V is orthogonal to the constants in $L^2(T^d, d\mu)$.]

$\hat{L}$ has discrete spectrum on $\mathscr{H}$, $\lambda_n\leqslant 0$, $n=0,1,\dots$, with $\lambda_0=0$ and $\lambda_n\to-\infty$ as $n\to\infty$. Moreover, $\lambda_0=0$ is a simple eigenvalue (i.e., $\lambda_1<0$) with a corresponding eigenfunction $\psi_0=1$. The spectral gap between λ_1 and $\lambda_0=0$ allows the second and third terms in (3.3) to be separated, so that

$$E_e[|\mathbf{X}_t-\mathbf{X}_0|^2]=Dt+C_0-C(t) \tag{3.5}$$

where D is as in (3.4), C_0 is a positive constant

$$C_0=2\langle\nabla V\cdot\hat{L}^{-2}\,\nabla V\rangle \tag{3.6}$$

and $C(t)$ is positive and exponentially decaying,

$$C(t)=2\langle\nabla V\cdot\hat{L}^{-2}[\exp(\hat{L}t)]\,\nabla V\rangle \tag{3.7}$$

In fact, we have the following bound:

$$C(t)\leqslant(\gamma/\lambda_1^2)\,e^{-|\lambda_1|t} \tag{3.8}$$

where

$$\gamma=\int_{T^d}|\nabla V|^2\,d\mu\geqslant 0 \tag{3.9}$$

Equations (3.2)–(3.4) are valid for a general stationary random potential with $\hat{L}$ the generator of a suitable "environment process."[1,2] However, in general there will be no spectral gap, and without additional detailed spectral information, the decomposition (3.5)–(3.7) is not possible.

We summarize these results in the following:

Theorem 3.1. For the process $\mathbf{X}_t$ in $\mathbb{R}^d$ which obeys (2.1) with smooth, periodic V and "starts in equilibrium,"

$$E_e[|\mathbf{X}_t - \mathbf{X}_0|^2] = Dt + C_0 + O(e^{-|\lambda_1| t}) \tag{3.10}$$

where D and C_0 are the positive constants in (3.4) and (3.6) and $\lambda_1 < 0$ is the first nonzero eigenvalue of $\hat{L}$ acting on $\mathscr{H} = L^2(T^d, d\mu)$.

A lower bound on $|\lambda_1|$ can be obtained by unitarily mapping $\hat{L}$ on $L^2(T^d, d\mu)$ to H on $L^2(T^d, d\mathbf{x})$ via $e^V H e^{-V} = \hat{L}$, where

$$H = \tfrac{1}{2}\Delta + q, \qquad q = \tfrac{1}{2}[\nabla V \cdot \nabla V - \Delta V]$$

Then, for $d = 1$,[14] with $q_-(x) = \min\{q(x), 0\}$,

$$|\lambda_1| \geq 2\pi^2 \left[1 + \frac{1}{8} \int_0^1 q_-(x)\, dx \right] \tag{3.11}$$

We now consider $\mathbf{X}_t$ satisfying (2.1) with fixed, periodic V, but with a fixed starting point $\mathbf{X}_0 = \mathbf{x}_0$. Again the MSD has the same structure as (3.10), although we cannot readily obtain such detailed information on the constants involved, as we see in the following result:

Theorem 3.2. For $\mathbf{X}_t$ satisfying (2.1) with fixed $\mathbf{X}_0 = \mathbf{x}_0$ and periodic V in any dimension,

$$E_{\mathbf{x}_0}[|\mathbf{X}_t - \mathbf{x}_0|^2] = Dt + B(\mathbf{x}_0) + O(e^{-bt}) \tag{3.12}$$

where D is the same as in Theorem 3.1, $\sup_{\mathbf{x}_0} |B(\mathbf{x}_0)| < \infty$, and $b > 0$.

In (3.11) and in the proof of the theorem, we use the notation $O(e^{-\gamma t})$ for a function $f(\mathbf{x}_0, t)$ satisfying $|f(\mathbf{x}_0, t)| \leq Ce^{-\gamma t}$ for some C independent of $\mathbf{x}_0$. The proof of Theorem 3.2 involves a coupling of the process with fixed $\mathbf{X}_0 = \mathbf{x}_0$ to one that starts in equilibrium. Since this proof employs different techniques than are used in the rest of the paper, we relegate it to the Appendix.

4. NASH ESTIMATES AND THEIR CONSEQUENCES

Here we collect results from Ref. 1 necessary in the analysis of the MSD $E(t)$ for nonperiodic potentials. We begin with the Nash estimates.

Theorem 4.1. Let $u(\mathbf{x}, t)$ be the fundamental solution of (2.3) in $\mathbb{R}^d$ with smooth, bounded V, $\mathbf{y}=\mathbf{x}_0$, and $t'=0$. Then

$$\frac{1}{Ct^{d/2}} \exp\left(-C\frac{|\mathbf{x}-\mathbf{x}_0|^2}{t}\right) \leqslant u(\mathbf{x}, t) \leqslant \frac{C}{t^{d/2}} \exp\left(-\frac{|\mathbf{x}-\mathbf{x}_0|^2}{Ct}\right) \quad (4.1)$$

where C depends only on $V_{\max}$, $V_{\min}$, and d.

We consider the Laplace transform in time of the transition density,

$$\tilde{u}(\mathbf{x}, s) = \int_0^\infty e^{-st} u(\mathbf{x}, t)\, dt, \qquad \operatorname{Re} s > 0 \quad (4.2)$$

which satisfies

$$L^* \tilde{u} - s\tilde{u} = -\delta(\mathbf{x}-\mathbf{x}_0) \quad (4.3)$$

As an immediate consequence of Theorem 4.1, we have the following result for $d=1$.

Corollary 4.1. For each $x \in \mathbb{R}^1$, there exist positive constants a_1 and a_2 such that for sufficiently small $s>0$,

$$a_1/\sqrt{s} \leqslant \tilde{u}(x, s) \leqslant a_2/\sqrt{s} \quad (4.4)$$

It also follows from (4.1) that for $d \leqslant 3$, $\tilde{u}(\cdot, s)$ is an $L^2(\mathbb{R}^d, e^{2V}\, d\mathbf{x})$-valued solution to (4.3). Using the fact that $L^* = \frac{1}{2}\nabla \cdot (e^{-2V} \nabla e^{2V})$ is self-adjoint in $L^2(\mathbb{R}^d, e^{2V}\, d\mathbf{x})$ with spectrum in the negative real axis, one can prove the following result.

Corollary 4.2. Let $d \leqslant 3$. For each $s \notin (-\infty, 0]$, (4.3) has a unique $L^2(\mathbb{R}^d, e^{2V}\, d\mathbf{x})$ solution $\tilde{u}(\cdot, s)$. As an $L^2(\mathbb{R}^d, e^{2V}\, d\mathbf{x})$-valued function on $C-(-\infty, 0]$, $\tilde{u}$ is holomorphic. Moreover, for any $\varepsilon>0$, there exists a $C>0$ such that for any s in the region $|\arg s| \leqslant \pi - \varepsilon$,

$$\|\tilde{u}(\cdot, s)\|_{L^2(\mathbb{R}^d, e^{2V}\, d\mathbf{x})} \leqslant \frac{C}{|s|^{1-d/4}} \quad (4.5)$$

It follows from Theorem 4.1 that for $\operatorname{Re} s > 0$,

$$\tilde{E}(s) = \int_{\mathbb{R}^d} |\mathbf{x}-\mathbf{x}_0|^2\, \tilde{u}(\mathbf{x}, s)\, d\mathbf{x} \quad (4.6)$$

Also, it is easy to see that $\tilde{E}(s) \to 0$ as $s \to \infty$ in the region $|\arg s| \leqslant \pi/2 - \varepsilon$, but extending this information, as well as (4.6), to the left half-plane requires work. This result is stated as follows:

Theorem 4.2. $\tilde{E}(s)$ can be analytically continued into $C-(-\infty, 0]$, where it is given by (4.6). Furthermore, for any $\varepsilon>0$, as $s \to \infty$ in the region $|\arg s| \leqslant \pi-\varepsilon$,

$$\tilde{E}(s) \to 0 \tag{4.7}$$

Finally, we consider diffusion in a smooth potential of the form $V+B$ in $\mathbb{R}^d$, where V is stationary random ergodic and B has compact support, satisfying

$$d\mathbf{X}_t = -\nabla(V(\mathbf{X}_t)+B(\mathbf{X}_t))\,dt + d\mathbf{W}_t \tag{4.8}$$

A rather involved proof employing Nash estimates at each major step implies that the addition of a bump does not affect the asymptotic MSD to leading order.

Theorem 4.3. For $\mathbf{X}_t$ in $\mathbb{R}^d$ obeying (4.8)

$$\lim_{t\to\infty} \frac{E[|\mathbf{X}_t-\mathbf{x}_0|^2]}{t} = D \tag{4.9}$$

where $D=D(V)$ is defined by (3.4). (If V is not periodic, the convergence here is in ρ-measure, where ρ is the probability measure on the space of potentials.)

5. MSD FOR A PERIODIC POTENTIAL WITH A LOCAL PERTURBATION ($d=1$)

We now give the structure of the MSD for the one-dimensional diffusion (4.8) with smooth V of period 1 and smooth B of compact support. Our analysis will focus on the Laplace transform $\tilde{u}(x, s)$ of the density $u(x, t)$, which is the fundamental solution of $\partial u/\partial t = L^*u$, $u(x, 0) = \delta(x-x_0)$, with $L^* = \frac{1}{2}\Delta + \nabla\cdot[\nabla(V+B)\cdot]$. Its structure as a function of s near $s=0$ will help us deduce the structure of the MSD.

6.1. Floquet Analysis of the Green's Function for the Periodic Potential

To facilitate the analysis of $\tilde{u}(x, s)$, we first consider $\tilde{u}_0(x, s)$ for the periodic potential V of period 1, which satisfies

$$\frac{1}{2}\frac{d^2\tilde{u}_0}{dx^2} + \frac{d}{dx}(V'\tilde{u}_0) - s\tilde{u}_0 = -\delta(x-x_0) \tag{5.1}$$

where $V' = dV/dx$. In terms of $H = \frac{1}{2}d^2/dx^2 + q(x)$, with $q(x) = \frac{1}{2}[V'' - (V')^2]$, (5.1) becomes

$$Hg - sg = -e^{V(x_0)}\,\delta(x - x_0) \tag{5.2}$$

where $g(x, s) = e^{V(x)}\,\tilde{u}_0(x, s)$ and H is self-adjoint on $L^2(\mathbb{R}, dx)$. The Green's function defined by (5.2) can be obtained from analysis of the homogeneous equation

$$\frac{1}{2}\frac{d^2y}{dx^2} + q(x)\,y = sy \tag{5.3}$$

where q has period 1. Much is known about (5.3), which is referred to as Hill's equation.[14,15] We mention some of the facts relevant to us.

Since $q(x)$ has period 1, if $\psi(x)$ is a solution to (5.3), so is $\psi(x+1)$. However, (nontrivial) periodic solutions of (6.3) need not exist. Nevertheless, there exist $\rho \neq 0$ and a nontrivial solution $\psi(x)$ to (5.3) such that $\psi(x+1) = \rho\psi(x)$. Let $\theta_1(x)$ and $\theta_2(x)$ be the normalized, linearly independent solutions of (5.3) satisfying $\theta_1(0) = 1$, $\theta_1'(0) = 0$, $\theta_2(0) = 0$, and $\theta_2'(0) = 1$. Then the condition that there exists a nontrivial solution $\psi(x)$ to (5.3) such that $\psi(x+1) = \rho\psi(x)$ is

$$\rho^2 - \mathscr{D}(s)\rho + 1 = 0 \tag{5.4}$$

where $\mathscr{D}(s) = \theta_1(1, s) + \theta_2'(1, s)$ is the discriminant of (5.3).

Qualitatively, for real s starting at $-\infty$, $\mathscr{D}(s)$ exhibits uniformly bounded oscillations between maxima at or above 2 and minima at or below -2. These oscillations cease at $s = \lambda_0$, the supremum of the spectrum of the negative H, where $\mathscr{D}(s = \lambda_0) = +2$. Beyond this point, $\mathscr{D}(s) > 2$, $s > \lambda_0$. The roots of $\mathscr{D}(s) = +2$ are precisely the $\lambda_0, \lambda_1, \ldots$ of Section 3. The roots of $\mathscr{D}(s) = -2$ are the eigenvalues $\mu_0, \mu_1, \ldots$ of H on $L^2(A, dx)$ with antiperiodic boundary conditions. The spectrum of H on $L^2(\mathbb{R}, dx)$ is purely absolutely continuous and is arranged in bands $[\mu_0, \lambda_0]$, $[\lambda_1, \mu_1]$, $[\mu_2, \lambda_2], \ldots$. In these "stability" bands, $|\mathscr{D}(s)| < 2$, $|\rho| = 1$, and the solutions of (5.3) are bounded. In the gaps (λ_0, ∞), (μ_1, μ_0), $(\lambda_2, \lambda_1), \ldots$, $|\mathscr{D}(s)| > 2$, $|\rho| \neq 1$, and the solutions of (5.3) are unbounded.

We are, of course, most interested in small, positive s. In order to see how the solutions depend on s, let us analyze the Floquet multiplier ρ, which from (5.4) is given by

$$\rho = \tfrac{1}{2}\mathscr{D} \pm \tfrac{1}{2}[(\mathscr{D} + 2)(\mathscr{D} - 2)]^{1/2} \tag{5.5}$$

As a function of the complex variable s, $\mathscr{D}(s)$ is entire, since θ_1 and θ_2 are.

At $s=0$, $\mathscr{D}(s)-2$ has a simple zero, so that $\lambda_0=0$ is nondegenerate. Thus, $\mathscr{D}(s)$ around $s=0$ has the expansion

$$\mathscr{D}(s)=2+a_1 s+a_2 s^2+\cdots, \qquad a_1>0 \tag{5.6}$$

so that

$$\rho(s)=(1+\tfrac{1}{2}a_1 s+\cdots)\pm\tfrac{1}{2}(4a_1 s+\cdots)^{1/2} \tag{5.7}$$

We see from (5.7) that $\rho(s)$ is analytic in $\sqrt{s}$ in a neighborhood of the origin $\sqrt{s}=0$. The two roots (5.5) of (5.4) can be written as

$$\rho_1=e^{-m}, \qquad \rho_2=e^{m} \tag{5.8}$$

where $m>0$ when $s>0$ and is continued analytically. Then

$$m(s)=\log(1+a_1\sqrt{s}+\cdots) \tag{5.9}$$

which proves the following result.

Lemma 5.1. The exponent m defined by (5.8) and (5.9) is analytic in $\zeta=\sqrt{s}$ in a neighborhood of $\zeta=0$ with

$$m(\zeta)=a_1\zeta+\cdots \tag{5.10}$$

From (5.8) there are two linearly independent solutions to (5.3) of the form [when $\mathscr{D}(s)\neq\pm 2$]

$$y_1(x,s)=e^{-m(s)x}p_1(x,s), \qquad y_2(x,s)=e^{m(s)x}p_2(x,s) \tag{5.11}$$

where p_1 and p_2 have period 1 in x and satisfy

$$\frac{1}{2}\frac{d^2p_1}{dx^2}-m\frac{dp_1}{dx}+\left[q(x)+\frac{1}{2}m^2-s\right]p_1=0 \tag{5.12}$$

$$\frac{1}{2}\frac{d^2p_2}{dx^2}+m\frac{dp_2}{dx}+\left[q(x)+\frac{1}{2}m^2-s\right]p_2=0 \tag{5.13}$$

Using y_1 and y_2, we can construct the Green's function $\tilde{u}_0(x,s)$ satisfying (5.1) and classify its dependence on s. We remind the reader that by Corollary 4.2, Eq. (5.1) has a unique L^2 solution.

Lemma 5.2. For V periodic and $s\notin(-\infty,0]$, the L^2 solution of (5.1) has the form

$$\tilde{u}_0(x,s)=\begin{cases} e^{-V(x)-m(s)(x-x_0)}p_1(x,s), & x>x_0 \\ e^{-V(x)+m(s)(x-x_0)}p_2(x,s), & x<x_0 \end{cases} \tag{5.14}$$

where p_1 and p_2 have the same period as V and satisfy (5.12) and (5.13).

Furthermore, for any fixed $x \neq x_0$, $\tilde{u}_0(x, \zeta)$ is analytic in $\zeta = \sqrt{s}$ in a punctured neighborhood of $\zeta = 0$ with

$$\tilde{u}_0(x, \zeta) = \frac{b_{-1}(x)}{\zeta} + b_0(x) + b_1(x)\zeta + \cdots, \qquad b_{-1} \neq 0 \tag{5.15}$$

Proof. For $x > x_0$, $g(x)$ satisfying (5.2) is a linear combination of y_1 and y_2 in (5.11), and similarly for $x < x_0$. Since $g \in L^2(\mathbb{R}, dx)$, $\tilde{u}_0$ has the structure (5.14). Let ϕ_1 and ψ_1 be the normalized solutions of (5.12) satisfying $\phi_1(0) = 1$, $\phi_1'(0) = 0$, $\psi_1(0) = 0$, $\psi_1'(0) = 1$, and similarly for ϕ_2 and ψ_2 satisfying (5.13). Then they are all entire in $\zeta = \sqrt{s}$. The periodic solutions p_1 and p_2 of (5.12) and (5.13) have the form $p_1 = b_1\phi_1 + c_1\psi_1$ and $p_2 = b_2\phi_2 + c_2\psi_2$. The coefficients b_1, c_1, b_2, and c_2 are determined by imposing periodicity on p_1 and p_2, continuity of g in (6.2) across $x = x_0$, and the jump condition in the first derivative of g at $x = x_0$. Note that for periodicity it suffices to consider boundary conditions on p_1 and p_2 and not their derivatives, since periodic solutions must exist, but not all solutions have the same value at 0 and 1. Thus, there are four linear equations for b_1, c_1, b_2, and c_2, and they have coefficients which are entire functions of ζ. Moreover, the determinant of this system cannot vanish identically, due to the existence and uniqueness of the L^2 solution of the differential equation (Corollary 4.2), and, in fact, has discrete zeros only on the negative real axis. Thus, the b_i and c_i, $i = 1, 2$, are rational functions of entire functions of ζ. As such, their worst singularities (at any finite ζ) are isolated poles. Thus, there exists a punctured neighborhood of $\zeta = 0$ in which the b_i and c_i are analytic in ζ. Corollary 4.1 assures us that the b_i and c_i have nonzero first-order poles at $\zeta = 0$, and no higher order poles. Tracing back to $\tilde{u}_0$ proves the lemma.

Lemma 5.2 says that the principal features of $\tilde{u}_0(x, s)$ for periodic V reflect those for the special case $V = 0$. In this special case,

$$\tilde{u}(x, s) = \frac{1}{(2s)^{1/2}} \exp[-(2s)^{1/2} |\mathbf{x} - \mathbf{x}_0|] \tag{5.16}$$

so that $p_1 = p_2 = 1/(2s)^{1/2}$ and $m = (2s)^{1/2}$.

5.2. Green's Function for $V + B$ and the MSD

We are now in a position to assess the effect of adding a local perturbation B to the periodic potential V. For simplicity we take $\operatorname{supp}(B) \subset (0, 1)$ and $x_0 \in (0, 1)$. Let $\tilde{u}(x, s)$ satisfy

$$\frac{1}{2}\frac{d^2\tilde{u}}{dx^2} + \frac{d}{dx}[(V' + B')\tilde{u}] - s\tilde{u} = -\delta(x - x_0) \tag{5.17}$$

Using Lemma 5.2, we can prove the following about the structure of $\tilde{u}$.

Lemma 5.3. For V periodic, B supported in $(0, 1)$, and $s \notin (-\infty, 0]$, the L^2 solution $\tilde{u}$ of (5.17) outside of $(0, 1)$ has the form

$$\tilde{u}(x, s) = \begin{cases} \gamma_1(s)\, \tilde{u}_0(x, s), & x > 1 \\ \gamma_2(s)\, \tilde{u}_0(x, s), & x < 0 \end{cases} \tag{5.18}$$

$$\begin{aligned} \gamma_1(s) &= 1 + \gamma_{11}\sqrt{s} + \gamma_{12}s + \cdots \\ \gamma_2(s) &= 1 + \gamma_{21}\sqrt{s} + \gamma_{22}s + \cdots \end{aligned} \tag{5.19}$$

where $\tilde{u}_0$ is as in Lemma 5.2. Furthermore, for any x, $\tilde{u}(x, \zeta)$ is analytic in $\zeta = \sqrt{s}$ in a punctured neighborhood N of $\zeta = 0$, and has a Laurent expansion there like (5.15).

Proof. Since for $x > 1$, $\tilde{u}(x, s)$ satisfies the same ordinary differential equation as $\tilde{u}_0(x, s)$, we have that $\tilde{u}(x, s) = \gamma_1 \tilde{u}_0(x, s)$. Similarly for $x < 0$. Inside $(0, 1)$, the homogeneous form of (5.17) has two normalized solutions ϕ and ψ (satisfying normalized boundary conditions at, say, $x = 0$), both of which are entire functions of s. For $x \in (0, x_0)$, $\tilde{u} = c_1\phi + c_2\psi$, for some c_1 and c_2. Similarly, for $x \in (x_0, 1)$, $\tilde{u} = b_1\phi + b_2\psi$, for some b_1 and b_2. Continuity of $\tilde{u}$ at $x = 0$, x_0, 1, continuity in $d\tilde{u}/dx$ at $x = 0, 1$, and the jump condition in the first derivative of $e^{(V+B)}\tilde{u}$ at $x = x_0$ give six linear equations for c_1, c_2, b_1, b_2, γ_1, and γ_2 with coefficients that are entire in $\zeta = \sqrt{s}$. An argument similar to the one given in the proof of Lemma 5.2, which appeals to Corollaries 4.1 and 4.2, tells us that these coefficients are analytic in $\zeta = \sqrt{s}$ with at worst discrete poles on the negative real axis. The coefficients c_1, c_2, b_1, and b_2 have at worst first-order poles in ζ at $\zeta = 0$, with no higher order poles. Furthermore, $\gamma_1 = \gamma_{10} + \gamma_{11}\sqrt{s} + \cdots$, and $\gamma_2 = \gamma_{20} + \gamma_{21}\sqrt{s} + \cdots$. The conditions that the mean displacement is $o(\sqrt{t})$, which follows from the invariance principle, and that both u and u_0 have integrals over $\mathbb{R}$ equal to 1, can be shown, using the techniques in the proof of the next theorem, to give two independent linear equations for γ_{10} and γ_{20}. The unique solution of these equations is $\gamma_{10} = \gamma_{20} = 1$, so that the lemma is proved.

Now we use the information about $\tilde{u}$ contained in Lemma 5.3 to obtain a Laurent series expansion for the Laplace transform $\tilde{E}(s)$ of the MSD.

Theorem 5.1. For X_t satisfying (4.8) in $d = 1$ with smooth, periodic V, compactly supported, smooth B, and fixed starting point x_0, the Laplace transform $\tilde{E}(s)$ of the MSD is analytic in $\zeta = \sqrt{s}$ in a punctured neighborhood of $\zeta = 0$, and has there a Laurent expansion

$$\tilde{E}(s) = \frac{D}{s^2} + \sum_{n=-3}^{\infty} \beta_n (\sqrt{s})^n \tag{5.20}$$

where D is the same as in Theorem 3.2, and the β_n depend on V, B, and x_0.

Proof. Using Lemma 5.3, we write

$$\tilde{E}(s) = \int_{-\infty}^{\infty} (x - x_0)^2\, \tilde{u}(x, s)\, dx$$

$$= \gamma_2 \int_{-\infty}^{\infty} (x - x_0)^2\, e^{-V + m(x - x_0)} p_2\, dx$$

$$+ \gamma_1 \int_0^{\infty} (x - x_0)^2\, e^{-V - m(x - x_0)} p_1\, dx + A(s) \tag{5.21}$$

where p_1 and p_2 are defined by (5.14), and

$$A(s) = \int_0^1 (x - x_0)^2\, \tilde{u}(x, s)\, dx - \gamma_1 \int_0^1 (x - x_0)^2\, \tilde{u}_0\, dx \tag{5.22}$$

so that

$$A(s) = \frac{a_{-1}}{\sqrt{s}} + a_0 + a_1 \sqrt{s} + \cdots \tag{5.23}$$

Equation (5.23) is justified by noting that $\tilde{u}$ and $\tilde{u}_0$ are analytic in $\sqrt{s}$ and jointly continuous in $\sqrt{s}$ and x in the product of a punctured neighborhood of 0 and $[0, 1]$. The periodicity of V, p_1, and p_2 allows (5.21) to be written as

$$\tilde{E}(s) = \gamma_2 \sum_{n=0}^{\infty} \int_0^1 (-n - \theta - x_0)^2\, e^{m(-n - \theta - x_0)} e^{-V(-\theta)} p_2(-\theta)\, d\theta$$

$$+ \gamma_1 \sum_{n=0}^{\infty} \int_0^1 (n + \theta - x_0)^2\, e^{-m(n + \theta - x_0)} e^{-V(\theta)} p_1(\theta)\, d\theta$$

$$+ A(s) \tag{5.24}$$

$$= A_2 + A_1 + A \tag{5.25}$$

We analyze A_1 in (5.25). With $\alpha = \theta - x_0$ we have

$$A_1 = \gamma_1 \int_0^1 d\theta\, e^{-V} p_1 \sum_{n=0}^{\infty} (n + \alpha)^2\, e^{-m(n + \alpha)} \tag{5.26}$$

Now,

$$\sum_{n=0}^{\infty} (n + \alpha)^2\, e^{-m(n + \alpha)} = \frac{\partial^2}{\partial m^2} \left(e^{-m\alpha} \sum_{n=0}^{\infty} e^{-mn} \right) \tag{5.27}$$

A simple calculation shows that

$$\sum_{n=0}^{\infty} (n+\alpha)^2 e^{-m(n+\alpha)} = \sum_{n=-3}^{\infty} c'_n(\alpha)(\sqrt{s})^n \tag{5.28}$$

for some c'_n, so that, as for (5.23),

$$A_1 = \sum_{n=-4}^{\infty} c_n(\sqrt{s})^n \tag{5.29}$$

and similarly for

$$A_2 = \sum_{n=-4}^{\infty} b_n(\sqrt{s})^n \tag{5.30}$$

Since the diffusion constant must be the same as that for the periodic potential V by Theorem 4.3, we must have $c_{-4} + b_{-4} = D$, which proves the theorem.

Finally, by inverting the Laplace transform, we have the following result.

Theorem 5.2. For X_t satisfying (4.8) in $d=1$ with smooth, periodic V, compactly supported, smooth B, and fixed starting point x_0, the MSD for any $\varepsilon > 0$ is analytic in t and has the asymptotic series representation as t approaches ∞ in the angular region $|\arg t| \leqslant \pi/2 - \varepsilon$,

$$E[|X_t - x_0|^2] = Dt + \alpha\sqrt{t} + C + \frac{1}{\sqrt{t}} \sum_{n=0}^{\infty} \frac{\alpha_n}{t^n} \tag{5.31}$$

where D is the same as in Theorem 3.2, and α, C, α_1, α_2,... depend on V, B, and x_0.

Proof. The theorem follows from Theorem 5.1. We employ Theorem 37.1 in Doetsch.[16] For this theorem to apply to our situation, we need that $\tilde{E}(s)$ is analytic in the region $|\arg s| \leqslant \pi - \varepsilon$ and that $\tilde{E}(s) \to 0$ as $s \to \infty$ in this region, which is the content of Theorem 4.2.

We remark that α, C, and the α_n are in general presumably nonzero. That $\alpha \neq 0$ in the special case of rapidly decaying potentials was discussed in Ref. 1.

Recall that the generator for periodic V,

$$L^* = \frac{1}{2}\frac{d^2}{dx^2} + \frac{d}{dx} V' \quad \text{on} \quad L^2(\mathbb{R}, e^{2V}\, dx)$$

has absolutely continuous spectrum arranged in bands, the first of which is immediately to the left of the origin. The effect of adding B to V[17] is to leave the continuous spectrum invariant, but cause eigenvalues to appear in the gaps between the bands [although not in $(0, \infty)$ for $L^* \leqslant 0$]. Let $H_0 = \frac{1}{2} d^2/dx^2 + q$, where $q = \frac{1}{2}[V'' - (V')^2]$, and $H_1 = \phi = \frac{1}{2}[B'' - (B')^2]$. Rofe-Beketov[17] has shown that if ϕ satisfies

$$\int_{-\infty}^{\infty} (1 + |x|)\, |\phi(x)|\, dx < \infty \tag{5.32}$$

then there are at most a finite number of eigenvalues in each gap of the continuous spectrum of H. For bounded ϕ of compact support, (5.32) is trivially satisfied.

The mild effect of the perturbation on the spectrum of H_0 is reflected in Lemma 5.3. If the perturbation were to, say, introduce eigenvalues arbitrarily close to zero, then the branch point structure $\tilde{u}$ exhibited in Lemma 5.3 would presumably not occur. Instead, 0 would be an essential singularity. However, because of the branch point structure in s, $\tilde{u}$ can be continued across the negative real axis near 0 in such a way that $\tilde{u}(x, s)$ is multiple-valued in a punctured neighborhood of $s = 0$. In fact, $\tilde{u}(x, s)$ is single-valued and analytic in a punctured neighborhood of the origin of a two-sheeted Riemann surface with parameter $\zeta = \sqrt{s}$.

We expect that for a "truly random" potential, $\tilde{u}(x, s)$ will have an essential singularity at $s = 0$. Nevertheless, since the Nash estimates still hold, $\tilde{u}(x, s)$ for $d = 1$ has the asymptotic behavior $1/\sqrt{s}$ as $s \to 0$, as indicated in Corollary 4.1.

We close by remarking that the arguments and techniques used in this paper also apply to diffusion processes with generator $L = \nabla \cdot \mathrm{a}\nabla$, as well as to the case of $L = b\nabla \cdot a\nabla$, with $a, b > 0$.

APPENDIX. PROOF OF THEOREM 3.2

Unless explicitly indicated otherwise, all constants are independent of $\mathbf{x}_0$. In the proof we shall use the following result.

Lemma A.1. For $\mathbf{X}_t$ satisfying (2.1) with fixed starting point $\mathbf{x}_0$ and periodic V,

$$E[\mathbf{X}_t - \mathbf{x}_0] = \mathbf{B}_0(\mathbf{x}_0) + O(e^{-|\lambda_1| t}) \tag{A.1}$$

where $\sup_{\mathbf{x}_0} |\mathbf{B}_0(\mathbf{x}_0)| < \infty$, and λ_1 is as in Theorem 3.1.

Proof. We may assume that $\mathbf{x}_0 \in A$, the period cell. From (2.1) and the periodicity of V we have that

$$E_{\mathbf{x}_0}[\mathbf{X}_t - \mathbf{x}_0] = -\int_0^t E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)]\, ds \tag{A.2}$$

We must analyze $E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)]$, which can be written as

$$E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)] = \int_A \nabla V(\mathbf{x})\, u_{\mathbf{x}_0}(\mathbf{x}, s)\, d\mathbf{x} \tag{A.3}$$

where $u_{\mathbf{x}_0}(x, s)$ is the solution in A of

$$\partial u/\partial t = L^* u, \qquad u(\mathbf{x}, 0) = \delta(\mathbf{x} - \mathbf{x}_0) \tag{A.4}$$

under periodic boundary conditions with L^* as in (2.5). Let $u_{\text{eq}}\, d\mathbf{x} = d\mu(\mathbf{x})$. We write

$$E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)] = \int_A \nabla V(\mathbf{x})\, [u_{\mathbf{x}_0}(\mathbf{x}, s) - u_{\text{eq}}(\mathbf{x})]\, d\mathbf{x} \tag{A.5}$$

since $\int_A \nabla V\, d\mu = 0$. Using the fact that for large enough s[18]

$$\|u_{\mathbf{x}_0}(\cdot, s) - u_{\text{eq}}(\cdot)\|_{L^2(A, d\mu)} = O(e^{-|\lambda_1| s}) \tag{A.6}$$

we obtain

$$E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)] = O(e^{-|\lambda_1| t}) \tag{A.7}$$

Then, writing (A.2) as

$$E_{\mathbf{x}_0}[\mathbf{X}_t - \mathbf{x}_0] = -\int_0^\infty E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)]\, ds + \int_t^\infty E_{\mathbf{x}_0}[\nabla V(\hat{\mathbf{X}}_s)]\, ds \tag{A.8}$$

yields (A.1).

At this point we restrict ourselves to $d = 1$. By a coupling of two processes $X_t^{(1)}$ and $X_t^{(2)}$ we mean a simultaneous realization of these processes on the same probability space $(\bar{S}, \bar{\mathscr{G}}, \bar{P})$.[19] Let $X_t^{(1)}$ and $X_t^{(2)}$ be the two proesses satisfying (2.1), starting in equilibrium on the period cell $[x_0 - 1, x_0) \equiv A_{x_0}$ and at fixed $x_0 \in [0, 1)$, respectively. For any particular sample of $X_t^{(1)}$ that starts at $y \in A_{x_0}$, consider its translate $X_t^{(1)} + 1$. Together they form a moving box and $X_t^{(2)}$ starts inside this box. The coupling of the processes $X_t^{(1)}$ and $X_t^{(2)}$ is such that they move independently until the time τ when $X_t^{(2)}$ hits the side of the box, i.e., until $X_t^{(2)} = X_t^{(1)}$ mod 1, after which $X_t^{(2)}$ is glued to the copy of $X_t^{(1)}$ that it hit. The gluing is permissible by the Markovian nature of the processes. Let $\varepsilon_t = X_t^{(2)} - X_t^{(1)}$, so that $0 \leqslant \varepsilon_t \leqslant 1$. For $t \geqslant \tau$, $\varepsilon_t = 0$ or 1.

Now we write

$$\bar{E}[(X_t^{(2)} - x_0)^2] = E[(X_t^{(2)})^2 - 2x_0 X_t^{(2)} + x_0^2] \tag{A.9}$$

By Lemma A.1,

$$\bar{E}[-2x_0 X_t^{(2)} + x_0] = B_1(x_0) + O(e^{-|\lambda_1| t}) \tag{A.10}$$

where $\sup_{x_0} |B_1(x_0)| < \infty$. Via the coupling, we write

$$\bar{E}[(X_t^{(2)})^2] = \bar{E}[(X_t^{(1)})^2 + 2\varepsilon_t X_t^{(1)} + \varepsilon_t^2] \tag{A.11}$$

The first term on the right can be written as

$$\begin{aligned}\bar{E}[(X_t^{(1)})^2] &= \bar{E}[(X_t^{(1)} - X_0^{(1)})^2 + 2(X_t^{(1)} - X_0^{(1)})\, X_0^{(1)} + (X_0^{(1)})^2] \\ &= E_e[(X_t - X_0)^2] + 2\int_{x_0 - 1}^{x_0} \mu(dy)\, y E_y(X_t - y) \\ &\quad + \int_{x_0 - 1}^{x_0} \mu(dy)\, y^2 \end{aligned} \tag{A.12}$$

Thus, from Theorem 3.1 and Lemma A.1 we obtain

$$\bar{E}[(X_t^{(1)})^2] = Dt + C_1(x_0) + O(e^{-|\lambda_1| t}) \tag{A.13}$$

where $\sup_{x_0} |C_1(x_0)| < \infty$.

To control the last two terms on the right in (A.11), we must analyze the probability $\bar{P}\{\tau > t\}$ that $X_t^{(2)}$ has not hit the box by time t. First, it is easy to see from (2.1) and the fact that ∇V is bounded and the properties of Brownian motion that $\inf_{x_0} \bar{P}\{\tau \leqslant 1\} \equiv \xi_1 > 0$, so that $\bar{P}\{\tau > 1\} \leqslant 1 - \xi_1$. By the Markov property, $\bar{P}\{\tau > n\} \leqslant (1 - \xi_1)^n$, and in general,

$$\bar{P}\{\tau > t\} \leqslant Ce^{-\xi t} \tag{A.14}$$

for some $\xi > 0$ and some constant $C < \infty$.

The last term on the right in (A.11) can be written as

$$\bar{E}[\varepsilon_t^2] = \bar{E}[\varepsilon_t^2 (I_{\{t > \tau\}} + I_{\{t \leqslant \tau\}})]$$

where $I_{\{t > \tau\}}$ is the indicator function for the event $\{t > \tau\}$, and similarly for $I_{\{t \leqslant \tau\}}$. Since

$$\bar{E}[\varepsilon_t^2 I_{\{t > \tau\}}] = \bar{E}[\varepsilon_\infty^2 I_{\{t > \tau\}}] = \bar{E}[\varepsilon_\infty^2] - \bar{E}[\varepsilon_\infty^2 I_{\{t \leqslant \tau\}}]$$

and $\bar{P}\{t \leqslant \tau\} \leqslant Ce^{-\xi t}$, we have

$$\bar{E}[\varepsilon_t^2] = C_2(x_0) + O(e^{-\xi t}) \tag{A.15}$$

where $\sup_{x_0} |C_2(x_0)| < \infty$.

Finally, for the second term in (A.11), again we split the expectation,

$$\bar{E}[\varepsilon_t X_t^{(1)}] = \bar{E}[\varepsilon_t X_t^{(1)}(I_{\{t>\tau\}} + I_{\{t\leqslant\tau\}})] \tag{A.16}$$

The second term in (A.16) gives, by the Schwarz inequality,

$$\bar{E}[\varepsilon_t X_t^{(1)} I_{\{t\leqslant\tau\}}] \leqslant C_3(t+1)^{1/2}\, e^{-\xi t/2} = O(e^{-bt}) \tag{A.17}$$

for some $b>0$. The first term in (A.16) can be written as

$$\bar{E}[\varepsilon_t X_t^{(1)} I_{\{t>\tau\}}] = \bar{E}[\varepsilon_\tau X_\tau^{(1)} I_{\{t>\tau\}}] + \bar{E}[\varepsilon_\tau (X_t^{(1)} - X_\tau^{(1)})] \tag{A.18}$$

$$= \mathrm{I} + \mathrm{II} \tag{A.19}$$

For I we have

$$\mathrm{I} = \bar{E}[\varepsilon_\tau X_\tau^{(1)}] - \bar{E}[\varepsilon_\tau X_\tau^{(1)} I_{\{t\leqslant\tau\}}] \tag{A.20}$$

with

$$|\bar{E}[\varepsilon_\tau X_\tau^{(1)}]| \leqslant \bar{E}[|X_\tau^{(1)}|] < \infty \tag{A.21}$$

uniformly in x_0, and

$$|\bar{E}[\varepsilon_\tau X_\tau^{(1)} I_{\{t\leqslant\tau\}}]| \leqslant \{\bar{E}[(X_\tau^{(1)})^2]\}^{1/2}\, [\bar{P}\{\tau>t\}]^{1/2} \tag{A.22}$$

$$= O(e^{-\xi t/2}) \tag{A.23}$$

Here we have used (A.14) to control the moments of $X_\tau^{(1)}$. Let $\mathscr{F}_\tau$ be the σ-algebra generated by the process up to time τ. Then, using (A.14) and Lemma A.1, we have

$$\begin{aligned}
\mathrm{I} &= \bar{E}[\varepsilon_\tau I_{\{t>\tau\}} E_{\mathscr{F}_\tau}(X_t^{(1)} - X_\tau^{(1)})] \\
&= \bar{E}[\varepsilon_\tau I_{\{t>\tau\}} E_{X_\tau}(X_{t-\tau} - X_0)] \\
&= \bar{E}[\varepsilon_\tau I_{\{t>\tau\}}(B_0(X_\tau) + O(e^{-|\lambda_1|(t-\tau)}))] \\
&= \bar{E}[\varepsilon_\tau B_0(X_\tau)] - \bar{E}[\varepsilon_\tau B_0(X_\tau)\, I_{\{t\leqslant\tau\}}] \\
&\quad + \bar{E}[\varepsilon_\tau I_{\{t\leqslant\tau\}} \cdot O(e^{-|\lambda_1|(t-\tau)})] \\
&= B_3(x_0) + O(e^{-\eta t})
\end{aligned} \tag{A.24}$$

where $\sup_{x_0} |B_3(x_0)| < \infty$ and $\eta = \min(|\lambda_1|, \xi/2)$. This concludes the proof for $d=1$.

In dimensions $d \geqslant 2$ the proof is essentially the same as in $d=1$, except that the coupling is not as readily obtainable as in $d=1$. However, we proceed as follows. Let $\hat{\mathbf{X}}_t^{(1)}$ be the process on A satisfying (2.1) that starts in equilibrium, and let $\hat{\mathbf{X}}_t^{(2)}$ be the same except that it starts at a fixed $\mathbf{x}_0 \in A$. Let $u_{\mathbf{x}_0}^{(2)}(\mathbf{x}, t)$ be the density of $\hat{\mathbf{X}}_t^{(2)}$. Since

$$\inf_{\mathbf{x}_0} \|u_{\text{eq}}^{(1)}(\mathbf{x}) \wedge u_{\mathbf{x}_0}^{(2)}(\mathbf{x}, 1)\|_{L^1(A)} > 0 \tag{A.25}$$

we are assured[19] of the existence of a coupling for which

$$\bar{P}[\hat{X}_s^{(1)} \neq \hat{X}_s^{(2)} \text{ for some } s \geqslant t] = O(e^{-\xi t}) \qquad \text{for some} \quad \xi > 0 \tag{A.26}$$

The key difference for $d \geqslant 2$ is that when we "unwrap" these processes onto $\mathbb{R}^d$ to obtain $X_t^{(1)}$ and $X_t^{(2)}$, $\boldsymbol{\varepsilon}_t = \mathbf{X}_t^{(2)} - \mathbf{X}_t^{(1)}$ can be unbounded, depending on how many times it "wrapped around" the torus before coupling. However, by (A.26), the probability of $\sup_t |\boldsymbol{\varepsilon}_t|$ being large is exponentially small, which allows the proof to proceed to a conclusion in a similar manner to $d = 1$.

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