# **1 BROWNIAN MOTION IN AN N-SCALE PERIODIC POTENTIAL**

2

A. B. DUNCAN \* AND G. A. PAVLIOTIS<sup>†</sup>

**Abstract.** We study the problem of Brownian motion in a multiscale potential. The potential is assumed to have N + 1 scales (i.e. N small scales and one macroscale) and to depend periodically on all the small scales. We show that for nonseparable potentials, i.e. potentials in which the microscales and the macroscale are fully coupled, the homogenized equation is an overdamped Langevin equation with multiplicative noise driven by the free energy, for which the detailed balance condition still holds. The calculation of the effective diffusion tensor requires the solution of a system of N coupled Poisson equations.

10 **Key words.** Brownian dynamics, multiscale analysis, reiterated homogenization, reversible 11 diffusions, free energy.

#### 12 AMS subject classifications. 35B27,35Q82,60H30

**1.** Introduction. The evolution of complex systems arising in chemistry and bi-13 ology often involve dynamic phenomena occuring at a wide range of time and length 14 scales. Many such systems are characterised by the presence of a hierarchy of barriers 15in the underlying energy landscape, giving rise to a complex network of metastable 16regions in configuration space. Such energy landscapes occur naturally in macromolecular models of solvated systems, in particular protein dynamics. In such cases 18 the rugged energy landscape is due to the many competing interactions in the energy 19 function [12], giving rise to frustration, in a manner analogous to spin glass models 20 [13, 38]. Although the large scale structure will determine the minimum energy con-21 22 figurations of the system, the small scale fluctuations of the energy landscape will still have a significant influence on the dynamics of the protein, in particular the be-23 haviour at equilibrium, the most likely pathways for binding and folding, as well as 24 the stability of the conformational states. Rugged energy landscapes arise in various 25other contexts, for example nucleation at a phase transition and solid transport in 26condensed matter. 27

To study the influence of small scale potential energy fluctuations on the system dynamics, a number of simple mathematical models have been proposed which capture the essential features of such systems. In one such model, originally proposed by Zwanzig [51], the dynamics are modelled as an overdamped Langevin diffusion in a rugged two-scale potential  $V^{\epsilon}$ ,

34 (1) 
$$dX_t^{\epsilon} = -\nabla V^{\epsilon}(X_t) dt + \sqrt{2\sigma} dW_t, \quad \sigma = \beta^{-1} = k_B T,$$

where T is the temperature and  $k_B$  is Boltmann's constant. The function  $V^{\epsilon}(x) =$ 35  $V(x, x/\epsilon)$  is a smooth potential which has been perturbed by a rapidly fluctuating 36 function with wave number controlled by the small scale parameter  $\epsilon > 0$ . See Figure 37 1 for an illustration. Zwanzig's analysis was based on an effective medium approxima-38 tion of the mean first passage time, from which the standard Lifson-Jackson formula 39 [31] for the effective diffusion coefficient was recovered. In the context of protein 40 41 dynamics, phenomenological models based on (1) are widespread in the literature, including but not limited to [5, 25, 33, 48]. Theoretical aspects of such models have 42

<sup>28</sup> 

<sup>\*</sup>Department of Mathematics/Department of Chemical Engineering, Imperial College London (a.duncan@imperial.ac.uk).

<sup>&</sup>lt;sup>†</sup>Department of Mathematics, Imperial College London (g.pavliotis@imperial.ac.uk).

43 also been previously studied. More recent studies include [15] where the authors

44 study diffusion in a strongly correlated quenched random potential constructed from

45 a periodically-extended path of a fractional Brownian motion, and [7] in which the

<sup>46</sup> authors perform a numerical study of the effective diffusivity of diffusion in a potential obtained from a realisation of a stationary isotropic Gaussian random field.



Fig. 1: Example of a multiscale potential. The left panel shows the isolines of the Mueller potential [46, 35]. The right panel shows the corresponding rugged energy landscape where the Mueller potential is perturbed by high frequency periodic fluctuations.

47

For the case where (1) possesses one characteristic lengthscale controlled by  $\epsilon > 0$ , 48 the convergence of  $X_t^{\epsilon}$  to a coarse-grained process  $X_t^0$  in the limit  $\epsilon \to 0$  over a finite 49 time interval is well-known. When the rapid oscillations are periodic, under a diffu-50sive rescaling this problem can be recast as a periodic homogenization problem, for 51which it can be shown that the process  $X_t^{\epsilon}$  converges weakly to a Brownian motion with constant effective diffusion tensor D (covariance matrix) which can be calculated 53 by solving an appropriate Poisson equation posed on the unit torus, see for example 54[44, 9]. The analogous case where the rapid fluctuations arise from a stationary ergodic random field has been studied in [27, Ch. 9]. The case where the potential  $V^{\epsilon}$  pos-5657 sesses periodic fluctuations with two or three well-separated characteristic timescales, i.e.  $V^{\epsilon}(x) = V(x, x/\epsilon, x\epsilon^2)$  follow from the results in [9, Ch. 3.7], in which case the 58 dynamics of the coarse-grained model in the  $\epsilon \to 0$  limit are characterised by an Itô SDE whose coefficients can be calculated in terms of the solution of an associated 60

61 Poisson equation. A generalization of these results to diffusion processes having N-

62 well separated scales was explored in Section 3.11.3 of the same text, but no proof of

63 convergence is offered in this case. Similar diffusion approximations for systems with 64 one fast scale and one slow scale, where the fast dynamics are not periodic have been

65 studied in [40].

66

Further properties of the homogenized dynamics, in addition to the calculation of 67 the mean first passage time, have been investigated. For potentials of the form 68  $V^{\epsilon}(x) = \alpha V(x) + p(x/\epsilon)$  for a smooth periodic function  $p(\cdot)$  it was shown in [43] that 69 the maximum likelihood estimator for the drift coefficients of the homogenized equa-70 tion, given observations of the slow variable of the full dynamics (1) is asymptotically 71*biased.* Further results on inference of multiscale diffusions including (1) can be found 72 73 in [29, 28]. In [17], asymptotically optimal importance sampling schemes for studying rare events associated with (1) of the form  $V^{\epsilon}(x) = V(x, x/\epsilon)$  were constructed by 74 studying the  $\epsilon \to 0$  limit of an associated Hamilton-Jacobi-Bellmann equation, the 75results were subsequently generalised to random stationary ergodic fluctuations in 76 [49]. In [21], the authors study optimal control problems for two-scale systems. Small 77  $\epsilon$  asymptotics for the exit time distribution of (1) were studied in [3]. 78

79

A model for Brownian dynamics in a potential V possessing infinitely many character-

81 istic lengthscales was studied in [8]. In particular, the authors studied the large-scale

82 diffusive behaviour of the overdamped Langevin dynamics in potentials of the form

83 (2) 
$$V^n(x) = \sum_{k=0}^n U_k\left(\frac{x}{R_k}\right),$$

obtained as a superposition of Hölder continuous periodic functions with period 1. It was shown in [8] that the effective diffusion coefficient decays exponentially fast with the number of scales, provided that the scale ratios  $R_{k+1}/R_k$  are bounded from above and below, which includes cases where the is no scale separation. From this the authors were able to show that the effective dynamics exhibits subdiffusive behaviour, in the limit of infinitely many scales.

In this paper we study the dynamics of diffusion in a rugged potential possessing N well-separated lengthscales. More specifically, we study the dynamics of (1) where the multiscale potential is chosen to have the form

$$V^{\epsilon}(x) = V(x, x/\epsilon, x/\epsilon^2, \dots, x/\epsilon^N),$$

where V is a smooth function, which is periodic in all but the first variable. Clearly, V can always be written in the form

86 (3) 
$$V(x_0, x_1, \dots, x_N) = V_0(x_0) + V_1(x_0, x_1, \dots, x_N),$$

where  $(x_0, x_1, \ldots, x_N) \in \mathbb{R}^d \times (\mathbb{T}^d)^N$ . In this paper, we shall assume that the large scale component of the potential  $V_0$  is smooth and confining on  $\mathbb{R}^d$ , and that the perturbation  $V_1$  is a smooth bounded function which is periodic in all but the first variable. Unlike [8], we work under the assumption of explicit scale separation, however we also permit more general potentials than those of the form (2), allowing possibly nonlinear interactions between the different scales, and even full coupling between scales <sup>1</sup>. To emphasize the fact that the potential (3) leads to a fully coupled

<sup>&</sup>lt;sup>1</sup>we will refer to potentials of the form  $V^{\epsilon}(x) = V_0(x) + V_1(x/\epsilon, \dots, x/\epsilon^N)$  where  $V_1$  is periodic in all variables as separable.

system across scales, we introduce the auxiliary processes  $X_t^{(j)} = X_t/\epsilon^j$ , j = 0, ..., N. The SDE (1) can then be written as a fully coupled system of SDEs driven by the same Brownian motion  $W_t$ ,

97 (4a) 
$$dX_t^{(0)} = -\sum_{i=0}^N \epsilon^{-i} \nabla_{x_i} V\left(X_t^{(0)}, X_t^{(1)}, \dots, X_t^{(N)}\right) dt + \sqrt{2\sigma} \, dW_t$$

98 (4b) 
$$dX_t^{(1)} = -\sum_{i=0}^N \epsilon^{-i+1} \nabla_{x_i} V\left(X_t^{(0)}, X_t^{(1)}, \dots, X_t^{(N)}\right) dt + \sqrt{\frac{2\sigma}{\epsilon^2}} dW_t$$

99

100 (4c) 
$$dX_t^{(N)} = -\sum_{i=0}^N \epsilon^{-i+N} \nabla_{x_i} V\left(X_t^{(0)}, X_t^{(1)}, \dots, X_t^{(N)}\right) dt + \sqrt{\frac{2\sigma}{\epsilon^{2N}}} dW_t$$

102 in which case  $X_t^{(0)}$  is considered to be a "slow" variable, while  $X_t^{(1)}, \ldots X_t^{(N)}$  are 103 "fast" variables. In this paper, we first provide an explicit proof of the convergence of 104 the solution of (1),  $X_t^{\epsilon}$  to a coarse-grained (homogenized) diffusion process  $X_t^0$  given 105 by the unique solution of the following Itô SDE:

106 (5) 
$$dX_t^0 = -\mathcal{M}(X_t^0)\nabla\Psi(X_t^0)\,dt + \sigma\nabla\cdot\mathcal{M}(X_t^0)\,dt + \sqrt{2\sigma\mathcal{M}(X_t^0)}\,dW_t,$$

where

$$\Psi(x) = -\sigma \log Z(x),$$

denotes the free energy, for

÷

$$Z(x) = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V(x,y_1,\dots,y_N)/\sigma} \, dy_1 \dots dy_N$$

and where  $\mathcal{M}(x)$  is a symmetric uniformly positive definite tensor which is independent of  $\epsilon$ . The formula of the effective diffusion tensor is given in Section 2. The multiplicative noise is due to the full coupling between the macroscopic and the Nmicroscopic scales.<sup>2</sup> In particular, we show that although the noise in  $X_t^{\epsilon}$  is additive, the coarse-grained dynamics will exhibit multiplicative noise, arising from the interaction between the microscopic fluctuations and the thermal fluctuations. For one-dimensional potentials, we are able to obtain an explicit expression for  $\mathcal{M}(x)$ , regardless of the number of scales involved. In higher dimensions,  $\mathcal{M}(x)$  will be expressed in terms of the solution of a recursive family of Poisson equations which can be solved only numerically. We also obtain a variational characterization of the effective diffusion tensor, analogous to the standard variational characterisations for the effective conductivity tensor for multiscale conductivity problems, see for example [26]. Using this variational characterisation, we are able to derive tight bounds on the effective diffusion tensor, and in particular, show that as  $N \to \infty$ , the eigenvalues of the effective diffusion tensor will converge to zero, suggesting that diffusion in potentials with infinitely many scales will exhibit anomalous diffusion. The focus of this paper is the rigorous analysis of the homogenization problem for (1) with  $V^{\epsilon}$  given by (3). In a companion paper, [16] we study in detail qualitative properties of the solution to

 $<sup>^{2}</sup>$ For additive potentials of the form (2), i.e. when there is no interaction between the macroscale and the microscales, the noise in the homogenized equation is additive.

the homogenized equation (5), including noise-induced transitions and noise-induced hysteresis behaviour.

For the cases N = 1, 2 the main result of this paper, namely the derivation of the coarse grained dynamics, arises as a special case of [9, Chapter 3.7]. However, to our knowledge, the results in this paper are the first which rigorously prove the existence of this limit for arbitrarily many scales. A standard tool for the rigorous analysis of periodic homogenization problems is two-scale convergence [1, 37]. This theory was extended to study reiterated homogenization problems in [2]. The techniques developed in these papers do not seem to be directly applicable to the problem here for several reasons: first, we work in an unbounded domain, second the operators that we consider, i.e. the infinitesimal generator of the diffusion process (1) cannot be written in divergence form. The application of two-scale convergence to our problem would require extending two-scale convergence to weighted  $L^2$ -spaces, that depend both on the large and small scale parameters, something which does not seem to be straightforward. Our method for proving the homogenization theorem, Theorem 3 is based on the well known martingale approach to proving limit theorems [9, 39, 40]. The main technical difficulty in applying such well known techniques is the construction of the corrector field/compensator. This turns out to be a very tedious task, since we consider the case where all scales, the macroscale and the N- microscales, are fully coupled.

Note that although we consider the homogenized process  $X_t^0$ , the solution of (17) to be a coarse grained version of the multiscale process  $X_t^\epsilon$ , both processes have the same configuration space. We must therefore distinguish this approach with other coarse graining methodologies where effective dynamics are obtained for a lower dimensional set of coordinates of the original system, see for example [30, 11, 23, 45]. Nonetheless, one can still draw parallels between our approach and method described in [30, 11]. Indeed, when writing (1) in the form (4) we can still view the limit  $\epsilon \to 0$  as a form of dimension reduction, approximating the fast-slow system (4) of N + 1 processes  $(X_t^{(0)}, X_t^{(1)}, \ldots, X_t^{(N)})$  taking values in  $\mathbb{R}^{dN}$  by a single  $\mathbb{R}^d$ -valued process  $X_t^0$  whose effective dynamics are characterised by the free energy Z(x) and an effective diffusion tensor

Our assumptions on the potential  $V^{\epsilon}$  in (3) guarantee that the full dynamics (1) is ergodic and reversible with invariant distribution  $\pi^{\epsilon}$ . Furthermore, the coarse-grained dynamics (5) is ergodic and reversible with respect to the equilibrium distribution

$$\pi^0(x) = Z(x)/\overline{Z}.$$

Indeed, the natural interpretation of  $\Psi(x) = -\sigma \log Z(x)$  is as the free energy cor-107 responding to the coarse-grained variable  $X_t$ . The weak convergence of  $X_t^{\epsilon}$  to  $X_t^0$ 108 implies in particular that the distribution of  $X_t^{\epsilon}$  will converge weakly to that of  $X_t^0$ , 109 uniformly over finite time intervals [0, T], which does not say anything about the con-110 vergence of the respective stationary distributions  $\pi^{\epsilon}$  to  $\pi^{0}$ . In Section 4 we study the 111 equilibrium behaviour of  $X_t^{\epsilon}$  and  $X_t^0$  and show that the long-time limit  $t \to \infty$  and the 112 coarse-graining limit  $\epsilon \to 0$  commute, and in particular that the equilibrium measure 113 $\pi^{\epsilon}$  of  $X_t^{\epsilon}$  converges in the weak sense to  $\pi^0$ . We also study the rate of convergence 114to equilibrium for both processes, and we obtain bounds relating the two rates. This 115116 question is naturally related to the study of the Poincaré constants for the full and 117 coarse-grained potentials.

118

129

6

119 The rest of the paper is organized as follows. In Section 2 we state the assumptions 120 on the structure of the multiscale potential and state the main results of this paper. 121 In Section 3 we study properties of the effective dynamics, providing expressions for 122 the diffusion tensor in terms of a variational formula, and derive various bounds. In 123 Section 4 we study properties of the effective potential, and prove convergence of the 124 equilibrium distribution of  $X_t^{\epsilon}$  to the coarse-grained equilibrium distribution  $\pi^0$ .

**2. Setup and Statement of Main Results.** In this section we provide conditions on the multiscale potential which are required to obtain a well-defined homogenization limit. In particular, we shall highlight assumptions necessary for the ergodicity of the full model as well as the coarse-grained dynamics.

130 We will consider the overdamped Langevin dynamics

$$\frac{131}{132} \quad (6) \qquad \qquad dX_t^{\epsilon} = -\nabla V^{\epsilon}(X_t^{\epsilon}) \, dt + \sqrt{2\sigma} \, dW_t,$$

133 where  $V^{\epsilon}(x)$  is of the form

134 (7) 
$$V^{\epsilon}(x) = V\left(x, \frac{x}{\epsilon}, \frac{x}{\epsilon^2}, \dots, \frac{x}{\epsilon^N}\right),$$

and where  $V : \mathbb{R}^d \times \mathbb{T}^d \times \ldots \times \mathbb{T}^d \to \mathbb{R}$  is a smooth function which is assumed to be periodic with period 1 in all but its first argument. The multiscale potentials we consider in this paper can be viewed as a smooth confining potential perturbed by smooth, bounded fluctuations which become increasingly rapid as  $\epsilon \to 0$ , see Figure 1 for an illustration. More specifically, we will assume that the multiscale potential V satisfies the following assumptions.<sup>3</sup>

141 ASSUMPTION 1. The potential V is given by  $V = \frac{1}{2} \int \frac{1}{2} \frac{1}{2}$ 

142 (8) 
$$V(x_0, x_1, \dots, x_N) = V_0(x_0) + V_1(x_0, x_1, \dots, x_N),$$

143 where:

- 144 1.  $V_0$  is a smooth confining potential, i.e.  $e^{-V_0(x)} \in L^1(\mathbb{R}^d)$  and  $V_0(x) \to \infty$  as 145  $|x| \to \infty$ .
- 146 2. The perturbation  $V_1(x_0, x_1, ..., x_N)$  is smooth and bounded uniformly in x, 147 independently of  $\epsilon$ .
- 148 3. There exists C > 0 such that  $\left\| \nabla^2 V_0 \right\|_{L^{\infty}(\mathbb{R}^d)} \leq C$ .

149 REMARK 2. We note that Assumption 3 quite stringent, since it implies that  $V_0$ 150 is quadratic to leading order. This assumption is also made in [40]. In cases where 151 the process  $X_0^{\epsilon} \sim \pi^{\epsilon}$ , i.e. the process is started in stationary, this condition can be 152 relaxed considerably.

153 The infinitesimal generator  $\mathcal{L}^{\epsilon}$  of  $X_t^{\epsilon}$  is the selfadjoint extension of

154 (9) 
$$\mathcal{L}^{\epsilon}f(x) = -\nabla V^{\epsilon}(x) \cdot \nabla f(x) + \sigma \Delta f(x), \quad f \in C_0^{\infty}(\mathbb{R}^d)$$

- 155 Since  $V_0$  is confining, it follows that the corresponding overdamped Langevin equation
- 156 (10)  $dZ_t = -\nabla V_0(Z_t) dt + \sqrt{2\sigma} dW_t,$

<sup>3</sup>We remark that we can always write (3) in the form (8) where  $V_0(x) = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} V(x, x_1, \dots, x_N) dx_1 \dots dx_N.$ 

is ergodic with unique stationary distribution

$$\pi_{ref}(x) = \frac{1}{Z} \exp(-V_0(x)/\sigma), \quad Z = \int_{\mathbb{R}^d} e^{-V_0(x)/\sigma} dx$$

Since  $V_1$  is bounded uniformly, by Assumption 1, it follows that the potential  $V^{\epsilon}$  is also confining, and therefore  $X_t^{\epsilon}$  is ergodic, possessing a unique invariant distribution given by  $\pi^{\epsilon}(x) = \frac{e^{-V^{\epsilon}(x)/\sigma}}{Z^{\epsilon}}$ , where  $Z^{\epsilon} = \int_{\mathbb{R}^d} e^{-V^{\epsilon}(x)/\sigma}$ . Moreover, noting that the generator  $\mathcal{L}^{\epsilon}$  of  $X_t^{\epsilon}$  can be written as

$$\mathcal{L}^{\epsilon}f(x) = \sigma e^{V^{\epsilon}(x)} \nabla \cdot \left( e^{-V^{\epsilon}(x)} \nabla f(x) \right), \quad f \in C_0^2(\mathbb{R}^d).$$

157 it follows that  $\pi^{\epsilon}$  is reversible with respect to the dynamics  $X_t^{\epsilon}$ , c.f. [42, 19]. 158

Our main objective in this paper is to study the dynamics (6) in the limit of infinite scale separation  $\epsilon \to 0$ . Having introduced the model and the assumptions we can now present the main result of the paper.

162 THEOREM 3 (Weak convergence of  $X_t^{\epsilon}$  to  $X_t^0$ ). Suppose that Assumption 1 holds 163 and let T > 0, and the initial condition  $X_0$  is distributed according to some probability 164 distribution  $\nu$  on  $\mathbb{R}^d$ . Then as  $\epsilon \to 0$ , the process  $X_t^{\epsilon}$  converges weakly in  $(C[0,T]; \mathbb{R}^d)$ 165 to the diffusion process  $X_t^0$  with generator defined by

166 (11) 
$$\mathcal{L}^0 f(x) = \frac{\sigma}{Z(x)} \nabla_x \cdot (Z(x)\mathcal{M}(x)\nabla_x f(X)), \quad f \in C_0^2(\mathbb{R}^d),$$

167 and where

168 (12) 
$$Z(x) = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V(x,x_1,\dots,x_N)/\sigma} dx_N \dots dx_1$$

169 *and* 

(13)

170 
$$\mathcal{M}(x) = \frac{1}{Z(x)} \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} (1 + \nabla_{x_N} \theta_N^\top) \cdots (1 + \nabla_{x_1} \theta_1^\top) e^{-V(x, x_1, \dots, x_N)/\sigma} \, dx_N \cdots dx_1.$$

171 The correctors are defined recursively as follows: define  $\theta_{N-k}$  to be the weak solution 172 of the PDE

173 (14) 
$$\nabla_{x_{N-k}} \cdot (\mathcal{K}_{N-k}(x_0, \dots, x_{N-k})(\nabla_{x_{N-k}}\theta_{x_{N-k}}(x_0, \dots, x_{N-k}) + I)) = 0,$$

174 where  $\theta_{N-k}(x_0, \dots, x_{N-k-1}, \cdot) \in H^1(\mathbb{T}^d)$  and where (15)  $\mathcal{K}_{N-k}(x_0, \dots, x_{N-k})$ 

$$= \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} (I + \nabla_N \theta_N^\top) \cdots (I + \nabla_{N-k+1} \theta_{N-k+1}^\top) e^{-V/\sigma} \, dx_N \dots dx_{N-k+1},$$

176 for 
$$k = 1, ..., N - 1$$
, and

177 (16) 
$$\mathcal{K}_N(x, x_1, \dots, x_N) = e^{-V(x, x_1, \dots, x_N)/\sigma} I$$

178 where I denotes the identity matrix in  $\mathbb{R}^{d \times d}$ . Provided that Assumptions 1 hold,

- 179 Proposition 16 guarantees existence and uniqueness (up to a constant) of solutions to
- 180 the coupled Poisson equations (14). Furthermore, the solutions will depend smoothly

181 on the slow variable x as well as the fast variables  $y_1, \ldots, y_N$ . The process  $X_t^0$  is the 182 unique solution to the Itô SDE

(17) 
$$dX_t^0 = -\mathcal{M}(X_t^0)\nabla\Psi(X_t^0)\,dt + \sigma\nabla\cdot\mathcal{M}(X_t^0)\,dt + \sqrt{2\sigma\mathcal{M}(X_t^0)}\,dW_t,$$

where

$$\Psi(x) = -\sigma \log Z(x) = -\sigma \log \left( \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V(x,y_1,\dots,y_N)/\sigma} \, dy_1 \dots dy_N \right).$$

The proof, which closely follows that of [40] is postponed to Section 5. Theorem 3 confirms the intuition that the coarse-grained dynamics is driven by the free energy. On the other hand, the corresponding SDE has multiplicative noise given by a space dependent diffusion tensor  $\mathcal{M}(x)$ . We can show that the homogenized process (17) is ergodic with unique invariant distribution

$$\pi^0(x) = \frac{Z(x)}{\overline{Z}} = \frac{1}{\overline{Z}} e^{-\Psi(x)/\sigma}, \quad \text{where} \quad \overline{Z} = \int_{\mathbb{R}^d} Z(x) \, dx$$

It is important to note that the reversibility of  $X_t^{\epsilon}$  with respect to  $\pi^{\epsilon}$  is preserved under the homogenization procedure. In particular, the homogenized SDE (17) will be reversible with respect to the Gibbs measure  $\pi^0(x)$ . Indeed, (17) has the form of the most general diffusion process that is reversible with respect to  $\pi^0(x)$ , see [42, Sec. 4.7].

While Theorem 3 only characterises the convergence of  $X_t^{\epsilon}$  to  $X_t^0$  over finite time intervals, quite often we are interested in the equilibrium behaviour and in the rate of convergence to equilibrium for the coarse–grained process. In Section 4 we study the properties of the invariant distributions  $\pi^{\epsilon}$  and  $\pi^0$  of  $X_t^{\epsilon}$  and  $X_t^0$ , respectively. In particular, we show that  $\pi^{\epsilon}$  converges to  $\pi^0$  in the sense of weak convergence of probability measures, and moreover characterise the rate of convergence to equilibrium for both  $X_t^{\epsilon}$  and  $X_t^0$  in terms of  $\epsilon$ , the parameter which measures scale separation.

As is characteristic with homogenization problems, when d = 1 we can obtain, up to quadratures, an explicit expression for the homogenized SDE. In this case, we obtain explicit expressions for the correctors  $\theta_1, \ldots, \theta_N$ , so that the intermediary coefficients  $\mathcal{K}_1, \ldots, \mathcal{K}_N$  can be expressed as

$$\mathcal{K}_i(x_0, x_1, \dots, x_i) = \left( \int e^{V(x_0, x_1, \dots, x_i, x_{i+1}, \dots, x_N)/\sigma} \, dx_{i+1} \dots dx_N \right)^{-1}, \quad i = 1, \dots, N.$$

184 PROPOSITION 4 (Effective Dynamics in one dimension). When d = 1, the effective 185 diffusion coefficient  $\mathcal{M}(x)$  in (17) is given by

186 (18) 
$$\mathcal{M}(x) = \frac{1}{Z_1(x)\widehat{Z}_1(x)},$$

where

$$Z_1(x) = \int \cdots \int e^{-V_1(x, x_1, \dots, x_N)/\sigma} dx_1 \dots dx_N,$$

and

$$\widehat{Z}_1(x) = \int \cdots \int e^{V_1(x, x_1, \dots, x_N)/\sigma} dx_1 \dots dx_N.$$

187 Equation (18) generalises the expression for the effective diffusion coefficient for 188a two-scale potential that was derived in [51] without any appeal to homogenization theory. In higher dimensions we will not be able to obtain an explicit expression 189 for  $\mathcal{M}(x)$ , however we are able to obtain bounds on the eigenvalues of  $\mathcal{M}(x)$ . In 190 particular, we are able to show that (18) acts as a lower bound for the eigenvalues of 191  $\mathcal{M}(x).$ 192

193 **PROPOSITION 5.** The effective diffusion tensor  $\mathcal{M}$  is uniformly positive definite over  $\mathbb{R}^d$ . In particular, 194

195 (19) 
$$0 < e^{-osc(V_1)/\sigma} \le \frac{1}{Z_1(x)\widehat{Z}_1(x)} \le e \cdot \mathcal{M}(x)e \le 1,$$

for all  $e \in \mathbb{R}^d$  such that |e| = 1, where

$$osc(V_1) = \sup_{\substack{x \in \mathbb{R}^d, \\ y_1, \dots, y_N \in \mathbb{T}^d}} V_1(x, y_1, \dots, y_N) - \inf_{\substack{x \in \mathbb{R}^d, \\ y_1, \dots, y_N \in \mathbb{T}^d}} V_1(x, y_1, \dots, y_N)$$

This result follows immediately from Lemmas 10 and 11 which are proved in Section 1963. 197

REMARK 6. The bounds in (19) highlight the two extreme possibilities for fluctu-198ations occurring in the potential  $V^{\epsilon}$ . The inequality  $\frac{1}{Z_1(x)\widehat{Z}_1(x)} \leq e \cdot \mathcal{M}(x)e$  is attained 199when the multiscale fluctuations  $V_1(x_0, \ldots, x_N)$  are constant in all but one dimension 200 (e.g. the analogue of a layered composite material, [14, Sec 5.4], [44, Sec 12.6.2]). 201 In the other extreme, the inequality  $e \cdot \mathcal{M}(x)e = 1$  is attained in the abscence of 202fluctuations, i.e. when  $V_1 = 0$ . 203

204 REMARK 7. Clearly, the lower bound in (19) becomes exponentially small in the limit as  $\sigma \to 0$ . 205

While Theorem 3 guarantees weak convergence of  $X_t^{\epsilon}$  to  $X_t^0$  in  $C([0,T]; \mathbb{R}^d)$  for fixed T, it makes no claims regarding the convergence at infinity, i.e. of  $\pi^{\epsilon}$  to  $\pi^{0}$ . However, under the conditions of Assumption 1 we can show that  $\pi^{\epsilon}$  converges weakly to  $\pi^0$ , so that the  $T \to \infty$  and  $\epsilon \to 0$  limits commute, in the sense that:

$$\lim_{\epsilon \to 0} \lim_{T \to \infty} \mathbb{E}[f(X_T^{\epsilon})] = \lim_{T \to \infty} \lim_{\epsilon \to 0} \mathbb{E}[f(X_T^{\epsilon})]$$

for all  $f \in L^2(\pi_{ref})$ . 206

**PROPOSITION 8** (Weak convergence of  $\pi^{\epsilon}$  to  $\pi^{0}$ ). Suppose that Assumption 1 207 holds. Then for all  $f \in L^2(\pi_{ref})$ , 208

209 (20) 
$$\int_{\mathbb{R}^d} f(x) \, \pi^{\epsilon}(dx) \to \int_{\mathbb{R}^d} f(x) \pi^0(dx),$$

as  $\epsilon \to 0$ . 210

If Assumption 1 holds, then for every  $\epsilon > 0$ , the potential  $V^{\epsilon}$  is confining, so that 211 the process  $X_t^{\epsilon}$  is ergodic. If the "unperturbed" process defined by (10) converges to 212equilibrium exponentially fast in  $L^2(\pi_{ref})$ , then so will  $X_t^{\epsilon}$  and  $X_t^0$ . Moreover, we can 213relate the rates of convergence of the three processes. 214

**PROPOSITION 9.** Suppose that Assumptions 1 holds and let  $P_t$  be the semigroup 215associated with the dynamics (10) and suppose that  $\pi_{ref}(x) = \frac{1}{Z_0} e^{-V_0(x)/\sigma}$  satisfies 216

217 Poincaré's inequality with constant  $\rho/\sigma$ , i.e.

218 (21) 
$$\operatorname{Var}_{\pi_{ref}}(f) \leq \frac{\sigma}{\rho} \int |\nabla f(x)|^2 \, \pi_{ref}(dx), \quad f \in H^1(\pi_{ref}),$$

219 or equivalently

220 (22) 
$$\operatorname{Var}_{\pi_{ref}}(P_t f) \le e^{-2\rho t/\sigma} \operatorname{Var}_{\pi_{ref}}(f), \quad f \in L^2(\pi_{ref}),$$

for all  $t \ge 0$ . Let  $P_t^{\epsilon}$  and  $P_t^0$  denote the semigroups associated with the full dynamics (6) and homogenized dynamics (17), respectively. Then for all  $f \in L^2(\pi_{ref})$ ,

223 (23) 
$$\operatorname{Var}_{\pi^{\epsilon}}(P_t^{\epsilon}f) \leq e^{-2\gamma t/\sigma} \operatorname{Var}_{\pi^{\epsilon}}(f),$$

224 and

225 (24) 
$$Var_{\pi^0}(P_t^0 f) \le e^{-2\tilde{\gamma}t/\sigma} Var_{\pi^0}(f).$$

226 for  $\gamma = \rho e^{-2osc(V_1)/\sigma}$  and  $\widetilde{\gamma} = \rho e^{-3osc(V_1)/\sigma}$ .

227 The proofs Propositions 8 and 18 will be deferred to Section 4.

**3.** Properties of the Coarse–Grained Process. In this section we study the properties of the coefficients of the homogenized SDE (17) and its dynamics.

**3.1. Separable Potentials.** Consider the special case where the potential  $V^{\epsilon}$  is *separable*, in the sense that the fast scale fluctuations do not depend on the slow scale variable, i.e.

$$V(x_0, x_1, \dots, x_N) = V_0(x_0) + V_1(x_1, x_2, \dots, x_N)$$

Then, it is clear from the construction of the effective diffusion tensor (13) that  $\mathcal{M}(x)$  will not depend on  $x \in \mathbb{R}^d$ . Moreover, since

$$Z(x) = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-\frac{V_0(x) + V_1(y_1, \dots, y_N)}{\sigma}} \, dy_1 \dots dy_N = \frac{1}{K} e^{-V_0(x)/\sigma},$$

where  $K = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} \exp(-V_1(y_1, \ldots, y_N)/\sigma) \, dy_1 \ldots dy_N$ , then it follows that the coarse-grained stationary distribution  $\pi^0$  equals the stationary distribution  $\pi_{ref} \propto$ exp $(-V_0(x)/\sigma)$  of the process (10). For general multiscale potentials however,  $\pi^0$  will be different from  $\pi_{ref}$ . Indeed, introducing multiscale fluctuations can dramatically alter the qualitative equilibrium behaviour of the process, including noise-inductioned transitions and noise induced hysteresis, as has been studied for various examples in [16].

3.2. Variational bounds on  $\mathcal{M}(x)$ . A first essential property is that the constructed matrices  $\mathcal{K}_N, \ldots, \mathcal{K}_1$  are uniformly elliptic with respect to all their parameters, which is shown in the following lemma. For convenience, we shall introduce the notation

241 (25) 
$$\mathbb{X}_k = \mathbb{R}^d \times \bigotimes_{i=1}^k \mathbb{T}^d$$

for k = 1, ..., N, and set  $\mathbb{X}_0 = \mathbb{R}^d$  for consistency. First we require the following existence and regularity result for a uniformly elliptic Poisson equation on  $\mathbb{T}^d$ .

## This manuscript is for review purposes only.

LEMMA 10. For k = 1, ..., N, the tensor  $\mathcal{K}_k(x_0, ..., x_{k-1}, \cdot)$  is uniformly positive definite and in particular satisfies, for all unit vectors  $e \in \mathbb{R}^d$ ,

246 (26) 
$$\frac{1}{\widehat{Z}_k(x_0, x_1, \dots, x_{k-1})} \le e \cdot \mathcal{K}_k(x_0, x_1, \dots, x_{k-1}, x_k) e, \quad x_k \in \mathbb{T}^d$$

where

$$\widehat{Z}_k(x_0, x_1, \dots, x_{k-1}) = \int \dots \int e^{V(x_0, x_1, \dots, x_{k-1}, x_k, \dots, x_N)/\sigma} dx_N dx_{N-1} \dots dx_k,$$

which is independent of  $x_k$ . Moreover, the tensor  $\mathcal{K}_k$  satisfies  $(\mathcal{K}_k)_{i,j} \in C_b^{\infty}(\mathbb{X}_k)$ , for all  $i, j \in \{1, \ldots, d\}$ .

249 Proof. We prove the result by induction on k starting from k = N. For k = N the 250 tensor  $\mathcal{K}_N$  is clearly uniformly positive definite for fixed  $x_0, \ldots, x_{N-1} \in \mathbb{X}_{N-1}$ . The 251 existence of the solution  $\theta_N$  of (14) is then ensured by the Lemma 10, and moreover 252 it follows that  $\mathcal{K}_{N-1}$  is well defined. To show that  $\mathcal{K}_{N-1}(x_0, \ldots, x_{N-2}, \cdot)$  is uniformly 253 elliptic on  $\mathbb{T}^d$  we first note that

254 (27) 
$$\int_{\mathbb{T}^d} (I + \nabla_{x_N} \theta_N)^\top (I + \nabla_{x_N} \theta_N) e^{-V/\sigma} dx_N = \int_{\mathbb{T}^d} (I + \nabla_{x_N} \theta_N + \nabla_{x_N} \theta_N^\top + \nabla_{x_N} \theta_N^\top \nabla_{x_N} \theta_N) e^{-V/\sigma} dx_N,$$

where  $V = V(x_0, x_1, \ldots, x_N)$ , for  $x_0, \ldots, x_{N-1} \in \mathbb{X}_{N-1}$  fixed, and where  $\top$  denotes the transpose. From the Poisson equation for  $\theta_N$  we have

$$\int \theta_N \cdot \nabla_{x_N} \cdot (e^{-V/\sigma} (\nabla_{x_N} \theta_N + I)) e^{-V/\sigma} \, dx_N = 0,$$

from which we obtain, after integrating by parts:

$$\int_{\mathbb{T}^d} \nabla_{x_N} \theta_N^\top \nabla_{x_N} \theta_N e^{-V/\sigma} \, dx_N = -\int \nabla_{x_N} \theta_N^\top e^{-V/\sigma} \, dx_N,$$

255 so that

256 257

$$\mathcal{K}_{N-1} = \int_{\mathbb{T}^d} (I + \nabla_{x_N} \theta_N)^\top (I + \nabla_{x_N} \theta_N) e^{-V/\sigma} \, dx_N.$$

We note that

$$\int_{\mathbb{T}^d} (I + \nabla_N \theta_N) \, dx_N = I,$$

therefore, it follows by Hölder's inequality that

$$|v|^{2} \leq \left| v \cdot \int_{\mathbb{T}^{d}} (I + \nabla_{N} \theta_{N}) v \right|^{2} \leq v \cdot (\mathcal{K}_{N-1}) v \int_{\mathbb{T}^{d}} e^{V/\sigma} dx_{N}$$

so that

$$\frac{|v|^2}{\widehat{Z}_N(x_0,\ldots,x_{N-1})} \le v \cdot \mathcal{K}_{N-1}(x_0,\ldots,x_{N-1})v, \quad \forall (x_0,x_1,\ldots,x_{N_1}).$$

258 Since  $V_1$  is uniformly bounded over  $x_0, \ldots, x_{N-1}$  it follows that  $\widehat{Z}_N$  is strictly posi-

tive, so that  $\mathcal{K}_{N-1}$  is uniformly elliptic, and arguing as above we obtain existence of

a unique  $\theta_{N-1}$ , up to a constant, solving (42) for k = 2.

261

Now, assume that the correctors have been constructed for  $i = N, \ldots, N - k + 1$ and consider the tensor

 $\int \cdots \int (I + \nabla_{i+1}\theta_{i+1})^\top \cdots (I + \nabla_{k+1}\theta_{k+1})^\top$ 

264 (28)

 $\mathcal{K}_k(I + \nabla_{k+1}\theta_{k+1}) \cdots (I + \nabla_{i+1}\theta_{i+1}) \, dx_N \dots dx_{i+1}.$ 

Integrating by parts the cell equation for  $\theta_{k+1}$  we see that

$$\int \left(I + \nabla_{k+1}\theta_{k+1}\right)^{\top} \mathcal{K}_k \left(I + \nabla_{k+1}\theta_{k+1}\right) \, dx_{k+1} = \mathcal{K}_{k-1}.$$

Continuining this approach by induction, it follows that (28) equals  $\mathcal{K}_{i+1}$ , thus proving the representation (27), as required. We now verify (26). First we note that

$$\int \cdots \int (I + \nabla_N \theta_N) \cdots (I + \nabla_{i+1} \theta_{i+1}) dx_N \dots dx_{i+1} = I.$$

265 Therefore, for any vector  $v \in \mathbb{R}^d$ :

$$266 |v|^{2} \leq \left| \left( \int \cdots \int (I + \nabla_{N} \theta_{N}) \cdots (I + \nabla_{i+1} \theta_{i+1}) dx_{N} \dots dx_{i+1} \right) v \right|^{2}$$

$$267 \qquad \leq v \cdot \left( \int \cdots \int (I + \nabla_{i+1} \theta_{i+1})^{\top} \cdots (I + \nabla_{i+1} \theta_{i+1}) e^{-V/\sigma} dx_{N} \dots dx_{i+1} \right) v \int e^{V/\sigma} dx_{N} \dots dx_{i+1}$$

$$268 \qquad = (v \cdot \mathcal{K}_{i+1}(x_{1}, \dots, x_{i})v) \,\widehat{Z}(x_{1}, \dots, x_{i}).$$

270 The fact that we have strict positivity for fixed  $x_1, \ldots x_i$  then follows immediately.

To obtain upper bounds for the effective diffusion coefficient, we will express the intermediary diffusion tensors  $\mathcal{K}_i$  as solutions of a quadratic variational problem. This variational formulation of the diffusion tensors can be considered as a generalisation of the analogous representation for the effective conductivity coefficient of a two-scale composite material, see for example [26, 32, 9].

276 LEMMA 11. For i = 1, ..., N, the tensor  $\mathcal{K}_i$  satisfies (29)  $e \cdot \mathcal{K}_i(x_0, ..., x_i)e$ 

$$= \inf_{v_{i+1},\dots,v_N \in H^1(\mathbb{T}^d)} \int_{(\mathbb{T}^d)^N} |e + \nabla v_{i+1}(x_i) + \dots + \nabla v_N(x_N)|^2 e^{-V(x_0,\dots,x_N)/\sigma} dx_N \dots dx_{i+1} dx$$

278 for all 
$$e \in \mathbb{R}^d$$
.

279 *Proof.* For i = 1, ..., N, from the proof of Lemma 10 we can express the inter-280 mediary diffusion tensor  $\mathcal{K}_{i-1}$  in the following recursive manner,

281 
$$e \cdot \mathcal{K}_{i-1}(x_0, \dots, x_{i-1})e$$
282
283 
$$= \int_{\mathbb{T}^d} (e + e \cdot \nabla_{x_i} \theta_i(x_0, \dots, x_i))^\top \mathcal{K}_i(x_0, \dots, x_i)(e + e \cdot \nabla_{x_i} \theta_i(x_0, \dots, x_i)) \, dx_i.$$

For fixed  $x_0, \ldots, x_{i-1} \in \mathbb{X}_{i-1}$  and  $e \in \mathbb{R}^d$ , consider the tensor  $\widetilde{\mathcal{K}}_{i-1}$  defined by the following quadratic minimization problem

286 (30) 
$$e \cdot \widetilde{\mathcal{K}}_{i-1}(x_0, \dots, x_{i-1})e = \inf_{v \in H^1(\mathbb{T}^d)} \int_{\mathbb{T}^d} (e + \nabla v(x_i)) \cdot \mathcal{K}_i(x_0, \dots, x_i)(e + \nabla v(x_i)) \, dx_i.$$

Since  $\mathcal{K}_i$  is a symmetric tensor, the corresponding Euler-Lagrange equation for the minimiser is given by

$$\nabla_{x_i} \cdot (\mathcal{K}_i(x_0, \dots, x_i)(\nabla_{x_i}\chi(x_0, \dots, x_i) + e)) = 0, \quad x \in \mathbb{T}^d,$$

with periodic boundary conditions. This equation has unique mean zero solution given by  $\chi(x_0, \ldots, x_i) = \theta_i(x_0, \ldots, x_i) \cdot e$ , where  $\theta_i$  is the unique mean-zero solution of (14).

It thus follows that  $e \cdot \mathcal{K}_{i-1}e = e \cdot \mathcal{K}_{i-1}e$ , where  $\mathcal{K}_{i-1}$  is given by (30). Expanding  $\mathcal{K}_i$ in a similar fashion, we obtain

291 
$$e \cdot \mathcal{K}_{i-1}(x_0,\ldots,x_{i-1})e$$

$$\underset{v_{i},v_{i+1}\in H^{1}(\mathbb{T}^{d})}{\inf} \int_{\mathbb{T}^{d}} \int_{\mathbb{T}^{d}} \int_{\mathbb{T}^{d}} \left( e + \nabla v_{i}(x_{i}) + \nabla v_{i+1}(x_{i+1}) \right) \cdot \mathcal{K}_{i+1}(x_{0},\ldots,x_{i+1}) (e + \nabla v_{i}(x_{i}) + \nabla v_{i+1}(x_{i+1})) \, dx_{i+1} dx_{i}.$$

294 Proceeding recursively, we arrive at

$$295 \quad e \cdot \mathcal{K}_{i-1}(x_0, \ldots, x_{i-1})e$$

296 =  $\inf_{v_i,...,v_N \in H^1(\mathbb{T}^d)} \int_{(\mathbb{T}^d)^N} |e + \nabla v_i(x_i) + \ldots + \nabla v_N(x_N)|^2 e^{-V(x_0,...,x_N)/\sigma} dx_N \ldots dx_i,$ 

298 as required.

REMARK 12. Proposition 5 follows immediately from Lemma 11 by choosing

$$v_1=v_2=\ldots=v_N=0,$$

299 in (29) in the case where i = 1.

4. Properties of the Equilibrium Distributions. In this section we study in more detail the properties of the equilibrium distributions  $\pi^{\epsilon}$  and  $\pi^{0}$  of the full (6) and homogenized (17) dynamics, respectively. We first provide a proof of Proposition 8. The approach we follow in this proof is based on properties of periodic functions, in a manner similar to [14, Sec. 2].

*Proof of Proposition 8.* First we note that, by Assumptions 1, there exists a C > 0 independent of  $\epsilon$ , such that

$$\int_{\mathbb{R}^d} \left| e^{-V_1(x, x/\epsilon, \dots, x/\epsilon^N)/\sigma} \right|^2 e^{-V_0(x)/\sigma} \, dx \le C < \infty.$$

It follows that there exists  $\Lambda \in L^2(\mathbb{R}^d; e^{-V_0/\sigma})$  and a subsequence  $(\epsilon_n)_{n \in \mathbb{N}}$  where  $\epsilon_n \to 0$  such that

$$\int_{\mathbb{R}^d} e^{-V_1(x, x/\epsilon_n, \dots, x/\epsilon_n^N)/\sigma} g(x) e^{-V_0(x)/\sigma} \, dx \xrightarrow{n \to \infty} \int_{\mathbb{R}^d} \Lambda(x) g(x) e^{-V_0(x)/\sigma} \, dx,$$

for all  $g \in L^2(\pi_{ref})$ . To identify the limit, we choose  $g = \mathbf{1}_{\Omega}$  where  $\Omega$  is an open bounded subset of  $\mathbb{R}^d$  where  $\partial\Omega$  is smooth; noting that the span of such functions is dense in  $L^2(\pi_{ref})$ .

Following [36] and [14, Sec. 2.3], given  $\Omega$  and  $\epsilon > 0$ , let  $\{Y_k\}_{k=1,\ldots,N(\epsilon)}$  be a collection of pairwise disjoint translations of  $\mathbb{T}^d$ , such that  $\epsilon^N Y_k \subset \Omega$ , for  $k = 1, \ldots, N(\epsilon)$  and for all  $\delta > 0$ , there exists  $\epsilon_0$  such that

$$\lambda\left(\Omega\setminus \cup_{k=1}^{N(\epsilon)}\epsilon^N Y_k\right)<\delta,$$

for all  $\epsilon < \epsilon_0$ , where  $\lambda(\cdot)$  denotes the Lebesgue measure on  $\mathbb{R}^d$ . Given  $\delta > 0$ , there 305 306 exists  $\epsilon_0$  such that for  $\epsilon < \epsilon_0$ ,

307 
$$\int_{\Omega} e^{-V^{\epsilon}(x)/\sigma} dx = \sum_{k=1}^{N(\epsilon)} \int_{\epsilon^{N} Y_{k}} e^{-V^{\epsilon}(x)/\sigma} dx + O(\delta)$$
208 
$$-\sum_{k=1}^{N(\epsilon)} \int_{\Omega} e^{-V(x,x/\epsilon,\dots,x/\epsilon^{N-1},x/\epsilon^{N})/\sigma} dx + O(\delta)$$

308

$$= \sum_{k=1}^{N} \int_{\epsilon^{N}(x_{k}+\mathbb{T}^{d})} e^{-V(\epsilon^{N}(x_{k}+y),\epsilon^{N-1}(x_{k}+y),\dots,\epsilon(x_{k}+y),y)/\sigma} dy + C(\delta)$$

309
$$=\epsilon^{Nd}\sum_{k=1}\int_{\mathbb{T}^d} e^{-V(\epsilon^N(x_k+y),\epsilon^{N-1}(x_k+y),\dots,\epsilon(x_k+y),y)/\sigma} \, dy + O(\delta)$$

310 
$$= \epsilon^{Nd} \sum_{k=1}^{\infty} \int_{\mathbb{T}^d} e^{-V(\epsilon^N x_k, \epsilon^{N-1} x_k, \dots, \epsilon x_k, y)/\sigma} \, dy + O(\delta)$$

311 
$$= \int_{\bigcup_{k=1}^{N(\epsilon)} Y_k} \int_{\mathbb{T}^d} e^{-V(x, x/\epsilon, \dots, x/\epsilon^{N-1}, y)/\sigma} \, dy \, dx + O(\delta)$$

$$= \int_{\Omega} \int_{\mathbb{T}^d} e^{-V(x,x/\epsilon,\dots,x/\epsilon^{N-1},y)/\sigma} \, dy \, dx + O(\delta),$$

where we use the fact that V is smooth with bounded derivatives on  $\Omega$ . Proceeding iteratively in the above manner, we obtain that for all  $\delta > 0$ , there exists  $\epsilon_0$  such that

$$\int_{\Omega} e^{-V^{\epsilon}(x)/\sigma} dx = \int_{\Omega} \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V(x,y_1,\dots,y_N)/\sigma} dy_N \dots dy_N dx + O(\delta),$$

for all  $\epsilon < \epsilon_0$ . Thus it follows that

$$\Lambda(x) = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V_1(x, y_1, \dots, y_N)/\sigma} \, dy_N \, dy_{N-1} \, \dots \, dy_1$$

In particular,

$$Z^{\epsilon} = \int_{\mathbb{R}^d} e^{-V^{\epsilon}(x)/\sigma} \, dx \to Z^0 = \int_{\mathbb{R}^d} \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V(x,y_1,\dots,y_N)/\sigma} \, dy_N \, \dots \, dy_1 \, dx,$$

and thus, for all  $h \in L^2(\mathbb{R}^d; e^{-V_0(x)/\sigma})$ 

$$\int h(x)\pi^{\epsilon}(x)\,dx \to \int h(x)\pi^{0}(x)\,dx,$$

as  $\epsilon \to 0$ , as required. 314

Proof of Proposition 9. Since  $V_1$  is bounded uniformly by Assumption 1, it is 315straightforward to check that 316

317 (31) 
$$\pi_{ref}(x)e^{-2osc(V_1)/\sigma} \le \pi^{\epsilon}(x) \le \pi_{ref}(x)e^{2osc(V_1)/\sigma}.$$

It thus follows directly from (21), or alternatively from [6, Lemma 5.1.7], that  $\pi^{\epsilon}$ satisfies Poincaré's inequality with constant

$$\gamma = \frac{\rho}{\sigma} e^{-2\mathrm{OSC}(V_1)/\sigma},$$

which implies (23). An identical argument follows for the coarse–grained density  $\pi^0(x)$ . Finally, using the fact that

$$|v|^2 e^{-osc(V_1)/\sigma} \le \frac{|v|^2}{Z(x)\widehat{Z}(x)} \le v \cdot \mathcal{M}(x)v,$$

for all  $v \in \mathbb{R}^d$ , we obtain 318

319  

$$\operatorname{Var}_{\pi^{0}}(f) \leq \frac{\sigma}{\rho} e^{2osc(V_{1})/\sigma} \int_{\mathbb{R}^{d}} |\nabla f(x)|^{2} \pi^{0}(x) \, dx$$
320  
321  

$$\leq \frac{\sigma}{\rho} e^{3osc(V_{1})/\sigma} \int \nabla f(x) \cdot \mathcal{M}(x) \nabla f(x) \, \pi^{0}(x) \, dx,$$

from which (24) follows. 322

REMARK 13. Note that one can similarly relate the constants in the Logarithmic 323 Sobolev inequalities for the measures  $\pi_{ref}$ ,  $\pi^{\epsilon}$  and  $\pi^{0}$  in an almost identical manner, 324based on the Holley-Stroock criterion [24]. 325

REMARK 14. Proposition 9 requires the assumption that the multiscale perturbation  $V_1$  is bounded uniformly. If this is relaxed, then it is no longer guaranteed that  $\pi^{\epsilon}$  will satisfy a Poincaré inequality, even though  $\pi_{ref}$  does. For example, consider the potential

$$V^{\epsilon}(x) = x^2 (1 + \alpha \cos(2\pi x/\epsilon)),$$

then the corresponding Gibbs distribution  $\pi^{\epsilon}(x)$  will not satisfy Poincaré's inequality for any  $\epsilon > 0$ . Following [22, Appendix A] we demonstrate this by checking that this choice of  $\pi^{\epsilon}$  does not satisfy the Muckenhoupt criterion [34, 4] which is necessary and sufficient for the Poincaré inequality to hold, namely that  $\sup_{r \in \mathbb{R}} B_{\pm}(r) < \infty$ , where

$$B_{\pm}(r) = \left(\int_{r}^{\pm\infty} \pi^{\epsilon}(x) \, dx\right)^{\frac{1}{2}} \left(\int_{[0,\pm r]} \frac{1}{\pi^{\epsilon}(x)} \, dx\right)^{\frac{1}{2}}.$$

Given  $n \in \mathbb{N}$ , we set  $r/\epsilon = 2\pi n + \pi/2$ . Then we have that 326

327 
$$B_{+}(r) \ge \left(\int_{\epsilon(2\pi n + 4\pi/3)}^{\epsilon(2\pi n + 4\pi/3)} e^{-|x|^{2}(1 - \alpha/2)/\sigma} dx\right)^{1/2} \left(\int_{\epsilon(2\pi n - \pi/3)}^{\epsilon(2\pi n + \pi/3)} e^{|x|^{2}(1 + \alpha/2)/\sigma} dx\right)^{1/2}$$

$$\geq \left(\frac{2\pi\epsilon}{3}\right) \exp\left(-\frac{|\pi\epsilon(2n+4/3)|^2}{2\sigma}\left(1-\frac{\alpha}{2}\right) + \frac{|\pi\epsilon(2n-1/3)|^2}{2\sigma}\left(1+\frac{\alpha}{2}\right)\right)$$

329 
$$= \left(\frac{2\pi\epsilon}{3}\right) \exp\left(-\frac{|2\pi\epsilon n|^2(1+2/3n)^2}{2\sigma}\left(1-\frac{\alpha}{2}\right) + \frac{|2\pi\epsilon n|^2(1-1/6n)^2}{2\sigma}\left(1+\frac{\alpha}{2}\right)\right)$$

$$\underset{331}{\overset{330}{331}} \approx \left(\frac{2\pi\epsilon}{3}\right) \exp\left(\frac{|2\pi\epsilon n|^2}{2\sigma} \left(\alpha + o(n^{-1})\right)\right) \to \infty, \quad as \ n \to \infty,$$

332 so that Poincaré's inequality does not hold for  $\pi^{\epsilon}$ .

A natural question to ask is whether the weak convergence of  $\pi^{\epsilon}$  to  $\pi^{0}$  holds 333 true in a stronger notion of distance such as total variation. The following simple 334 one-dimensional example demonstrates that the convergence cannot be strengthened 335336 to total variation.

EXAMPLE 15. Consider the one dimensional Gibbs distribution

$$\pi^{\epsilon}(x) = \frac{1}{Z^{\epsilon}} e^{-V^{\epsilon}(x)/\sigma},$$

where

$$V^{\epsilon}(x) = \frac{x^2}{2} + \alpha \sin\left(2\pi \frac{x}{\epsilon}\right),$$

and where  $Z^{\epsilon}$  is the normalization constant and  $\alpha \neq 0$ . Then the measure  $\pi^{\epsilon}$  converges weakly to  $\pi^{0}$  given by

$$\pi^0(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-x^2/2\sigma}$$

From the plots of the stationary distributions in Figure 2a it becomes clear that the density of  $\pi^{\epsilon}$  exhibits rapid fluctuations which do not appear in  $\pi^{0}$ , thus we do not expect to be able to obtain convergence in a stronger metric. First we consider the distance between  $\pi^{\epsilon}$  and  $\pi^{0}$  in total variation <sup>4</sup>

$$\|\pi^{\epsilon} - \pi^{0}\|_{TV} = \int_{\mathbb{R}^{d}} |\pi^{\epsilon}(x) - \pi^{0}(x)| \, dx = \int_{\mathbb{R}^{d}} \frac{e^{-x^{2}/2\sigma}}{\sqrt{2\sigma}} \left| 1 - \frac{e^{-\frac{\alpha}{\sigma}\cos(2\pi x/\epsilon)}}{K^{\epsilon}} \right| \, dx,$$

343 where  $K^{\epsilon} = Z^{\epsilon}/\sqrt{2\pi\sigma}$ . It follows that

344 
$$\|\pi^{\epsilon} - \pi^{0}\|_{TV} \ge \sum_{n \ge 0} \int_{\epsilon(2\pi n - \pi/3)}^{\epsilon(2\pi n + \pi/3)} \frac{e^{-x^{2}/2\sigma}}{\sqrt{2\pi\sigma}} \, dx \left| 1 - \frac{e^{-\frac{\alpha}{2\sigma}}}{K^{\epsilon}} \right|$$

345 
$$\geq \sum_{n\geq 0} \frac{2\epsilon\pi}{3} \frac{e^{-\epsilon^2 (2n\pi+\pi/3)^2/2\sigma}}{\sqrt{2\pi\sigma}} \left| 1 - \frac{e^{-\frac{\alpha}{2\sigma}}}{K^{\epsilon}} \right|$$

$$\geq \int_0^\infty \frac{2\pi}{3} \frac{e^{-2\pi^2 (x+\epsilon/6)^2/\sigma}}{\sqrt{2\pi\sigma}} \left| 1 - \frac{e^{-\frac{\alpha}{2\sigma}}}{K^\epsilon} \right|,$$

where we use the fact that  $e^{-\alpha/2\sigma}/K^{\epsilon} \leq 1$ . In the limit  $\epsilon \to 0$ , we have  $K^{\epsilon} \to I_0(\alpha/\sigma)$ , where  $I_n(\cdot)$  is the modified Bessel function of the first kind of order n. Therefore, as  $\epsilon \to 0$ ,

351 (32) 
$$\|\pi^{\epsilon} - \pi^{0}\|_{TV} \ge \int_{0}^{\infty} \frac{2\pi}{3} \frac{e^{-2\pi^{2}(x+\epsilon/6)^{2}/\sigma}}{\sqrt{2\pi\sigma}} \left|1 - \frac{e^{-\frac{\alpha}{2\sigma}}}{K^{\epsilon}}\right| = \frac{1}{6} \left|1 - \frac{e^{-\frac{\alpha}{2\sigma}}}{I_{0}(\alpha/\sigma)}\right|,$$

which converges to  $\frac{1}{6}$  as  $\frac{\alpha}{\sigma} \to \infty$ . Since relative entropy controls total variation distance by Pinsker's theorem, it follows that  $\pi^{\epsilon}$  does not converge to  $\pi^{0}$  in relative entropy, either. Nonetheless, we shall compute the distance in relative entropy between  $\pi^{\epsilon}$  and  $\pi^{0}$  to understand the influence of the parameters  $\sigma$  and  $\alpha$ . Since both  $\pi^{0}$  and  $\pi^{\epsilon}$  have strictly positive densities with respect to the Lebesgue measure on  $\mathbb{R}$ , we have that

$$\frac{d\pi^{\epsilon}}{d\pi^{0}}(x) = \frac{\sqrt{2\pi\sigma}}{Z^{\epsilon}} e^{-V^{\epsilon}(x)/\sigma + \frac{1}{2}x^{2}/\sigma}.$$

<sup>&</sup>lt;sup>4</sup>we are using the same notation for the measure and for its density with respect to the Lebesgue measure on  $\mathbb{R}^d$ .

352 Then, for 
$$Z^0 = \sqrt{2\pi\sigma}I_0(1/\sigma)$$
,  
353  $H\left(\pi^{\epsilon} \mid \pi^0\right) = \frac{1}{Z^{\epsilon}} \int \left(\frac{1}{2}\log(2\pi\sigma) - \log Z^{\epsilon}\right) e^{-V^{\epsilon}(x)/\sigma} dx$ 

$$+ \frac{1}{Z^{\epsilon}} \int \left( -V^{\epsilon}(x)/\sigma + x^2/2\sigma \right) e^{-V^{\epsilon}(x)/\sigma} dx$$

355 
$$\xrightarrow{\epsilon \to 0} -\log I_0(\alpha/\sigma) + \frac{\alpha}{\sigma Z^0} \lim_{\epsilon \to 0} \int \cos(2\pi x/\epsilon) e^{-x^2/2\sigma - \alpha \cos(2\pi x/\epsilon)/\sigma} dx$$

$$= -\log I_0(\alpha/\sigma) + \frac{\alpha}{\sigma} \frac{I_1(\alpha/\sigma)}{I_0(\alpha/\sigma)} =: K(\alpha/\sigma).$$

and it is straightfoward to check that K(s) > 0, and moreover

$$K(s) \to \begin{cases} +\infty & as \ s \to 0, \\ 0 & as \ s \to \infty \end{cases}$$

In Figure 2b we plot the value of K(s) as a function of s. From this result, we see 358 that for fixed  $\alpha > 0$ , the measure  $\pi^{\epsilon}$  will converge in relative entropy only in the limit 359 360 as  $\sigma \to \infty$ , while the measures will become increasingly mutually singular as  $\sigma \to 0$ .



Fig. 2: Error between  $\pi^{\epsilon}(x) \propto \exp(-V^{\epsilon}(x)/\sigma)$  and effective distribution  $\pi^{0}$ .

5. Proof of weak convergence. In this section we show that over finite time 361 intervals [0,T], the process  $X_t^{\epsilon}$  converges weakly to a process  $X_t^0$  which is uniquely 362identified as the weak solution of a coarse-grained SDE. The approach we adopt is 363 based on the classical martingale methodology of [9, Section 3]. The proof of the 364 homogenization result is split into three steps. 365

- 1. We construct an appropriate test function which is used to decompose the 366 fluctuations of the process  $X_t^{\epsilon}$  into a martingale part and a term which goes 367 368 to zero as  $\epsilon \to 0$ .
- 2. Using this test function, we demonstrate that the path measure  $\mathbb{P}^{\epsilon}$  corre-369 sponding to the family  $\left\{ (X_t^{\epsilon})_{t \in [0,T]} \right\}_{0 < \epsilon \leq 1}$  is tight in  $C([0,T]; \mathbb{R}^d)$ . 3. Finally, we show that any limit point of the family of measures must solve a 370
- 371 372 well-posed martingale problem, and is thus unique.

The test functions will be constructed by solving a recursively defined sequence 373 of Poisson equations on  $\mathbb{R}^d$ . We first provide a general well-posedness result for this 374375 class of equations.

PROPOSITION 16. For fixed  $(x_0, \ldots, x_{k-1}) \in \mathbb{X}_{k-1}$ , let  $S_k$  be the operator given by

378 
$$S_k = \frac{1}{\rho(x_0, \dots, x_k)} \nabla_{x_k} \cdot (\rho(x_0, \dots, x_k) D(x_0, \dots, x_k) \nabla_{x_k} u(x_0, \dots, x_k)), \quad f \in C^2(\mathbb{T}^d),$$

and suppose that  $\rho$  is smooth and uniformly positive and bounded, and the tensor  $D(x_0, \ldots, x_k)$  is smooth and uniformly positive definite on  $\mathbb{X}_k$ . Given a function h which is smooth with bounded derivatives, such that for each  $(x_0, \ldots, x_{k-1}) \in \mathbb{X}_{k-1}$ :

382 (34) 
$$\int h(x_0, \dots, x_k) \rho(x_0, \dots, x_k) \, dx_k = 0.$$

Then there exists a unique, mean-zero solution  $u \in H^1(\mathbb{T}^d)$ , to the Poisson equation on  $\mathbb{T}^d$  given by

385 (35) 
$$S_k u(x_0, \dots, x_k) = h(x_0, \dots, x_k),$$

which is smooth and bounded with respect to the variable  $x_k \in \mathbb{T}^d$  as well as the parameters  $x_0, \ldots, x_{k-1} \in \mathbb{X}_{k-1}$ .

*Proof.* Since  $\rho(\cdot)$  and  $D(\cdot)$  are strictly positive, for fixed values of  $x_0, \ldots, x_{k-1}$ , the operator  $S_k$  is uniformly elliptic, and since  $\mathbb{T}^d$  is compact,  $S_k$  has compact resolvent in  $L^2(\mathbb{T}^d)$ , see [18, Ch. 6] and [44, Ch 7]. The nullspace of the adjoint  $S^*$  is spanned by a single function  $\rho(x_0, \ldots, x_{k-1}, \cdot)$ . By the Fredholm alternative, a necessary and sufficient condition for the existence of u is (34) which is assumed to hold. Thus, there exists a unique solution  $u(x_0, \ldots, x_{k-1}, \cdot) \in H^1(\mathbb{T}^d)$  having mean zero with respect to  $\rho(x_0, \ldots, x_k)$ . By elliptic estimates and Poincaré's inequality, it follows that there exists C > 0 satisfying

$$||u(x_0,\ldots,x_{k-1},\cdot)||_{H^1(\mathbb{T}^d)} \le C ||h(x_0,\ldots,x_{k-1},\cdot)||_{L^2(\mathbb{T}^d)},$$

for all  $(x_0,\ldots,x_{k-1}) \in \mathbb{X}_{k-1}$ . Since the components of D and  $\rho$  are smooth 388 with respect to  $x_k$ , standard interior regularity results [20] ensure that, for fixed 389 $x_0,\ldots,x_{k-1}\in\mathbb{X}_{k-1}$ , the function  $u(x_0,\ldots,x_{k-1},\cdot)$  is smooth. To prove the smooth-390 ness and boundedness with respect to the other parameters  $x_0, \ldots, x_{k-1}$ , we can apply 391 an approach either similar to [9], by showing that the finite differences approximation 392 of the derivatives of u with respect to the parameters has a limit, or otherwise, by 393 directly differentiating the transition density of the semigroup associated with the 394 395 generator  $\mathcal{S}_k$ , see for example [40, 50, 41] as well as [20, Sec 8.4].

REMARK 17. Suppose that the function h in Proposition 16 can be expressed as

$$h(x_0,\ldots,x_k) = a(x_0,x_1,\ldots,x_k) \cdot \nabla \phi_0(x_0)$$

where a is smooth with all derivatives bounded. Then the mean-zero solution of (35) can be written as

$$u(x_0, x_1, \dots, x_k) = \chi(x_0, x_1, \dots, x_k) \cdot \nabla \phi_0(x_0),$$

where  $\chi$  is the classical mean-zero solution to the following Poisson equation

$$\mathcal{S}_k \chi(x_0, \dots, x_k) = a(x_0, \dots, x_k), \quad (x_0, \dots, x_k) \in \mathbb{X}_k$$

In particular,  $\chi$  is smooth and bounded over  $x_0, \ldots, x_k$ , so that for some C > 0,

$$\|\nabla^{\alpha} u(x_0, \dots, x_k)\|_F \le C \sum_{k=0}^{\alpha_0} \|\nabla^{k+1} \phi_0(x_0)\|_F, \quad \forall x_0, x_1, \dots, x_k,$$

for all multi-indices  $\alpha = (\alpha_0, \ldots, \alpha_k)$  on the indices  $(0, \ldots, k)$ , where  $\|\cdot\|_F$  denotes the Frobenius norm. A similar decomposition is possible for

$$g(x_0,...,x_k) = A(x_0,x_1,...,x_k) : \nabla^2 \phi_0(x_0),$$

396 where  $\nabla^2$  denotes the Hessian.

**5.1.** Contructing the test functions. It is clear that we can rewrite (6) as

398 (36) 
$$dX_t^{\epsilon} = -\sum_{i=0}^N \epsilon^{-i} \nabla_{x_i} V(x_1, \dots, x_N) \Big|_{x_j = X_t^{\epsilon}/\epsilon^j} dt + \sqrt{2\sigma} \, dW_t$$

The generator of  $X_t^{\epsilon}$  denoted by  $\mathcal{L}^{\epsilon}$  can be decomposed into powers of  $\epsilon$  as follows

$$\mathcal{L}^{\epsilon} = -\sum_{n=0}^{N} \epsilon^{-n} \nabla_{x_n} V \cdot \nabla_x + \sigma \Delta_x.$$

For functions of the form  $f^{\epsilon}(x) = f(x, x/\epsilon, \dots, x/\epsilon^N)$  we write

$$\mathcal{L}^{\epsilon} f^{\epsilon}(x) = \sum_{n=0}^{2N} \epsilon^{-n} \mathcal{L}_n f(x_0, x_1 \dots, x_N) \big|_{x_i = x/\epsilon^i},$$

where

$$\mathcal{L}_n = e^{V/\sigma} \sum_{\substack{i,j \in \{1,\dots,N\}\\i+j=n}} \nabla_{x_i} \cdot \left(\sigma e^{-V/\sigma} \nabla_{x_j} \cdot\right)$$

399 Given  $\phi_0$ , our objective is to construct a test function  $\phi^{\epsilon}$  such that

400 
$$\phi^{\epsilon}(x) = \phi_0(x) + \epsilon \phi_1(x, x/\epsilon) + \ldots + \epsilon^N \phi_N(x, x/\epsilon, \ldots, x/\epsilon^N) + \epsilon^{N+1} \phi_{N+1}(x, x/\epsilon, \ldots, x/\epsilon^N) + \ldots + \epsilon^{2N} \phi_{2N}(x, x/\epsilon, \ldots, x/\epsilon^N),$$

403 where  $\phi_1, \ldots, \phi_{2N}$  satisfy

404 (37) 
$$\mathcal{L}^{\epsilon}\phi^{\epsilon}(x) = F(x) + O(\epsilon),$$

for some F which is independent of  $\epsilon$ . This is equivalent to the following sequence of N + 1 equations.

407 (38a) 
$$\mathcal{L}_{2N}\phi_N + \mathcal{L}_{2N-1}\phi_{N-1} + \dots \mathcal{L}_N\phi_0 = 0,$$

408 (38b) 
$$\mathcal{L}_{2N}\phi_{N+1} + \mathcal{L}_{2N-1}\phi_N + \dots + \mathcal{L}_{N-1}\phi_0 = 0,$$

409

410 (38c) 
$$\mathcal{L}_{2N}\phi_{2N-1} + \ldots + \mathcal{L}_1\phi_0 = 0,$$

÷

411 (38d)  $\mathcal{L}_{2N}\phi_{2N} + \ldots + \mathcal{L}_0\phi_0 = F(x),$ 

where F(x) is a function of x only. This generalizes the analogous expansion found in [9, III-11.3], written for three scales. These N+1 equations correspond to the different powers of  $\epsilon$  in an expansion of  $\mathcal{L}^{\epsilon}\phi^{\epsilon}$ , from  $O(\epsilon^{-N})$  to O(1). For  $k = 1, \ldots, N$ , we note that each term in (38a), (38b) to (38c) has the form

$$\sigma e^{V(x_0,\ldots,x_N)/\sigma} \nabla_{x_s} \cdot \left( e^{-V(x_0,\ldots,x_N)/\sigma} \nabla_t \phi_r \right),$$

where  $k = s + t - r \in \{1, \ldots, N\}$ . Suppose that s = 0, so that t = k + r, where  $t \in \{1, \ldots, N\}$  and  $r \in \{0, \ldots, N-1\}$ . Thus r < t, which is a contradiction. It follows necessarily that s > 1, for every term in the first N equations. In particular, since we have

$$V(x_0,...,x_N) = V_0(x_0) + V_1(x_0,...,x_N),$$

we can rewrite the first N equations as 413

414 (39a) 
$$\mathcal{A}_{2N}\phi_N + \mathcal{A}_{2N-1}\phi_{N-1} + \dots + \mathcal{A}_N\phi_0 = 0,$$

415 (39b) 
$$\mathcal{A}_{2N}\phi_{N+1} + \mathcal{A}_{2N-1}\phi_N + \dots + \mathcal{A}_{N-1}\phi_0 = 0,$$

416

416  

$$4_{1\overline{8}}$$
 (39c)  
 $\mathcal{A}_{2N}\phi_{2N-1} + \ldots + \mathcal{A}_{1}\phi_{0} = 0,$ 

where

$$\mathcal{A}_{n}f = \sigma e^{V_{1}(x_{0},...,x_{N})/\sigma} \sum_{\substack{i \in \{1,...,N\}\\j \in \{0,...,N-1\}\\i+i=n}} \nabla_{x_{i}} \cdot \left(e^{-V_{1}(x_{0},...,x_{N})/\sigma} \nabla_{x_{j}}f\right)$$

Before constructing the test functions, we first we introduce the sequence of spaces on which the sequence of correctors will be constructed. Define  $\mathcal{H}$  to be the space of functions on the extended state space, i.e.  $\mathcal{H} = L^2(\mathbb{X}_k)$ , where  $\mathbb{X}_k$  is defined by (25). We construct the following sequence of subspaces of  $\mathcal{H}$ . Let

$$\mathcal{H}_N = \left\{ f \in \mathcal{H} : \int f(x_0, \dots, x_N) e^{-V_1/\sigma} \, dx_N = 0 \right\}.$$

Then clearly  $\mathcal{H} = \mathcal{H}_N \oplus \mathcal{H}_N^{\perp}$ . Suppose we have defined  $\mathcal{H}_{N-k+1}$  then we can define  $\mathcal{H}_{N-k}$  inductively by

$$\mathcal{H}_{N-k} = \left\{ f \in \mathcal{H}_{N-k+1} : \int f(x_0, \dots, x_{N-k}) Z_{N-k}(x_0, \dots, x_{N-k}) \, dx_{N-k} = 0 \right\},$$

where  $Z_i(x_0, \ldots, x_i) = \int \ldots \int e^{-V_1(x_0, \ldots, x_N)/\sigma} dx_{i+1} dx_{i+2} \ldots dx_N = 0$ . Clearly, we have that  $\mathcal{H}_1 \oplus \mathcal{H}_1^{\perp} \oplus \ldots \oplus \mathcal{H}_N^{\perp} = \mathcal{H}$ . We now construct a series of correctors  $\theta_1, \ldots, \theta_N$ which are used to define the test functions. Define

$$\mathcal{K}_N(x_0, x_1, \dots, x_N) = e^{-V_1(x_0, x_1, \dots, x_N)/\sigma^2} I.$$

We note that the matrix  $\mathcal{K}_N$  is uniformly positive definite over  $\mathbb{X}_N$ . Fixing 419 $x_0, x_1, \ldots, x_{N-1}$ , let  $\theta_N$  be the solution of the vector-valued Poisson equation 420

421 (40) 
$$\nabla_{x_N} \cdot (\mathcal{K}_N (\nabla_{x_N} \theta_N + I)) = 0, \quad x_N \in \mathbb{T}^d,$$

where the notation  $(\nabla_x \theta)_{i,j} = \partial_{x_j} \theta_i$ ,  $i, j \in \{1, \dots, d\}$  is used. By Proposition 16, for 422each  $(x_0, \ldots, x_{N-1})$  there exists a unique smooth solution  $\theta_N(x_0, \ldots, x_{N-1}, \cdot)$  which 423

is also smooth with respect to the parameters  $x_0, \ldots, x_{N-1}$ . Now, suppose that  $\mathcal{K}_i$ and  $\theta_i$  have been defined for  $i \in \{N, \ldots, N-k+1\}$ , define

(41) 
$$\mathcal{K}_{N-k}(x_0, x_1, \dots, x_{N-k}) = \int (I + \nabla_N \theta_N^\top) \cdots (I + \nabla_{N-k+1} \theta_{N-k+1}^\top) e^{-V_1/\sigma^2} dx_N \dots dx_{N-k+1}.$$

427 Then by Lemma 10 the matrix  $\mathcal{K}_{N-k}$  is strictly positive definite over  $(x_0, \ldots, x_{N-k})$ 

and so there exists a unique vector-valued solution  $\theta_{N-k}$  in  $(H^1(\mathbb{T}^d) \cap \mathcal{H}_{N-k})^d$  to the Poisson equation:

430 (42) 
$$\nabla_{x_{N-k}} \cdot \left( \mathcal{K}_{N-k} (\nabla_{x_{N-k}} \theta_{N-k} + I) \right) = 0, \quad x_{N-k} \in \mathbb{T}^d.$$

431 PROPOSITION 18. Given  $\phi_0 \in C^{\infty}(\mathbb{R}^d)$ , there exist smooth functions  $\phi_i$  for i =432 1,..., 2N-1 such that equations (39a)-(39c) are satisfied, and moreover we have the 433 following pointwise estimates, which hold uniformly on  $x_0, \ldots, x_k \in \mathbb{X}_k$ :

434 (43) 
$$\|\nabla^{\alpha}\phi_i(x_0,\ldots,x_k)\|_F \le C \sum_{l=1}^{\alpha_0+2} \|\nabla_{x_0}^l\phi_0(x_0)\|_F,$$

for some constant C > 0, and all multiindices  $\alpha$  on  $(0, \ldots, k)$ , and all  $0 \le k \le i \le$ 2N - 1. Finally, equation (38d) is satisfied with

437 (44) 
$$F(x) = \frac{1}{Z(x)} \nabla_{x_0} \left( \mathcal{K}_1(x) \nabla_{x_0} \phi_0(x) \right).$$

*Proof.* We start from the  $O(\epsilon^{-N})$  equation. Since the operator  $\mathcal{A}_{2N}$  has a compact resolvent in  $L^2(\mathbb{T}^d)$ , by the Fredholm alternative a necessary and sufficient condition for  $\phi_N$  in (38a) to have a solution is that

$$\int \left(\mathcal{A}_{2N-1}\phi_{N-1} + \mathcal{A}_{2N-2}\phi_{N-2} + \ldots + \mathcal{A}_N\phi_0\right) e^{-V/\sigma} dx_N = 0.$$

We can check that the only non-zero terms in the above summation are:

$$\mathcal{A}_i \phi_i = \sigma e^{V/\sigma} \nabla_{x_N} \cdot \left( e^{-V/\sigma} \nabla_{x_{N-i}} \phi_i \right),$$

for i = 1, ..., N, so that the compatibility condition holds, by the periodicity of the domain. Then  $\theta_N$  defined by (40) is the unique mean-zero solution of

$$\mathcal{A}_{2N}\theta_N = \nabla_{x_N} \cdot e^{-V/\sigma},$$

438 then the solution  $\phi_N$  to (38a) can be written as

439 (45) 
$$\phi_N = \theta_N \cdot \left( \nabla_{x_{N-1}} \phi_{N-1} + \ldots + \nabla_{x_0} \phi_0 \right) + r_N^{(1)}(x_0, \ldots, x_{N-1}),$$

where

$$\theta_N \cdot (\nabla_{x_N-1}\phi_{N-1} + \ldots + \nabla_{x_0}\phi_0) \in \mathcal{H}_N$$

440 and  $r_N^{(1)} \in \mathcal{H}_N^{\perp}$  has not yet been specified. A sufficient condition for  $\phi_{N+1}$  to have a 441 solution in (38b) is that

442 (46) 
$$\int (\mathcal{A}_{2N-1}\phi_N + \ldots + \mathcal{A}_{N-2}\phi_1 + \mathcal{A}_{N-1}\phi_0) e^{-V/\sigma} dx_N = 0$$

Since  $r_N^{(1)}$  does not depend on  $x_N$  it follows that:

$$\int e^{-V/\sigma} \mathcal{A}_{2N-1} \phi_N \, dx_N = \nabla_{x_{N-1}} \cdot \left( \int e^{-V/\sigma} \nabla_{x_N} \theta_N \left( \nabla_{x_{N-1}} \phi_{N-1} \dots + \nabla_{x_0} \phi_0 \right) \, dx_N \right),$$

443 thus (46) can be written as

444 
$$0 = \nabla_{x_{N-1}} \cdot \left( \int e^{-V/\sigma} \nabla_{x_N} \theta_N \left( \nabla_{x_{N-1}} \phi_{N-1} \dots + \nabla_{x_0} \phi_0 \right) \, dx_N \right)$$
  
445  
445  
446  

$$+ \nabla_{x_{N-1}} \cdot \left( \int e^{-V/\sigma} \, dx_N \left( \nabla_{x_{N-1}} \phi_{N-1} + \dots + \nabla_{x_0} \phi_0 \right) \right),$$

resulting in the following equation for  $\phi_{N-1}$ : 447

448 (47) 
$$\nabla_{x_{N-1}} \cdot \left( \mathcal{K}_N \nabla_{x_{N-1}} \phi_{N-1} \right) = -\nabla_{x_{N-1}} \cdot \mathcal{K}_N \left( \nabla_{x_{N-2}} \phi_{N-2} + \ldots + \nabla_{x_0} \phi_0 \right) = 0,$$

where

$$\mathcal{K}_N = \int \left( I + \nabla_{x_N} \theta_N \right) e^{-V/\sigma} \, dx_N$$

By Lemma 10, for fixed  $x_0, x_1, \ldots, x_{N-1}$  the tensor  $\mathcal{K}_N$  is uniformly positive definite over  $x_{N-1} \in \mathbb{T}^d$ . As a consequence, the operator defined in (47) is uniformly elliptic, with adjoint nullspace spanned by  $Z_N(x_0, x_1, \ldots, x_{N-1})$ . Since the right hand side has mean zero, this implies that a solution  $\phi_{N-1}$  exists. Indeed, we can write  $\phi_{N-1}$  $\mathbf{as}$ 

$$\phi_{N-1} = \theta_{N-1} \cdot \left( \nabla_{x_{N-2}} \phi_{N-2} + \ldots + \nabla_{x_0} \phi_0 \right) + r_{N-1}^{(1)}(x_0, \ldots, x_{N-2}),$$

where  $r_{N-1}^{(1)} \in \mathcal{H}_{N-1}^{\perp}$  is still unspecified. Since (46) has been satisfied, it follows from Proposition 16 that there exists a unique decomposition of  $\phi_{N+1}$  into

$$\phi_{N+1}(x_0, x_1, \dots, x_N) = \widetilde{\phi}_{N+1}(x_0, x_1, \dots, x_N) + r_{N+1}^1(x_0, x_1, \dots, x_{N-1}),$$

where  $\tilde{\phi}_{N+1} \in \mathcal{H}_N$  and  $r_{N+1}^{(1)} \in \mathcal{H}_N^{\perp}$ , such that  $r_{N+1}^{(1)}$  is still unspecified. For the sake of illustration we now consider the  $O(\epsilon^{-(N-2)})$  equation in (39). This equation for  $\phi_{N+2}$  has a solution if and only if

$$\int \left(\mathcal{A}_{2N-1}\phi_{N+1} + \mathcal{A}_{2N-2}\phi_N + \ldots + \mathcal{A}_{N-2}\phi_0\right) e^{-V/\sigma} dx_N = 0.$$

Fixing the variables  $x_0, \ldots, x_{N-2}$ , we can rewrite the above equation as: 449

450 (48) 
$$\widetilde{\mathcal{A}}_{2N-2}r_N^{(1)} := \nabla_{N-1} \cdot \left( Z_{N-1} \nabla_{N-1} r_N^{(1)} \right) = -RHS$$

where the RHS contains all the remaining terms. We note that all the functions of  $x_{N-1}$  in the RHS are known, so that all the remaining undetermined terms can be viewed as constants for fixed  $x_0, \ldots, x_{N-2} \in \mathbb{X}_{N-2}$ . A necessary and sufficient condition for a unique mean zero solution to exist to (48) is that the RHS has integral zero with respect to  $x_{N-1}$ , which is equivalent to:

$$\nabla_{N-2} \cdot \left( \int \int \left( \nabla_N \phi_N + \nabla_{N-1} \phi_{N-1} + \ldots + \nabla_0 \phi_0 \right) e^{-V/\sigma} \, dx_N dx_{N-1} \right) = 0,$$

or equivalently:

$$\nabla_{N-2} \cdot \left( \mathcal{K}_{N-2} \left( \nabla_{N-2} \phi_{N-2} + \ldots + \nabla_0 \phi_0 \right) \right) = 0.$$

Once again, this implies that

$$\phi_{N-2} = \theta_{N-2} \cdot (\nabla_{N-3}\phi_{N-3} + \ldots + \nabla_0\phi_0) + r_{N-2}^{(1)}(x_0, \ldots, x_{N-3}),$$

where  $r_{N-2}^{(1)} \in \mathcal{H}_{N-2}^{\perp}$  is unspecified. Since the compatibility condition holds, by Proposition 16 equation (48) has a solution, so that we can write

$$r_N^{(1)}(x_0,\ldots,x_{N-1}) = \tilde{r}_N^{(1)}(x_0,\ldots,x_{N-1}) + r_N^{(2)}(x_0,\ldots,x_{N-2})$$

where  $\tilde{r}_N^{(1)} \in \mathcal{H}_{N-1}$  is the unique smooth solution of (48) and for some  $r_N^{(2)} \in \mathcal{H}_{N-1}^{\perp}$ .

For the inductive step, suppose that for some k < N, the functions  $\phi_N, \ldots \phi_{N\pm(k-1)}$  have all been determined. We shall consider the case when k is even, noting that the k odd case follows *mutatis mutandis*. From the previous steps, each term in

$$\phi_{N+k-2}, \phi_{N+k-4}, \ldots, \phi_{N-k-2},$$

admits a decomposition such that in each case we can write:

$$\phi_{N+k-2i} = \widetilde{\phi}_{N+k-2i} + r_{N+k-2i}^{(k/2-i)},$$

where

$$\phi_{N+k-2i} \in \mathcal{H}_{k/2-i}$$

has been uniquely specified, and the remainder term

$$r_{N+k-2i}^{(k/2-i)} \in \mathcal{H}_{k/2-i}^{\perp},$$

451 remains to be determined. The  $O(\epsilon^{N-k})$  equation is given by

452 (49) 
$$\mathcal{A}_{2N}\phi_{N+k} + \mathcal{A}_{2N-1}\phi_{N+k-1} + \ldots + \mathcal{A}_{N-k}\phi_0 = 0.$$

Following the example of the  $O(\epsilon^{N-2})$  step. In descending order we successively apply the compatibility conditions which must be satisfied for the equations involving  $r_{N+k}^{(1)}, \ldots, r_{N-k-2}^{(k-1)}$  of the form

456 (50) 
$$\widetilde{\mathcal{A}}_{2N-2k-2i}r_{N+k-2i}^{(k/2-i)} = RHS,$$

where in (50), all terms dependent on the variable  $x_{k/2-i}$  have been specified uniquely and where

$$\widehat{A}_{2N-2k-2i}u = \nabla_{x_{N-k-i}} \cdot \left( Z_{N-k-i} \nabla_{x_{N-k-i}} u \right).$$

This results in (49) being integrated with respect to the variables  $N, \ldots, N - k + 1$ . In particular, all terms  $\mathcal{A}_{2N-j}\phi$  for  $j = 0, \ldots, k-1$  will have integral zero, and thus

458 In particular, all terms  $\mathcal{A}_{2N-j}\phi$  for  $j = 0, \ldots, k$ -459 vanish. The resulting equation is then

460 (51) 
$$\int \dots \int (\mathcal{A}_{2N-k}\phi_N + \dots + \mathcal{A}_{N-k}\phi_0) e^{-V/\sigma} dx_N \dots dx_{N-k+1} = 0.$$

Moreover, since the function  $\phi_{N-i}$  depends only on the variables  $x_0, \ldots, x_{N-i}$ , then (51) must be of the form

$$\nabla_{N-k} \cdot \left( \int \dots \int \left( \nabla_{x_N} \phi_N + \dots \nabla_{x_{N-1}} \phi_{N-1} + \dots \nabla_{x_0} \phi_0 \right) e^{-V/\sigma} \, dx_N \dots dx_{N-k+1} \right) = 0.$$

## This manuscript is for review purposes only.

461 We now apply the inductive hypothesis to see that

$$462 \quad \int \left( \nabla_{x_N} \phi_N + \dots \nabla_0 \phi_0 \right) e^{-V/\sigma} \, dx_N \cdots dx_{N-k+1} 
463 \quad = \int \int \left( \nabla_{x_N} \theta_N + I \right) dx_N \left( \nabla_{N-1} \phi_{N-1} + \dots + \nabla_{x_0} \phi_0 \right) e^{-V/\sigma} \, dx_{N-1} \cdots dx_{N-k+1} 
464 \quad = \int \int \int \left( \nabla_{x_N} \theta_N + I \right) \, dx_N \left( \nabla_{x_{N-1}} \theta_{N-1} + I \right) \, dx_{N-1} \left( \nabla_{x_{N-2}} \phi_{N-2} + \dots + \nabla_{x_0} \phi_0 \right) e^{-V/\sigma} \, dx_{N-2} \cdots dx_{N-k+1}$$

465 :

465 =  $\mathcal{K}_{N-k+1} \left( \nabla_{x_{N-k}} \phi_{N-k} + \dots \nabla_{x_0} \phi_0 \right).$ 

Thus, the compatibility condition for the  $O(\epsilon^{N-k})$  equation reduces to the elliptic PDE

$$\nabla_{x_k} \cdot \left( \mathcal{K}_{x_{N-k}} \left( \nabla_{N-k} \phi_{x_{N-k}} + \dots \nabla_{x_0} \phi_0 \right) \right) = 0,$$

so that  $\phi_{N-k}$  can be written as

$$\phi_{N-k} = \theta_{N-k} \left( \nabla_{x_{N-k-1}} \phi_{x_{N-k-1}} + \dots \nabla_{x_0} \phi_0 \right) + r_{N-k}^{(1)}$$

where  $r_{N-k}^{(1)}$  is an element of  $\mathcal{H}_{N-k}^{\perp}$ , which is yet to be determined. Moreover, each remainder term  $r_{N+k-2i}^{(k/2-i)}$  can be further decomposed as

$$r_{N+k-2i}^{(k/2-i)} = \tilde{r}_{N+k-2i}^{(k/2-i)} + r_{N+k-2i}^{(k/2-i+1)},$$

where

$$\widetilde{r}_{N+k-2i}^{(k/2-i)} \in \mathcal{H}_{k/2-i+1},$$

is uniquely determined and

$$r_{N+k-2i}^{(k/2-i+1)} \in \mathcal{H}_{k/2-i+1}^{\perp},$$

468 is still unspecified. Continuing the above procedure inductively, starting from a 469 smooth function  $\phi_0$  we construct a series of correctors  $\phi_1, \ldots, \phi_{2N-1}$ .

470

471 We now consider the final equation (38d). Arguing as before, we note that we can 472 rewrite (53) as

473 (52) 
$$\mathcal{A}_{2N}\phi_{2N} + \dots + \mathcal{A}_{N+1}\phi_{N+1} = F(x) - \sum_{i=1}^{N} \mathcal{L}_i\phi_i.$$

474 A necessary and sufficient condition for  $\phi_{2N}$  to have a solution is that

475 (53)  
$$\int_{\mathbb{T}^d} (\mathcal{A}_{2N-1}\phi_{2N-1} + \dots + \mathcal{A}_{N+1}\phi_{N+1}) e^{-V/\sigma} dx_N$$
$$= \int_{\mathbb{T}^d} \left( F(x) - \sum_{i=1}^N \mathcal{L}_i \phi_i \right) e^{-V/\sigma} dx_N.$$

At this point, the remainder terms will be of the form

$$r_{2N-2}^{(1)}, r_{2N-4}^{(2)}, \dots, r_{2N-2k}^{(k)}, \dots, r_{2}^{(1)},$$

476 such that  $r_{2N-2i}^{(i)} \in \mathcal{H}_i^{\perp}$ , is unspecified. Starting from  $r_{2N-2}^{(1)}$  a necessary and sufficient 477 condition for the remainder  $r_{2N-2i}^{(i)}$  to exist is that the integral of the equation with 478 respect to  $dx_{N-i}$  vanishes, i.e.

(54)  

$$F(x)Z(x) = \int_{(\mathbb{T}^d)^N} (\mathcal{A}_{2N-1}\phi_{2N-1} + \dots + \mathcal{A}_{N+1}\phi_{N+1}) e^{-V/\sigma} dx_N dx_{N-1} \dots dx_1 + \int_{(\mathbb{T}^d)^N} (\mathcal{L}_N\phi_N + \dots + \mathcal{L}_1\phi_1) e^{-V/\sigma} dx_N dx_{N-1} \dots dx_1$$

where

4

$$Z(x) = \int_{\mathbb{T}^d} \dots \int_{\mathbb{T}^d} e^{-V/\sigma} \, dx_N \dots dx_1.$$

As above, after simplification, (54) becomes

$$\nabla_{x_0} \cdot (\nabla_{x_N} \phi_N + \ldots + \nabla_{x_0} \phi_0) = Z(x) F(x),$$

which can be written as

$$\frac{\sigma}{Z(x)}\nabla_{x_0}\cdot\left(\int_{(\mathbb{T}^d)^N}\left(I+\nabla_{x_N}\theta_N\right)\cdot\ldots\cdot\left(I+\nabla_{x_1}\theta_1\right)e^{-V/\sigma}\,dx_N\ldots dx_1\nabla_{x_0}\phi_0\right)=F(x),$$

or more compactly

$$F(x) = \frac{\sigma}{Z(x)} \nabla_{x_0} \cdot \left( \mathcal{K}_1(x) \nabla_{x_0} \phi_0(x) \right),$$

where the terms in the right hand side have been specified and are unique. Thus, the O(1) equation (54) provides a unique expression for F(x). Moreover, for each  $i = 1, \ldots, N-1$ , there exists a smooth unique solution  $r_{2N-2i}^{(i)} \in \mathcal{H}_{i-1}$  and  $\phi_{2N} \in \mathcal{H}_{2N}$ by Proposition 16.

Note that we have not uniquely identified the functions  $\phi_1, \ldots, \phi_{2N}$ , since after the above N steps there will be remainder terms which are still unspecified. However, conditions (39a)-(39c) will hold for any choice of remainder terms which are still unspecified. In particular, we can set all the remaining unspecified remainder terms to 0. Moreover, every Poisson equation we have solved in the above steps has been of the form:

$$S_k u(x_0, \dots, x_k) = a(x_0, \dots, x_k) \cdot \nabla_{x_0} \phi_0(x_0) + A(x_0, \dots, x_k) : \nabla_{x_0}^2 \phi_0(x_0),$$

480 where  $S_k$  is of the form (33), and a and A are uniformly bounded with bounded 481 derivatives. In particular, from the remark following Proposition 16 the pointwise 482 estimates (43) hold.

REMARK 19. Although we do not have an explicit formula for the test functions, for i = 1, ..., N, we have that an expression for the gradient of  $\phi_i$  in terms of the correctors  $\theta_i$ :

$$\nabla_{x_i}\phi_i = \nabla_{x_i}\theta_i(1+\nabla_{x_{i-1}}\theta_{x_{i-1}})\cdots(1+\nabla_{x_1}\theta_{x_1})\nabla_{x_0}\phi_0$$

483 As we shall see, these are the only terms that are required for the calculation of the

homogenized diffusion tensor, thus we can obtain an explicit characterisation of the effective coefficients.

5.2. Tightness of Measures. In this section we establish the weak compactness 486 of the family of measures corresponding to  $\{X_t^{\epsilon}: 0 \leq t \leq T\}_{0 < \epsilon < 1\}}$  in  $C([0,T]; \mathbb{R}^d)$ 487 by establishing tightness. Following [40], we verify the following two conditions which 488 are a slight modification of the sufficient conditions stated in [10, Theorem 8.3]. 489

LEMMA 20. The collection  $\{X_t^{\epsilon} : 0 \leq t \leq T\}_{\{0 < \epsilon < 1\}}$  is relatively compact in 490  $C([0,T];\mathbb{R}^d)$  if it satisfies: 491

1. For all  $\delta > 0$ , there exists M > 0 such that

$$\mathbb{P}\left(\sup_{0 \le t \le T} |X_t^{\epsilon}| > M\right) \le \delta, \quad 0 < \epsilon \le 1$$

2. For any  $\delta > 0$ , M > 0, there exists  $\epsilon_0$  and  $\gamma$  such that

$$\gamma^{-1} \sup_{0 < \epsilon < \epsilon_0} \sup_{0 \le t_0 \le T} \mathbb{P}\left( \sup_{t \in [t_0, t_0 + \gamma]} \left| X_t^{\epsilon} - X_{t_0}^{\epsilon} \right| \ge \delta; \sup_{0 \le s \le T} \left| X_s^{\epsilon} \right| \le M \right) \le \delta.$$

To verify condition 1 we follow the approach of [40] and consider a test function 492 of the form  $\phi_0(x) = \log(1+|x|^2)$ . The motivation for this choice is that while  $\phi_0(x)$ 493is increasing, we have that 494

495 (55) 
$$\sum_{k=1}^{3} (1+|x|)^{l} \|\nabla_{x}^{l}\phi_{0}(x)\|_{F} \leq C.$$

Let  $\phi_1, \ldots, \phi_{2N-1}$  be the first 2N-1 test functions constructed in Proposition 18. 496 Consider the test function

497

498 (56) 
$$\phi^{\epsilon}(x) = \phi_0(x) + \epsilon \phi_1(x, x/\epsilon) + \ldots + \epsilon^{2N-1} \phi_{2N-1}(x, x/\epsilon, \ldots, x/\epsilon^{2N-2}, x/\epsilon^{2N-1}).$$

Applying Itô's formula, we have that

$$\phi^{\epsilon}(X_t^{\epsilon}) = \phi^{\epsilon}(x) + \int_0^t G(X_s^{\epsilon}) \, ds + \sum_{i=0}^N \sum_{k=0}^{2N-1} \epsilon_i \int_0^t \nabla_{x_i} \phi_j \, dW_s,$$

where G(x) is a smooth function consisting of terms of the form: 499

500 (57) 
$$\epsilon^{i+j-k} e^{V/\sigma} \nabla_{x_i} \cdot \left( e^{-V/\sigma} \nabla_j \phi_k \right) (x, x/\epsilon, \dots, x/\epsilon^N),$$

To obtain relative compactness we need to individually control the terms arising in 501

the drift. More specifically, we must show that 502

503 (58) 
$$\mathbb{E}\sup_{0\le t\le T}\int_0^t \left| e^{V/\sigma} \nabla_{x_i} \cdot \left( e^{-V/\sigma} \nabla_j \phi_k \right) \left( X_s^{\epsilon}, X_s^{\epsilon}/\epsilon, \dots, X_s^{\epsilon}/\epsilon^N \right) ds \right| < \infty,$$

where  $i + j - k \ge 0$ , and moreover, for terms arising from the martingale part, 504

505 (59) 
$$\mathbb{E} \left| \sup_{0 \le t \le T} \int_0^t \nabla_{x_j} \phi_k(X_s^{\epsilon}, X_s^{\epsilon}/\epsilon, \dots, X_s^{\epsilon}/\epsilon^N) \, dW_s \right|^2 < \infty,$$

506 together with

507 (60) 
$$\sup_{0 \le t \le T} |\phi_j(X_t^{\epsilon})| < \infty.$$

Terms of the type (58) can be bounded above by: 508

$$\underset{510}{\overset{509}{=}} \mathbb{E} \sup_{0 \le t \le T} \int_0^t \left| \left( \nabla_{x_i} V \cdot \nabla_{x_j} \phi_k \right) \left( X_s^{\epsilon}, \dots, X_s^{\epsilon} / \epsilon^N \right) \right| + \left| \sigma \nabla_{x_i} \cdot \nabla_{x_j} \phi_k \left( X_s^{\epsilon}, \dots, X_s^{\epsilon} / \epsilon^N \right) \right| \, ds.$$

If i > 0, then  $\nabla_{x_i} V$  is uniformly bounded, and so the above expectation is bounded 511above by 512

513  

$$C \mathbb{E} \int_{0}^{T} |\nabla_{x_{j}} \phi_{k}(X_{s}^{\epsilon}, \dots, X_{s}^{\epsilon}/\epsilon^{N})| + |\nabla_{x_{i}} \cdot \nabla_{x_{j}} \phi_{k}(X_{s}^{\epsilon}, \dots, X_{s}^{\epsilon}/\epsilon^{N})| ds$$
514  
515  

$$= C \mathbb{E} \int_{0}^{T} \sum_{m=1}^{3} \left\| \nabla_{x_{0}}^{m} \phi_{0}(X_{s}^{\epsilon}) \right\|_{F} ds \leq KT,$$

515

using (55), for some constant K > 0. For the case when i = 0, an additional term 516arises from the derivative  $\nabla_{x_0} V_0$  and we obtain an upper bound of the form 517

518 (61)  
$$\mathbb{E} \int_{0}^{T} \sum_{m=1}^{3} \left\| \nabla_{x_{0}}^{m} \phi_{0}(X_{t}^{\epsilon}) \right\| (1 + |\nabla_{x_{0}} V_{0}(X_{t}^{\epsilon})|) dt$$
$$\leq \mathbb{E} \int_{0}^{T} \sum_{m=1}^{3} \left\| \nabla_{x_{0}}^{m} \phi_{0}(X_{t}^{\epsilon}) \right\| (1 + \|\nabla \nabla V_{0}\|_{L^{\infty}} |X_{t}^{\epsilon}|) dt$$

and which is bounded by Assumption 1 and (55). For (59), we have 519

$$\sum_{\substack{b \leq t \leq T \\ 522}} \mathbb{E} \left| \sup_{0 \leq t \leq T} \int_{0}^{t} \nabla_{x_{j}} \phi_{k}(X_{s}^{\epsilon}, X_{s}^{\epsilon}/\epsilon, \dots, X_{s}^{\epsilon}/\epsilon^{N}) dW_{s} \right|^{2} \leq 4\mathbb{E} \int_{0}^{T} |\nabla_{x_{j}} \phi_{k}(X_{s}^{\epsilon}, X_{s}^{\epsilon}/\epsilon, \dots, X_{s}^{\epsilon}/\epsilon^{N})|^{2} ds$$

$$\leq C \mathbb{E} \int_{0}^{T} \sum_{m=1}^{3} \left\| \nabla_{x_{0}}^{m} \phi_{0}(X_{s}^{\epsilon}) \right\|_{F} ds,$$

which is again bounded. Terms of the type (60) follow in a similar manner. Condition 5231 then follows by an application of Markov's inequality. 524

525

To prove Condition 2, we set  $\phi_0(x) = x$  and let  $\phi_1, \ldots, \phi_{2N-1}$  be the test func-526tions which exist by Proposition 18. Applying Itô's formula to the corresponding 527 multiscale test function (56), so that for  $t_0 \in [0, T]$  fixed, 528

529 (62) 
$$X_t^{\epsilon} - X_{t_0}^{\epsilon} = \int_{t_0}^t G \, ds + \sum_{i=0}^N \sum_{k=0}^{2N-1} \epsilon^i \int_{t_0}^t \nabla_{x_i} \phi_j \, dW_s,$$

where G is of the form given in (57). Let M > 0, and let 530

531 (63) 
$$\tau_M^{\epsilon} = \inf\{t \ge 0; |X_t^{\epsilon}| > M\}.$$

Following [40], it is sufficient to show that 532(64)

533 
$$\mathbb{E}\left[\sup_{t_0 \le t \le T} \int_{t_0 \land \tau_M^{\epsilon}}^{t \land \tau_M^{\epsilon}} \left| e^{V/\sigma} \nabla_{x_i} \cdot \left( e^{-V/\sigma} \nabla_j \phi_k \right) \left( X_s^{\epsilon}, X_s^{\epsilon}/\epsilon, \dots, X_s^{\epsilon}/\epsilon^N \right) ds \right|^{1+\nu} \right] < \infty$$

and 534

535 (65) 
$$\mathbb{E}\left(\sup_{t_0 \le t \le t_0 + \gamma} \left| \int_{t_0 \land \tau_M^{\epsilon}}^{t \land \tau_M^{\epsilon}} \nabla_{x_i} \phi_j(X_s^{\epsilon}, X_s^{\epsilon}/\epsilon, \dots, X_s^{\epsilon}/\epsilon^N) \, dW_s \right|^{2+2\nu} \right) < \infty$$

536 for some fixed  $\nu > 0$ . For (64), when i > 0, the term  $\nabla_{x_i} V$  is uniformly bounded. Moreover, since  $\nabla \phi_0$  is bounded, so are the test functions  $\phi_1, \ldots, \phi_{2N+1}$ . Therefore, 537 538 by Jensen's inequality one obtains a bound of the form

539 
$$C\gamma^{\nu} \mathbb{E} \int_{t_0}^{t_0+\gamma} \left| e^{V/\sigma} \nabla_{x_i} \cdot \left( e^{-V/\sigma} \nabla_j \phi_k \right) \left( X_s^{\epsilon}, X_s^{\epsilon}/\epsilon, \dots, X_s^{\epsilon}/\epsilon^N \right) \right|^{1+\nu} ds$$
540
541
$$\leq C\gamma^{\nu} \int_{t_0}^{t_0+\gamma} |K|^{1+\nu} ds \leq K' \gamma^{1+\nu}.$$

541

When i = 0, we must control terms involving  $\nabla_{x_0} V_0$  of the form,

$$\mathbb{E}\left[\sup_{t_0 \le t \le t_0 + \gamma} \int_{t_0 \land \tau_M^{\epsilon}}^{t \land \tau_M^{\epsilon}} \left| \nabla V_0 \cdot \nabla_{x_j} \phi_k \right|^{1+\nu} ds \right]$$

where  $\tau_M^{\epsilon}$  is given by (63). However, applying Jensen's inequality, 542

543 
$$\mathbb{E}\left[\sup_{t_0 \le t \le t_0 + \gamma} \int_{t_0 \wedge \tau_M^{\epsilon}}^{t \wedge \tau_M^{\epsilon}} \left| \nabla V_0 \cdot \nabla_{x_j} \phi_k \right|^{1+\nu} ds \right] \le C \gamma^{\nu} \int_{t_0 \wedge \tau_M^{\epsilon}}^{(t_0 + \gamma) \wedge \tau_M^{\epsilon}} \mathbb{E}\left| \nabla V_0 \cdot \nabla_{x_j} \phi_k \right|^{1+\nu} ds$$
544 
$$\le C \gamma^{\nu} \int_{t_0 \wedge \tau_M^{\epsilon}}^{(t_0 + \gamma) \wedge \tau_M^{\epsilon}} \mathbb{E}\left| \nabla V_0(X_s^{\epsilon}) \right|^{1+\nu} ds$$

544

545 
$$\leq C\gamma^{\nu} \left\|\nabla^2 V_0\right\|_{\infty}^{1+\nu} \int_{t_0 \wedge \tau_M^{\epsilon}}^{(t_0+\gamma)\wedge \tau_M^{\epsilon}} \mathbb{E}|X_s^{\epsilon}|^{1+\nu} ds$$

546 (66) 
$$\leq CM\gamma^{1+\nu} \|\nabla^2 V_0\|_{L^{\infty}}^{1+\nu},$$

as required. Similarly, to establish (65) we follow a similar argument, first using the 548Burkholder-Gundy-Davis inequality to obtain: 549

550 
$$\mathbb{E}\left(\sup_{t_0 \le t \le t_0 + \gamma} \int_{t_0}^t |\nabla_{x_i} \phi_j \, dW_s|^{2+2\nu}\right) \le \mathbb{E}\left(\int_{t_0}^{t_0 + \gamma} |\nabla_{x_i} \phi_j|^2 \, ds\right)^{1+\nu}$$
551 
$$\le \gamma^{\nu} \int_{t_0}^{t_0 + \gamma} \mathbb{E}\left|\nabla_{x_i} \phi_j\right|^{2+2\gamma} \, ds$$
552 
$$\le C \gamma^{1+\nu}$$

$$553 \leq C\gamma^{1+}$$

We note that Assumption 1 (3) is only used to obtain the bounds (61) and (66). 554A straightforward application of Markov's inequality then completes the proof of 555condition 2. It follows from Prokhorov's theorem that the family  $\{X_t^{\epsilon}; t \in [0,T]\}_{0 < \epsilon < 1}$ 556is relatively compact in the topology of weak convergence of stochastic processes 557taking paths in  $C([0,T]; \mathbb{R}^d)$ . In particular, there exists a process  $X^0$  whose paths lie 558in  $C([0,T]; \mathbb{R}^d)$  such that  $\{X^{\epsilon_n}; t \in [0,T]\} \Rightarrow \{X^0; t \in [0,T]\}$  along a subsequence  $\epsilon_n$ . 559

5.3. Identifying the Weak Limit. In this section we uniquely identify any limit point the set  $\{X_t^{\epsilon}; t \in [0,T]\}_{0 < \epsilon \leq 1}$ . Given  $\phi_0 \in C_c^{\infty}(\mathbb{R}^d)$  define  $\phi^{\epsilon}$  to be

$$\phi^{\epsilon}(x) = \phi_0(x) + \epsilon \phi_1(x/\epsilon) + \dots \epsilon^N \phi_N(x, x/\epsilon, \dots, x/\epsilon^N) + \dots + \epsilon^{2N} \phi_{2N}(x, x/\epsilon, \dots, x/\epsilon^N)$$

where  $\phi_1, \ldots, \phi_N$  are the test functions obtained from Proposition 18. Since each test function is smooth, we can apply Itô's formula to  $\phi^{\epsilon}(X_{t}^{\epsilon})$  to see that

$$\mathbb{E}\left[\phi_0(X_t^{\epsilon}) - \int_s^t \frac{\sigma}{Z(X_u^{\epsilon})} \nabla_{x_0} \cdot \left(Z(X_u^{\epsilon})\mathcal{M}(X_u^{\epsilon})\nabla\phi_0(X_u^{\epsilon})\right) \, du + \epsilon R_\epsilon \, \Big| \, \mathcal{F}_s\right] = \phi_0(X_s^{\epsilon}),$$

where  $R_{\epsilon}$  is a remainder term which is bounded in  $L^2(\pi^{\epsilon})$  uniformly with respect to  $\epsilon$ , and where the homogenized diffusion tensor  $\mathcal{M}(x)$  is defined in Theorem 3. Taking  $\epsilon \to 0$  we see that any limit point is a solution of the martingale problem

$$\mathbb{E}\left[\phi_0(X_t^0) - \int_s^t \frac{\sigma}{Z(X_u^0)} \nabla_{x_0} \cdot \left(Z(X_u^0)\mathcal{M}(X_u^0)\nabla\phi_0(X_u^0)\right) \, du \, \Big| \, \mathcal{F}_s\right] = \phi_0(X_s^0).$$

This implies that  $X^0$  is a solution to the martingale problem for  $\mathcal{L}^0$  given by

$$\mathcal{L}_0 f(x) = \frac{\sigma}{Z(x)} \nabla \cdot (Z(x)\mathcal{M}(x)\nabla f(x))$$

560From Lemma 10, the matrix  $\mathcal{M}(x)$  is smooth, strictly positive definite and has 561 bounded derivatives. Moreover,

$$Z(x) = \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V(x,x_1,\dots,x_N)/\sigma} dx_1 \dots dx_N$$

$$= e^{-V_0(x)/\sigma} \int_{\mathbb{T}^d} \cdots \int_{\mathbb{T}^d} e^{-V_1(x,x_1,\dots,x_N)/\sigma} dx_1 \dots dx_N$$
563

where the term in the integral is uniformly bounded. It follows from Assumption 1, that for some C > 0,

$$|\mathcal{M}(x)\nabla\Psi(x)| \le C(1+|x|), \quad \forall x \in \mathbb{R}^d,$$

where  $\Psi = -\log Z$ . Therefore, the conditions of the Stroock-Varadhan theorem 565[47, Theorem 24.1] holds, and therefore the martingale problem for  $\mathcal{L}^0$  possesses a 566 unique solution. Thus  $X^0$  is the unique (in the weak sense) limit point of the family 567  $\{X^{\epsilon}\}_{0 \le \epsilon \le 1}$ . Moreover, by [47, Theorem 20.1], the process  $\{X^0_t; t \in [0,T]\}$  will be the 568 unique solution of the SDE (17), completing the proof. 569

570 6. Acknowledgements. The authors thank S. Kalliadasis and M. Pradas for useful discussions. They also thank B. Zegarlinski for useful discussions and for point-571ing out Ref. [22]. We acknowledge financial support by the Engineering and Physical 572Sciences Research Council of the UK through Grants Nos. EP/J009636, EP/L020564, 573EP/L024926 and EP/L025159. 574

#### REFERENCES

- [1] G. ALLAIRE, Homogenization and two-scale convergence, SIAM Journal on Mathematical Anal-576577 ysis, 23 (1992), pp. 1482-1518.
- [2] G. ALLAIRE AND M. BRIANE, Multiscale convergence and reiterated homogenisation, Proceed-578ings of the Royal Society of Edinburgh: Section A Mathematics, 126 (1996), pp. 297-342.

- [3] S. A. ALMADA AND K. SPILIOPOULOS, Scaling limits and exit law for multiscale diffusions,
   Asymptotic Analysis, 87 (2014), pp. 65–90.
- 582 [4] C. ANÉ ET AL., Sur les inégalités de Sobolev logarithmiques, (2000).
- [5] A. ANSARI, Mean first passage time solution of the Smoluchowski equation: Application to
   relaxation dynamics in myoglobin, The Journal of Chemical Physics, 112 (2000), pp. 2516–
   2522.
- [6] D. BAKRY, I. GENTIL, AND M. LEDOUX, Analysis and geometry of Markov diffusion operators,
   vol. 348, Springer Science & Business Media, 2013.
- [7] S. BANERJEE, R. BISWAS, K. SEKI, AND B. BAGCHI, Diffusion in a rough potential revisited,
   (2014), arXiv:1409.4581.
- [8] G. BEN AROUS AND H. OWHADI, Multiscale homogenization with bounded ratios and anomalous
   slow diffusion, Communications on Pure and Applied Mathematics, 56 (2003), pp. 80–113.
- [9] A. BENSOUSSAN, J. LIONS, AND G. PAPANICOLAOU, Asymptotic analysis for periodic structures,
   vol. 5, North Holland, 1978.
- 594 [10] P. BILLINGSLEY, Probability and measure, John Wiley & Sons, 2008.
- [11] X. BLANC, C. LE BRIS, F. LEGOLL, AND C. PATZ, Finite-temperature coarse-graining of onedimensional models: mathematical analysis and computational approaches, Journal of Nonlinear Science, 20 (2010), pp. 241–275.
- [12] J. D. BRYNGELSON, J. N. ONUCHIC, N. D. SOCCI, AND P. G. WOLYNES, Funnels, pathways,
   and the energy landscape of protein folding: a synthesis, Proteins: Structure, Function,
   and Bioinformatics, 21 (1995), pp. 167–195.
- [13] J. D. BRYNGELSON AND P. G. WOLYNES, Spin glasses and the statistical mechanics of protein
   folding, Proceedings of the National Academy of Sciences, 84 (1987), pp. 7524–7528.
- 603 [14] D. CIORANESCU AND P. DONATO, Introduction to homogenization, (2000).
- [15] D. S. DEAN, S. GUPTA, G. OSHANIN, A. ROSSO, AND G. SCHEHR, Diffusion in periodic, correlated random forcing landscapes, Journal of Physics A: Mathematical and Theoretical, 47 (2014), p. 372001.
- [16] A. DUNCAN, S. KALLIADASIS, G. PAVLIOTIS, AND M. PRADAS, Noise-induced transitions in rugged energy landscapes, (2016), arXiv:1604.04530.
- [17] P. DUPUIS, K. SPILIOPOULOS, AND H. WANG, Rare event simulation for rough energy land scapes, in Simulation Conference (WSC), Proceedings of the 2011 Winter, IEEE, 2011,
   pp. 504–515.
- 612 [18] L. C. EVANS, Partial differential equations, Graduate Studies in Mathematics, 19 (1998).
- 613 [19] C. GARDINER, *Stochastic methods*, Springer Series in Synergetics, Springer-Verlag, Berlin, 614 fourth ed., 2009. A handbook for the natural and social sciences.
- [20] D. GILBARG AND N. S. TRUDINGER, Elliptic partial differential equations of second order,
   springer, 2015.
- C. HARTMANN, J. C. LATORRE, W. ZHANG, AND G. A. PAVLIOTIS, Optimal control of multiscale systems using reduced-order models, Journal of Computational Dynamics, 1 (2014), pp. 279–306.
- [22] W. HEBISCH AND B. ZEGARLIŃSKI, Coercive inequalities on metric measure spaces, Journal of
   Functional Analysis, 258 (2010), pp. 814–851.
- [23] C. HIJÓN, P. ESPAÑOL, E. VANDEN-EIJNDEN, AND R. DELGADO-BUSCALIONI, Mori-Zwanzig
   formalism as a practical computational tool, Faraday discussions, 144 (2010), pp. 301–322.
- [24] R. HOLLEY AND D. STROOCK, Logarithmic Sobolev inequalities and stochastic Ising models,
   Journal of statistical physics, 46 (1987), pp. 1159–1194.
- [25] C. HYEON AND D. T., Can energy landscape roughness of proteins and RNA be measured by us ing mechanical unfolding experiments?, Proceedings of the National Academy of Sciences,
   100 (2003), pp. 10249–10253.
- [26] V. V. JIKOV, S. M. KOZLOV, AND O. A. OLEINIK, Homogenization of differential operators and integral functionals, Springer Science & Business Media, 2012.
- [27] T. KOMOROWSKI, C. LANDIM, AND S. OLLA, Fluctuations in Markov processes: time symmetry
   and martingale approximation, vol. 345, Springer Science & Business Media, 2012.
- [28] S. KRUMSCHEID, Perturbation-based inference for diffusion processes: Obtaining coarse-grained
   models from multiscale data, (2014), arXiv:1409.4685.
- [29] S. KRUMSCHEID, G. A. PAVLIOTIS, AND S. KALLIADASIS, Semiparametric drift and diffusion
   estimation for multiscale diffusions, Multiscale Modeling & Simulation, 11 (2013), pp. 442–
   473.
- [30] F. LEGOLL AND T. LELIEVRE, Effective dynamics using conditional expectations, Nonlinearity,
   23 (2010), p. 2131.
- [31] S. LIFSON AND J. L. JACKSON, On the self-diffusion of ions in a polyelectrolyte solution, The
   Journal of Chemical Physics, 36 (1962), pp. 2410–2414.

[32] G. W. MILTON, The theory of composites, Materials and Technology, 117 (1995), pp. 483–93.

643

- [33] D. MONDAL, P. K. GHOSH, AND D. S. RAY, Noise-induced transport in a rough ratchet potential, The Journal of chemical physics, 130 (2009), p. 074703.
- [34] B. MUCKENHOUPT, Hardy's inequality with weights, Studia Mathematica, 44 (1972), pp. 31–38.
- [35] K. MÜLLER, Reaction paths on multidimensional energy hypersurfaces, Angewandte Chemie
   International Edition in English, 19 (1980), pp. 1–13.
- [36] M. NEUSS-RADU, Homogenization techniques, PhD thesis, University of Cluj-Napoca, Romania,
   and University of Heidelberg, Germany, 1992.
- [37] G. NGUETSENG, A general convergence result for a functional related to the theory of homoge nization, SIAM Journal on Mathematical Analysis, 20 (1989), pp. 608–623.
- [38] J. N. ONUCHIC, Z. LUTHEY-SCHULTEN, AND P. G. WOLYNES, Theory of protein folding: the energy landscape perspective, Annual review of physical chemistry, 48 (1997), pp. 545–600.
- [39] G. C. PAPANICOLAOU, D. STROOCK, AND S. R. S. VARADHAN, Martingale approach to some limit theorems, in Duke Turbulence Conference (Duke Univ., Durham, NC, 1976), vol. 6, 1977.
- [40] È. PARDOUX AND A. Y. VERETENNIKOV, On the Poisson equation and diffusion approximation.
   I, Ann. Probab., 29 (2001), pp. 1061–1085.
- [41] È. PARDOUX AND A. Y. VERETENNIKOV, On Poisson equation and diffusion approximation. II,
   Ann. Probab., 31 (2003), pp. 1166–1192.
- [42] G. A. PAVLIOTIS, Stochastic processes and applications, vol. 60 of Texts in Applied Mathe matics, Springer, New York, 2014. Diffusion processes, the Fokker-Planck and Langevin
   equations.
- [664 [43] G. A. PAVLIOTIS AND A. M. STUART, Parameter estimation for multiscale diffusions, Journal
   665 of Statistical Physics, 127 (2007), pp. 741–781.
- [44] G. A. PAVLIOTIS AND A. M. STUART, Multiscale methods: averaging and homogenization,
   Springer Verlag, 2008.
- [668 [45] E. A. J. F. PETERS, Projection-operator formalism and coarse-graining, (2008),
   arXiv:0810.2894.
- [46] W. REN AND E. VANDEN-EIJNDEN, Probing multi-scale energy landscapes using the string
   method, (2002), arXiv:0205528.
- [47] L. C. G. ROGERS AND D. WILLIAMS, Diffusions, Markov processes and martingales: Volume
   2, Itô calculus, vol. 2, Cambridge university press, 2000.
- [48] J. G. SAVEN, J. WANG, AND P. G. WOLYNES, Kinetics of protein folding: the dynamics of globally connected rough energy landscapes with biases, J. Chem. Phys., 101 (1994), pp. 11037– 11043.
- [49] K. SPILIOPOULOS, Rare event simulation for multiscale diffusions in random environments,
   Multiscale Modeling & Simulation, 13 (2015), pp. 1290–1311.
- [50] A. Y. VERETENNIKOV, On Sobolev solutions of Poisson equations in  $\mathbb{R}^d$  with a parameter, J. Math. Sci. (N. Y.), 179 (2011), pp. 48–79. Problems in mathematical analysis. No. 61.
- [51] R. ZWANZIG, Diffusion in a rough potential, Proceedings of the National Academy of Sciences,
   85 (1988), pp. 2029–2030.