

# From ballistic to diffusive behavior in periodic potentials

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## Abstract

The long-time/large-scale, small-friction asymptotic for the one dimensional Langevin equation with a periodic potential is studied in this paper. It is shown that the Freidlin-Wentzell and central limit theorem (homogenization) limits commute. We prove that, in the combined small friction, long-time/large-scale limit the particle position converges weakly to a Brownian motion with a singular diffusion coefficient which we compute explicitly. We show that the same result is valid for a whole one parameter family of space/time rescalings. The proofs of our main results are based on some novel estimates on the resolvent of a hypoelliptic operator.

## 1 Introduction and Main Results

Random perturbations of dynamical systems has been the subject of intense study over the last several decades [FW84]. One of the most extensively studied randomly perturbed dynamical systems is given by the Langevin equation modelling the interaction of a classical particle with a heat bath at inverse temperature  $\beta$ :

$$\ddot{q} = -\nabla V(q) - \gamma \dot{q} + \sqrt{2\gamma\beta^{-1}}\xi(t). \quad (1.1)$$

Here,  $V(q)$  denotes a smooth potential,  $\gamma$  is a friction coefficient which should be interpreted as the strength of the coupling to the heat bath, and  $\xi(t)$  denotes standard  $d$ -dimensional white noise, i.e. a mean zero generalized Gaussian process with correlation structure

$$\langle \xi_i(t)\xi_j(s) \rangle = \delta_{ij}\delta(t-s), \quad i, j = 1, \dots, d.$$

There are various applications of this model to solid state physics, e.g. surface diffusion, Josephson junctions and superionic conductors. As a result, equation (1.1) has been one of the most popular stochastic models in the physics and the mathematics literature. See, e.g., [Ris89, Rei02, HTB90, HN05] and the references therein.

Various asymptotic limits for the Langevin equation (1.1) have been studied, both in finite [Nel67, Fre04] and in infinite dimensions [SCF06, PS05]. It is well known, for example, that for large values of the friction coefficient  $\gamma$ , solutions the rescaled process

$$q_\gamma(t) = q(t/\gamma) \quad (1.2)$$

converges to the solution of the Smoluchowski equation

$$\gamma \dot{z} = -\nabla V(z) + \sqrt{2\gamma\beta^{-1}}\xi(t). \quad (1.3)$$

This is usually called the *Kramers to Smoluchowski* limit.

Clearly, in the limit as the friction coefficient converges to zero, and for fixed finite time intervals, we retrieve the deterministic dynamics which is governed by the Hamiltonian system

$$\ddot{q} = -\nabla V(q).$$

The small  $\gamma$ , large-time asymptotic is much more interesting and was originally studied by Freidlin and Wentzell [FW84, FW94]. It was shown in these references that, for  $d = 1$ , and under appropriate assumptions on the potential, the Hamiltonian of the rescaled process

$$q^\gamma = \gamma q(t/\gamma), \quad (1.4)$$

converges weakly, in the limit as  $\gamma \rightarrow 0$ , to a diffusion process on a graph. This result was obtained for one dimensional Langevin equations with periodic potentials—the problem we study in this paper—in [FW99]. From this limit theorem one can infer the limiting behavior of the rescaled particle position, which actually converges to a non-Markovian process; see Corollary 2.2 and Remark 2.3 in this paper. Results similar to those of the Freidlin-Wentzell theory were obtained in [Sow03, Sow05] using singular perturbation theory.

On the other hand, when the potential is either periodic or random, and for fixed  $\gamma > 0$ , the long time behavior of solutions to (1.1) is described by an effective Brownian motion. Indeed, the rescaled particle position

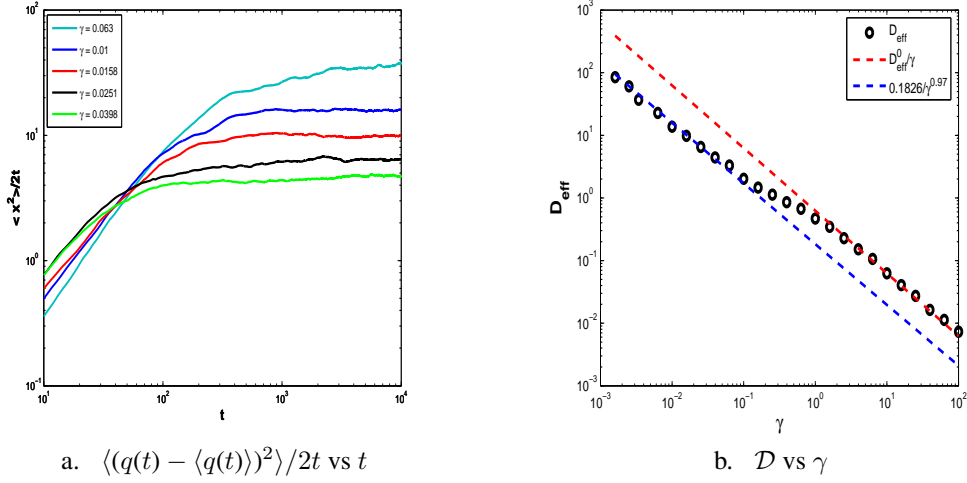
$$q^\varepsilon(t) := \varepsilon q(t/\varepsilon^2) \quad (1.5)$$

converges weakly, in the limit as  $\varepsilon \rightarrow 0$ , to a Brownian motion with a nonnegative diffusion coefficient  $D_\gamma$ . An expression for the diffusion coefficient can be obtained implicitly via the solution of a suitable Poisson equation [Rod89, HP04, PV85, Oll94, Koz89]. See also Section 3 below.

The above limit theorem for the rescaled process  $q^\varepsilon(t)$  does not provide us with a complete understanding of the long time asymptotic behavior of (1.1) for two reasons. First, it does not contain any information on the time needed for the process  $q(t)$  to reach the asymptotic diffusive regime, the *diffusive time scale*  $\tau_{\text{diff}}$ . Second, it does not provide us with any information on the dependence of the effective diffusion coefficient  $D_\gamma$  on the friction coefficient  $\gamma$  and on the inverse temperature  $\beta$ . The large- $\gamma$ /large- $\beta$  regime is the most interesting one from the point of view of applications and it has been studied quite extensively by means of formal asymptotics and numerical experiments, see [SLL<sup>+</sup>04, LSR<sup>+</sup>04] and the references therein. An asymptotic formula for the diffusion coefficient which is valid at small temperatures was obtained rigorously by Kozlov in [Koz89]. The formula obtained in that paper, however, is not valid uniformly in  $\gamma$ , but only for large or intermediate values of the friction coefficient. The purpose of this paper is to study the dependence of the diffusive time scale  $\tau_{\text{diff}}$  and of the effective diffusion coefficient  $D_\gamma$  on the friction coefficient, in particular in the limit as  $\gamma$  tends to 0, and to obtain results which are uniform in  $\beta$ . We also derive various results related to the large  $\gamma$  asymptotic.

To get some intuition on the dependence of  $\tau_{\text{diff}}$  and  $D_\gamma$  on  $\gamma$ , we calculate numerically  $D_\gamma$  for the nonlinear pendulum with dissipation and noise through the formula

$$D_\gamma = \lim_{t \rightarrow \infty} \frac{\langle (q(t) - \langle q(t) \rangle)^2 \rangle}{2t},$$

Figure 1: Second moment and effective diffusivity for various values of  $\gamma$ .

where  $\langle \cdot \rangle$  denotes ensemble average. In Figure 1a we plot the second moment of the particle position divided by  $2t$  as a function of time, for various values of the friction coefficient. In Figure 1b we plot the diffusion coefficient as a function of  $\gamma$ . All simulations were performed at a fixed temperature  $\beta^{-1} = 0.1$ . The numerical simulations suggest that

$$\tau_{\text{diff}} \sim \frac{1}{\gamma}, \quad \text{for } \gamma \ll 1, \quad (1.6)$$

and that

$$D_\gamma \sim \frac{1}{\gamma}, \quad \text{for both } \gamma \ll 1 \text{ and } \gamma \gg 1. \quad (1.7)$$

The central result of this article is a rigorous justification of the above two (actually three) scaling limits, and the explicit calculation of the prefactors for both the large and the small  $\gamma$  asymptotics of  $D_\gamma$ . We will restrict our attention to the one-dimensional case. We study the long time/small  $\gamma$  asymptotic of the one-dimensional Langevin equation

$$\ddot{q} = -\partial_q V(q) - \gamma \dot{q} + \sqrt{2\gamma\beta^{-1}} \xi(t) \quad (1.8)$$

when  $V(q)$  is a smooth, *periodic* potential and  $\xi(t)$  is white noise. Our first result can be summarized in the following.

**Theorem 1.1.** *The Freidlin–Wentzell scaling limit (1.4) and the diffusive scaling limit (1.5) ‘commute’. In particular, the rescaled process*

$$\varepsilon \gamma q(t / (\gamma \varepsilon^2))$$

*converges weakly, both in the  $\lim_{\varepsilon \rightarrow 0} \lim_{\gamma \rightarrow 0}$  limit and the  $\lim_{\gamma \rightarrow 0} \lim_{\varepsilon \rightarrow 0}$  limit, to a Brownian motion with diffusion coefficient  $D^*$  given by formula (2.8) below.*

*Furthermore, the Kramers to Smoluchowski scaling limit (1.2) and the diffusive scaling limit (1.5) also ‘commute’: the rescaled process*

$$\varepsilon q(t / (\gamma \varepsilon^2))$$

converges weakly, both in the  $\lim_{\varepsilon \rightarrow 0} \lim_{\gamma \rightarrow \infty}$  limit and the  $\lim_{\gamma \rightarrow \infty} \lim_{\varepsilon \rightarrow 0}$  limit, to a Brownian motion with diffusion coefficient  $\bar{D}$  given by formula (4.2) below.

The above theorem justifies rigorously the expressions (1.6) and (1.7), for  $\gamma \ll 1$  and  $\gamma \gg 1$ .

Clearly, the above theorem implies that

$$\lim_{\gamma \rightarrow 0} \gamma D_\gamma = D^* \quad \text{and} \quad \lim_{\gamma \rightarrow \infty} \gamma D_\gamma = \bar{D}.$$

In fact, we can say slightly more: in Section 4, we prove the two-sided bound

$$\frac{D^*}{\gamma} \leq D_\gamma \leq \frac{\bar{D}}{\gamma}, \quad \forall \gamma \in (0, \infty).$$

We also compute the next order correction in the large  $\gamma$  expansion of the diffusion coefficient  $D_\gamma$ .

More generally, we are going to study the small- $\gamma$  asymptotic of the rescaled process

$$q^\gamma(t) = \lambda_\gamma q(t/\mu_\gamma) \tag{1.9}$$

for a suitable one-parameter family of space-time rescalings  $\lambda_\gamma, \mu_\gamma$ . It turns out that the “right” scalings – the ones giving rise to a non-trivial limiting process – are of the form

$$\lambda_\gamma = \gamma^{1+\alpha}, \quad \mu_\gamma = \gamma^{1+2\alpha}, \quad \alpha \in [0, \infty). \tag{1.10}$$

Note that the case  $\alpha = 0$  corresponds to the Freidlin-Wentzell rescaling (1.4), whereas the case  $\alpha = \infty$  corresponds to the diffusive rescaling (1.5). Our second result is the following.

**Theorem 1.2.** *Assume that the Markov process  $(q(t), p(t))$  is stationary on  $\mathbf{T} \times \mathbf{R}$ . Then the rescaled process  $q^\gamma(t)$  defined in (1.9) converges weakly to a Brownian motion for every  $\alpha \in (1/2, +\infty)$ . The diffusion coefficient of the limiting Brownian motion is independent of  $\alpha$  and is given by (2.8).*

**Remark 1.3.** *We believe that this theorem is also true for  $\alpha \in (0, 1/2)$ . However, we haven't been able to prove this. See also Remark 1.8 below.*

**Remark 1.4.** *The stationarity assumption is not necessary and can be replaced with the assumption that the distribution of the initial condition has an  $L^2$  density with respect to the Maxwell-Boltzmann distribution  $\mu(dp dq) = Z^{-1} \exp(-\beta H(p, q)) dp dq$ . For purely technical reasons it seems to be more difficult to obtain the same result for deterministic initial conditions.*

The, perhaps, surprising result is that the diffusion coefficient is *independent of the exponent  $\alpha$* : as long as we are at length and time scales which are long compared to the Freidlin-Wentzell length and time scales, the particle performs an effective Brownian motion with the same diffusion coefficient.

**Remark 1.5.** *A similar result holds for the large  $\gamma$  limit: Under the assumption of stationarity, we have that*

$$\lim_{\gamma \rightarrow \infty} \gamma^{-\alpha} q(t\gamma^{1+2\alpha}) = \sqrt{2\bar{D}} W(t)$$

*weakly on  $C([0, T], \mathbf{R})$  for every  $\alpha > 0$ , where  $\bar{D}$  is given by formula 4.2 below.*

Similar scalings to the one considered in (1.9) were considered for the passive tracer dynamics

$$\dot{q} = v(q) + \sqrt{2\sigma}\xi, \quad \nabla \cdot v = 0$$

by Fannjiang in [Fan02]. There it was shown that the diffusive time scale depends crucially on the ergodic properties of the vector field  $v(q)$  on  $\mathbf{T}^d$ . On the contrary, for the problem studied in this paper, the small  $\gamma$  asymptotic of  $\tau_{\text{diff}}$  and  $D$  are independent of the specific properties of the potential  $V(q)$ . This is because the Hamiltonian vector field can never generate an ergodic flow on the phase space  $\mathbf{T} \times \mathbf{R}$  due to the presence of the integral of the energy.

The proofs of Theorems 1.1 and 1.2 are based on a careful analysis of the generator of the Markov process  $(q(t), p(t))$  on  $\mathbf{T} \times \mathbf{R}$ . It turns out to be notationally more convenient to study the rescaled generator of (1.8)

$$L_\gamma = \frac{1}{\gamma} \mathcal{A} + L_{\text{OU}}, \quad (1.11)$$

on  $\mathbf{T} \times \mathbf{R}$ , where  $\mathcal{A} = p\partial_q - V'(q)\partial_p$  is the Liouville operator describing the unperturbed deterministic dynamic and  $L_{\text{OU}} = \beta^{-1}\partial_p^2 - p\partial_p$  is the generator of the Ornstein-Uhlenbeck process describing the interaction with the heat bath.

The main technical results which are needed for the proof of Theorem 1.1 are an estimate on the resolvent of  $L_\gamma$ , as well as estimates on derivatives of solutions to Poisson equation of the form  $-L_\gamma u = h$ . We obtain an estimate on the semigroup generated by  $L_\gamma$  which is independent of  $\gamma$ :

**Theorem 1.6.** *There exist constants  $C$  and  $\alpha$  independent of  $\gamma$  such that*

$$\|e^{L_\gamma t} f\| \leq C e^{-\alpha t} \|f\|, \quad (1.12)$$

holds for every  $t > 0$ , every  $\gamma < 1$ , and every  $f \in L^2(\mu)$  such that  $\int f d\mu = 0$ , where  $\mu(dp dq) = Z^{-1} \exp(-\beta H(q, p)) dp dq$ .

The Poisson equation that we need to analyze is

$$-L_\gamma \varphi_\gamma = p. \quad (1.13)$$

The boundary conditions for this PDE are that the solution is periodic in  $q$  and that it belongs to  $L^2(\mu)$ . Our estimate on derivatives of  $\varphi_\gamma$  is uniform in  $\gamma$ :

**Proposition 1.7.** *Assume that  $V(q)$  is smooth and let  $\varphi_\gamma$  be the solution to (1.13). There exists a constant  $C$  which is independent of  $\gamma$  such that*

$$\|\varphi_\gamma\|^2 + \|\partial_p \varphi_\gamma\|^2 + \|\partial_q \varphi_\gamma\|^2 + \gamma \left( \|\partial_p^2 \varphi_\gamma\|^2 + \|\partial_p \partial_q \varphi_\gamma\|^2 + \|\partial_q^2 \varphi_\gamma\|^2 \right) \leq C, \quad (1.14)$$

independently of  $\gamma$ . Furthermore,  $\partial_p \varphi_\gamma$  is an element of  $L^4(\mu)$  and

$$\|\partial_p \varphi_\gamma\|_{L^4(\mu)} \leq C(1 + \gamma^{-1/4}). \quad (1.15)$$

**Remark 1.8.** *We believe that estimate 1.15 should actually be uniform in  $\gamma$ . However, we haven't been able to prove this. The reason for this is that we obtain (1.15) as a consequence of Sobolev embedding, but  $\partial_p^2 \varphi_\gamma$  is not uniformly bounded in any weighted  $L^2$  space.*

The proof of estimates 1.12 and 1.15 is based on the commutator techniques that were developed recently by Villani [Vil06]. Somewhat similar estimates to the ones we prove in this paper were recently derived by Hérau in [Hér07].

The rest of the paper is organized as follows. In Section 2 we analyze the Freidlin-Wentzell scaling (1.4). In Section 3, we then study the diffusive scaling (1.5). In Section 4 we obtain upper and lower bounds on the diffusion coefficient and we study the large  $\gamma$  asymptotic. The intermediate scalings (1.9) for  $\alpha \in (0, +\infty)$  are investigated in Section 5. The necessary estimates on the resolvent of the generator  $L_\gamma$  are presented in Section 6.

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## 2 Critical Scaling: the $\alpha = 0$ case

Let us rewrite the Langevin equation (1.1) in one space dimension as a first order system:

$$dq(t) = p(t) dt, \quad (2.1a)$$

$$dp(t) = -\partial_q V(q(t)) dt - \gamma p(t) dt + \sqrt{2\gamma\beta^{-1}} dW, \quad (2.1b)$$

where  $V(q)$  is a smooth periodic potential with period 1 and  $W(t)$  is a standard one-dimensional Wiener process.

This section is devoted to the study of the critical scaling

$$q^\gamma(t) = \gamma q(t/\gamma), \quad (2.2)$$

which corresponds to the limiting case which is not covered by Theorem 1.2. It turns out that under this scaling,  $q^\gamma$  does *not* converge to a Brownian motion, but to a non-Markovian process that will be described in this section.

The behavior at the critical scaling can be understood with the help of the Freidlin-Wentzell theory of averaging for small random perturbations of a Hamiltonian system [FW94, FW98, FW99]. Recall that one can associate to a Hamiltonian system on the symplectic manifold  $\mathcal{M} = \mathbf{T} \times \mathbf{R}$  a graph  $\Gamma$  in such a way that every point in the graph corresponds to a connected component of a level set of  $H$ . Vertices of the graph correspond to level sets containing a critical point of  $H$ . See Figure 2 for an example.

We identify points on the graph  $\Gamma$  with elements of  $\mathbf{R} \times \mathbf{Z}$  by ordering the edges of the graph and taking the value of the Hamiltonian as a local coordinate along each edge. We denote by  $\tilde{H}: \mathcal{M} \rightarrow \Gamma \approx \mathbf{R} \times \mathbf{Z}$  the ‘extended’ Hamiltonian which associates each point to its energy, together with the number of the edge to which the corresponding connected component belongs.

Denoting by  $\lambda$  the Lebesgue measure on  $\mathcal{M}$ , the measure  $\tilde{\lambda} = \tilde{H}^* \lambda$  on  $\Gamma$  then has a density with respect to Lebesgue measure on  $\Gamma$ , which we denote by  $T(z)$ . The notation  $T(z)$  is justified by the fact that it is actually equal to the period of the orbit corresponding to the point  $z$ . It is therefore a straightforward exercise to see that

$$T(z) \approx |\log(z - z_0)|,$$

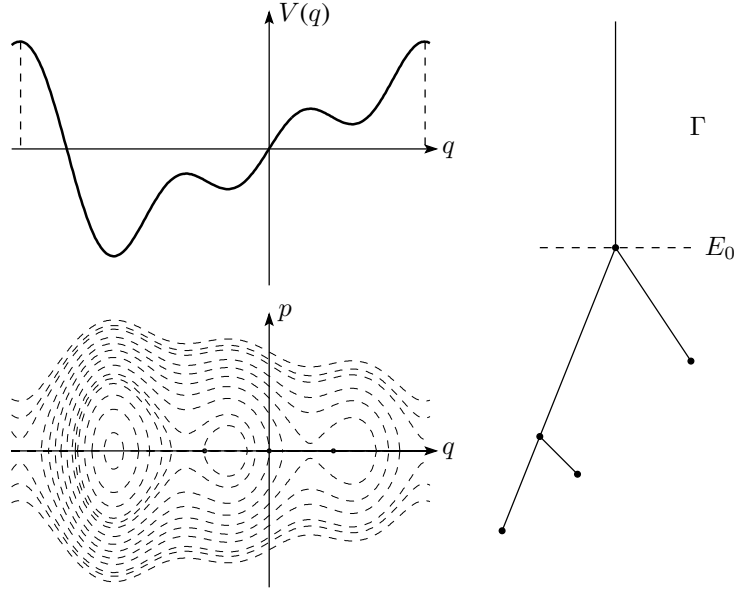


Figure 2: Example of a potential with the orbits of the Hamiltonian flow and the corresponding Freidlin-Wentzell graph  $\Gamma$ .

near the vicinity of a critical orbit  $z_0$  which corresponds to a maximum of the potential. For a point  $z \in \Gamma$ , denote by  $\ell_z$  the measure on  $\tilde{H}^{-1}(z)$  which is such that

$$\int_{\mathcal{M}} f(x) \lambda(dx) = \int_{\Gamma} \int_{\tilde{H}^{-1}(z)} f(x) \ell_z(dx) dz ,$$

for every integrable function  $f: \mathcal{M} \rightarrow \mathbf{R}$ . The measure  $\ell_z$  is not a probability measure but has mass  $T(z)$ . With this notation at hand, we define the function

$$S(z) = \int_{\tilde{H}^{-1}(z)} p^2 \ell_z(dx) ,$$

where we used the notation  $x = (q, p)$  for elements of  $\mathcal{M}$ . The function  $S(z)$  has non-trivial limits as  $z$  approaches the vertices of  $\Gamma$ . Note that these limits are in general different for different ways of approaching the same vertex, so that  $S$  is discontinuous on  $\Gamma$ . It is also possible to check [FW84] that  $S$  satisfies the relation  $S'(z) = T(z)$  in the interior of the edges.

The main result of [FW99] is then

**Theorem 2.1.** *Let  $X^\gamma(t)$  be defined by  $X^\gamma(t) = (p(t/\gamma), q(t/\gamma))$ , where  $(p, q)$  is a solution to (2.1). Then, the process  $\tilde{H}(X^\gamma(t))$  converges weakly to a Markov process  $Y$  on  $\Gamma$  whose generator is given by the expression*

$$Lv(z) = \frac{1}{\beta T(z)} \frac{d}{dz} \left( S(z) \frac{dv(z)}{dz} \right) - \frac{S(z)}{T(z)} \frac{dv(z)}{dz} , \quad (2.3)$$

for  $z$  in the interior of the edges of  $\Gamma$ . The domain of  $L$  consists of functions  $v$  such that the above expression is square integrable, and such that at each interior vertex,

the derivatives of  $v$  along the edges satisfy the ‘gluing’ conditions

$$\sum_{k \sim z_0} \sigma(z_0, k) \lim_{z \rightarrow_k z_0} S(z) \frac{dv(z)}{dz} = 0.$$

Here,  $z_0$  denotes an interior vertex of  $\Gamma$ , the sum runs over all edges  $k$  adjacent to  $z_0$ , and  $z \rightarrow_k z_0$  means that  $z$  converges to  $z_0$  along the edge  $k$ . The factor  $\sigma(z_0, k)$  is equal to 1 if  $H(z) > H(z_0)$  for  $z$  in the  $k$ th edge and  $-1$  otherwise.

Note that the gluing conditions are such that the process  $Y$  is reversible with respect to the probability measure  $\mu_\beta(dz) = Z_\beta^{-1} e^{-\beta z} \tilde{\lambda}(dz) = Z_\beta^{-1} e^{-\beta z} T(z) dz$  on  $\Gamma$ . This in turn is precisely the push-forward under  $\tilde{H}$  of the probability measure  $Z_\beta^{-1} e^{-\beta H(x)} \lambda(dx)$  on  $\mathcal{M}$  which is invariant for the process  $X^\gamma$ .

**Corollary 2.2.** *Let  $f: \mathcal{M} \rightarrow \mathbf{R}$  be smooth with at most polynomial growth and define  $\bar{f}: \Gamma \rightarrow \mathbf{R}$  by*

$$\bar{f}(z) = \frac{1}{T(z)} \int_{\tilde{H}^{-1}(z)} f(x) \ell_z(dx).$$

Then, the process  $\int_0^t f(X^\gamma(s)) ds$  converges weakly to the process  $\int_0^t \bar{f}(Y(s)) ds$ .

*Proof.* If  $f \equiv 0$  in a neighborhood of the critical orbits, the result follows from a standard averaging argument which will not be reproduced here. We refer to [] for a similar calculation. We can now construct smooth functions  $f^\delta$  such that  $f^\delta \equiv 0$  in a  $\delta$ -neighborhood of the critical orbits and  $f^\delta = f$  outside of a  $2\delta$ -neighborhood of the critical orbits. The result then follows immediately from the fact that there exists a function  $h$  with  $\lim_{\delta \rightarrow 0} h(\delta) = 0$  such that the expectation of the time that the process  $X^\gamma$  spends in the region where  $f^\varepsilon \neq f$  is bounded by  $h(\delta)$ , uniformly in  $\gamma$  (see [FW84, p. 294]).  $\square$

**Remark 2.3.** *An important particular case of Corollary 2.2 is that of  $f(p, q) = p$ . It shows that the process  $q^\gamma$  defined in (2.2) converges weakly to the process*

$$q^*(t) = \int_0^t \bar{p}(Y(s)) ds,$$

where the function  $\bar{p}: \Gamma \rightarrow \mathbf{R}$  is defined from  $p$  as in Corollary 2.2.

It is clear that the process  $q^*$  is not Markov by itself, but requires the computation of  $Y$  first. Note also that the function  $\bar{p}(z)$  vanishes identically for values of  $z$  corresponding to closed orbits, so that the process  $q^*$  is constant on intervals of time of positive length. On values of  $z$  for which the orbits are open, one has

$$\bar{p}(z) = \pm \frac{1}{T(z)}, \quad (2.4)$$

since the average velocity is given by the size of the torus (which was set to 1), divided by the period of the orbit.

Denote by  $\mathcal{P}_t$  the semigroup over  $\Gamma$  generated by  $L$ . It follows from the central limit theorem for additive functionals of reversible Markov processes [KV86] that the process  $\varepsilon q^*(t/\varepsilon^2)$  converges weakly as  $\varepsilon \rightarrow 0$  to a Brownian motion with diffusivity given by

$$D^* = \int_0^\infty \int_\Gamma \bar{p}(z) \mathcal{P}_t \bar{p}(z) \mu_\beta(dz) dt.$$



Since  $L$  is self-adjoint in  $L^2(\Gamma, \mu_\beta)$  and has a spectral gap, this integral converges and is given by

$$D^* = -\langle \bar{p}, L^{-1}\bar{p} \rangle_\beta, \quad (2.5)$$

where we denoted by  $\langle \cdot, \cdot \rangle_\beta$  the scalar product in  $L^2(\Gamma, \mu_\beta)$ .

It turns out that in our case, this expression can be computed in a very explicit way. Note that in  $L^2(\Gamma, \mu_\beta)$ , one has  $L = -A^*A$ , where the first order differential operator  $A$  is given by

$$Av(z) = \sqrt{\frac{S(z)}{\beta T(z)}} \frac{dv(z)}{dz} \equiv a(z) \frac{dv(z)}{dz}.$$

The domain of  $A$  consists of all continuous functions  $f$  on  $\Gamma$  such that  $f$  is weakly differentiable in the interior of each edge and such that  $Af \in L^2(\Gamma, \mu_\beta)$ .

The adjoint of  $A$  is given by the operator that acts in the interior of the edges of  $\Gamma$  like

$$\begin{aligned} A^*w(z) &= -\frac{e^{\beta z}}{T(z)} \frac{d}{dz} (T(z)e^{-\beta z} a(z)w(z)) \\ &= -\frac{d}{dz} (a(z)w(z)) - w(z)a(z) \left( \frac{T'(z)}{T(z)} - \beta \right), \end{aligned}$$

endowed with the ‘boundary conditions’

$$\sum_{k \sim z_0} \sigma(z_0, k) \lim_{z \rightarrow_k z_0} T(z)a(z)w(z) = 0. \quad (2.6)$$

Here, we used the same notations as in the statement of Theorem 2.1. One then has the following variational formulation of  $D^*$ :

$$D^* = \inf\{\|g\|_\beta^2 \mid A^*g = \bar{p}\}. \quad (2.7)$$

Functions satisfying the relation  $A^*g = \bar{p}$  are of the form

$$g(z) = \frac{\sqrt{\beta}e^{\beta z}}{\sqrt{S(z)T(z)}} \left( V_k + \int_{z_0}^z T(z)\bar{p}(z)e^{-\beta z} dz \right),$$

where we denote by  $k$  the index of the edge to which  $z$  belongs and by  $z_0$  the vertex with the lowest energy adjacent to that edge. The constants  $V_k$  are determined by the requirements that  $g$  satisfies the conditions (2.6) and that  $g \in L^2$ . By (2.7), remaining degrees of freedom should be dealt with by minimising over  $\|g\|_\beta$ .

In our case, the graph  $\Gamma$  contains two infinite edges and a number of finite ones. Since  $\bar{p}$  vanishes on the finite edges and is given by (2.4) on the two infinite edges, it follows that the function  $g$  minimizing (2.7) is given by

$$g(z) = \sigma(z) \frac{1}{\sqrt{\beta S(z)T(z)}},$$

where the function  $\sigma(z)$  vanishes on all the finite edges and is equal to  $\pm 1$  on the infinite edges, with the same sign as  $\bar{p}$ . Therefore, we finally obtain for  $D^*$  the expression

$$D^* = \frac{2}{\beta Z_\beta} \int_{E_0}^\infty \frac{e^{-\beta z}}{S(z)} dz, \quad (2.8)$$

where  $E_0$  is the energy of the vertex at which the two infinite edges join. (The reason for the factor 2 in front of the above expression is that there are exactly two infinite edges starting at  $E_0$ .) The function  $S(z)$  is asymptotic to  $2zT(z) \approx \sqrt{2z}$  at infinity and converges to a non-zero constant as  $z \rightarrow E_0$ . Furthermore, the partition function  $Z_\beta$  behaves like  $T_0/\beta$  for large values of  $\beta$  (here  $T_0$  is the value of  $T(z)$  as  $z$  approaches the orbit where the energy attains its global minimum).

In order to compute the behavior of  $Z_\beta$  for small values of  $\beta$ , we use the fact that  $T(z) \approx \frac{1}{\sqrt{2z}}$  for large values of  $z$ . Therefore

$$Z_\beta \approx \int_0^\infty \frac{e^{-\beta z}}{\sqrt{2z}} dz = \sqrt{\frac{\pi}{2\beta}}.$$

A similar calculation allows to evaluate the behavior of the integral over  $e^{-\beta z}/S(z)$  for small values of  $\beta$ . Collecting these asymptotic estimates, one obtains

$$\begin{aligned} D^* &\approx \frac{2}{\beta} & \beta \rightarrow 0, \\ D^* &\approx \frac{2e^{-\beta E_0}}{\beta T_0 S(E_0)} & \beta \rightarrow \infty. \end{aligned}$$

**Remark 2.4.** *It is unsurprising to see that the high-temperature limit  $\beta \rightarrow 0$  coincides with the result that one obtains when  $V \equiv 0$ .*

### 3 The Central Limit Theorem Regime: The $\alpha = \infty$ Case.

Just as in the previous section, the long time behavior of solutions to (1.1) for a fixed value of  $\gamma$  is governed by an effective Brownian motion. Indeed, the following central limit theorem holds [Rod89, PV85, HP04, Koz89].

**Theorem 3.1.** *Let  $V(q) \in C_{per}^\infty(\mathbf{T})$  and define the rescaled process*

$$q^\varepsilon(t) := \varepsilon q(t/\varepsilon^2).$$

*Then  $q^\varepsilon(t)$  converges weakly, on  $C([0, T], \mathbf{R})$ , in the limit as  $\varepsilon \rightarrow 0$ , to a Brownian motion with diffusion coefficient*

$$D_\gamma = \frac{1}{\gamma} \int_{\mathbf{T} \times \mathbf{R}} p \varphi_\gamma \mu(dp dq), \quad (3.1)$$

*where  $\mu(dp dq) = Z^{-1} \exp(-\beta H(p, q)) dp dq$ , and the function  $\varphi_\gamma$  is the unique mean-zero solution of the Poisson equation*

$$-L_\gamma \varphi_\gamma = p. \quad (3.2)$$

*Here  $L_\gamma$  is the rescaled generator defined in (1.11) and  $\varphi_\gamma$  is periodic in  $q$  and an element of  $L^2(\mu)$ .*

**Remark 3.2.** *This theorem is valid in arbitrary dimensions. It is also valid when the force field in (1.1) is not the gradient of a scalar function, provided that  $\mu(dp dq)$  is replaced by the corresponding invariant measure; see [HP04].*

The main result of this section is that, in the limit as the friction coefficient  $\gamma$  tends to 0, the rescaled effective diffusion coefficient given by (3.1) converges to the Freidlin-Wentzell effective diffusivity (2.5).

**Proposition 3.3.** *One has  $\lim_{\gamma \rightarrow 0} \gamma D_\gamma = D^*$ , where  $D^*$  is obtained by (2.5).*

*Proof.* Denote as before by  $L_\gamma$  the generator of the critically rescaled dynamic (2.2) given in eqn. (1.11) and by  $\mathcal{P}_t^\gamma$  the corresponding semigroup acting on  $L^2(\mathcal{M}, \mu)$ . Denote furthermore as previously by  $L$  the generator of the limiting Feidlin-Wentzell dynamic (2.3) and by  $\mathcal{P}_t$  the corresponding semigroup acting on  $L^2(\Gamma, \mu)$ . Finally, we introduce the averaging operator  $\Pi$  defined (on continuous functions  $f: \mathcal{M} \rightarrow \mathbf{R}$ ) by

$$(\Pi f)(z) = \frac{1}{T(z)} \int_{\tilde{H}^{-1}(z)} f(y) \ell_z(dy), \quad z \in \Gamma. \quad (3.3)$$

Note that  $\Pi f$  is a function from  $\Gamma$  to  $\mathbf{R}$ . Furthermore, it is immediate that  $\Pi$  is a contraction from  $L^2(\mathcal{M}, \mu)$  to  $L^2(\Gamma, \mu)$  and can therefore be extended uniquely to all of  $L^2(\mathcal{M}, \mu)$ .

We also define the isometric embedding operator  $\iota: L^2(\Gamma, \mu) \rightarrow L^2(\mathcal{M}, \mu)$  by

$$(\iota f)(x) = f(\tilde{H}(x)).$$

With these notations, one has  $D^* = \langle \Pi p, L^{-1} \Pi p \rangle$  and  $\gamma D_\gamma = \langle p, L_\gamma^{-1} p \rangle$ , so that the result follows if one can show that the strong limit in  $L^2(\mathcal{M}, \mu)$

$$\lim_{\gamma \rightarrow 0} L_\gamma^{-1} f = \iota L^{-1} \Pi f, \quad (3.4)$$

holds for every element  $f \in L^2(\mathcal{M}, \mu)$  such that  $\int f(x) \mu(dx) = 0$ .

This will be the consequence of the following two lemmas:

**Lemma 3.4.** *For every function  $f \in L^2(\mathcal{M}, \mu)$ , the limit  $\lim_{\gamma \rightarrow 0} \mathcal{P}_t^\gamma f = \iota \mathcal{P}_t \Pi f$  holds in  $L^2(\mathcal{M}, \mu)$ .*

*Proof.* Assume first that  $f$  is bounded and continuous. It then follows from Corollary 2.2 that  $\lim_{\gamma \rightarrow 0} (\mathcal{P}_t^\gamma f)(x) = (\iota \mathcal{P}_t \Pi f)(x)$  for every  $x \in \mathcal{M}$ . The claim then follows from Lebesgue's dominated convergence theorem. The fact that the claim holds for every  $f \in L^2(\mathcal{M}, \mu)$  is now a simple consequence of the density of bounded continuous functions, together with the fact that  $\mathcal{P}_t^\gamma$  is a contraction operator in  $L^2(\mathcal{M}, \mu)$ .  $\square$

This, together with Theorem 1.6 yields:

**Lemma 3.5.** *There exist constants  $C$  and  $\alpha$  (independent of  $\gamma < 1$ ) such that*

$$\|\mathcal{P}_t^\gamma f\| + \|\mathcal{P}_t f\| \leq C e^{-\alpha t} \|f\|,$$

for every  $f \in L^2(\Gamma, \mu)$  such that  $\int f(x) \mu(dx) = 0$ , and for every  $t > 0$ .

*Proof.* The bound on  $\|\mathcal{P}_t^\gamma f\|$  is precisely the one given in Theorem 1.6. Since this bound is uniform in  $\gamma$ , the bound on  $\mathcal{P}_t f$  follows at once from Lemma 3.4.  $\square$

We now have all the necessary ingredients for the proof of (3.4). Fix  $\varepsilon > 0$  and choose  $T$  sufficiently large such that

$$\left\| L_\gamma^{-1} f - \int_0^T \mathcal{P}_t^\gamma f dt \right\| \leq \varepsilon, \quad \left\| L^{-1} \Pi f - \int_0^T \mathcal{P}_t \Pi f dt \right\| \leq \varepsilon.$$

Such a  $T$  can be chosen independently of  $\gamma$  by Lemma 3.5. On the other hand, it follows from Lemma 3.4 and Lebesgue's dominated convergence theorem that

$$\lim_{\gamma \rightarrow 0} \left\| \int_0^T (\mathcal{P}_t^\gamma f - \iota \mathcal{P}_t \Pi f) dt \right\| = 0,$$

and the result follows.  $\square$

**Remark 3.6.** *Following the methodology advertised in [PS07], it would be satisfying to obtain an expansion for  $\varphi_\gamma$  of the type  $\varphi_\gamma = \varphi_0 + \gamma\varphi_1 + \varrho$  for some error term  $\varrho$  and therefore to get better explicit control over the convergence in (3.4). The problem with this approach is the loss of regularizing properties of the resolvent  $L_\gamma^{-1}$  as  $\gamma \rightarrow 0$ . In particular, the limiting function  $\varphi_0$  is not  $C^\infty$ , but only Lipschitz continuous. As a consequence, the first corrector is not of order  $\gamma$ , but expected to be of order  $\gamma^{1/2}$ , see [Sow03, Sow05], thus leading to a breakdown of the naive perturbative expansion.*

## 4 Estimates on the Effective Diffusion Coefficient

In this section we present some estimates on the diffusion coefficient  $D_\gamma$  defined in (3.1). To state the upper bound we need to define the diffusion coefficient for the Smoluchowski equation

$$\dot{z} = -\partial_z V(z) + \sqrt{\frac{2}{\beta}} \xi(t), \quad (4.1)$$

with  $V(z)$  being the smooth periodic potential in (1.1). It is well known, see e.g. [Oll94] or [PS07, Ch. 13], that the rescaled process  $\varepsilon z(t/\varepsilon^2)$  converges weakly in the limit as  $\varepsilon \rightarrow 0$  to  $\sqrt{2\bar{D}}W(t)$  where  $W(t)$  is a standard Brownian motion and the diffusion coefficient is given by the formula

$$\bar{D} = \beta^{-1} \int_{\mathbf{T}} |1 + \partial_q \chi|^2 \nu(dq) =: \beta^{-1} \|1 + \partial_q \chi\|^2, \quad (4.2)$$

where

$$\nu(dq) = \frac{1}{Z} e^{-\beta V(q)} dq, \quad Z = \int_{\mathbf{T}} e^{-\beta V(q)} dq,$$

and the function  $\chi$  is the solution to the Poisson equation

$$\bar{L}\chi = \partial_q V(q), \quad \bar{L} = -\partial_q V(q)\partial_q + \beta^{-1}\partial_q^2, \quad (4.3)$$

equipped with periodic boundary conditions. It is well known that  $\bar{D} \leq \beta^{-1}$ . The upper bound in the theorem below shows that diffusion for the Langevin dynamics is depleted even further.

**Proposition 4.1.** *Let  $D^*$  be as in (2.8) and let  $\bar{D}$  be as above. Then, the bound*

$$\frac{D^*}{\gamma} \leq D_\gamma \leq \frac{\bar{D}}{\gamma}, \quad (4.4)$$

is valid for every  $\gamma \in (0, \infty)$ .

*Proof.* We multiply equation (3.2) by a smooth test function  $\psi \in L^2(\mu)$  to obtain

$$\frac{1}{\gamma} \int_{\mathbf{T} \times \mathbf{R}} \varphi_\gamma \mathcal{A}\psi \mu(dp dq) + \beta^{-1} \int_{\mathbf{T} \times \mathbf{R}} \partial_p \varphi_\gamma \partial_p \psi \mu(dp dq) = \int_{\mathbf{T} \times \mathbf{R}} p\psi \mu(dp dq). \quad (4.5)$$

We choose a test function which is independent of  $p$ ,  $\psi = \psi(q)$  to obtain

$$\int_{\mathbf{T} \times \mathbf{R}} \varphi_\gamma p \partial_q \psi \mu(dp dq) = 0. \quad (4.6)$$

We introduce the decomposition

$$\bar{\varphi}_\gamma(q) = \int \varphi_\gamma(p, q) \nu_\beta(dp), \quad \tilde{\varphi}_\gamma(p, q) = \varphi_\gamma(p, q) - \bar{\varphi}_\gamma(q), \quad (4.7)$$

where  $\nu_\beta(p) = Z^{-1} \exp(-\beta p^2/2)$ . Note that if  $\varphi$  is a function from  $\mathbf{R}$  to  $\mathbf{R}$  such that  $\int \varphi(p) \nu_\beta(dp) = 0$ , then it follows from the spectral decomposition of the harmonic oscillator Schrödinger operator that  $\|\partial_p \varphi\|^2 \geq \beta \|\varphi\|^2$ , where the norms are in  $L^2(\nu_\beta)$ . This inequality can be applied pointwise to  $\tilde{\varphi}_\gamma$ , so that he bound

$$\|\partial_p \varphi_\gamma\|^2 = \|\partial_p \tilde{\varphi}_\gamma\|^2 \geq \beta \|\tilde{\varphi}_\gamma\|^2 \quad (4.8)$$

holds.

Substituting the decomposition (4.7) and (4.6) into the expression for  $D_\gamma$ , we obtain

$$\begin{aligned} D_\gamma &= \int_{\mathbf{T} \times \mathbf{R}} \tilde{\varphi}_\gamma p \mu(dp dq) = \int_{\mathbf{T} \times \mathbf{R}} \tilde{\varphi}_\gamma p (1 + \partial_q \psi) \mu(dp dq) \\ &\leq \|\tilde{\varphi}_\gamma\| \|p(1 + \partial_q \psi)\| \leq \sqrt{\beta^{-1}} \|\partial_p \varphi_\gamma\| \|1 + \partial_q \psi\| \|p\| \\ &\leq \sqrt{\gamma D_\gamma} \|1 + \partial_q \psi\| \sqrt{\beta^{-1}}. \end{aligned}$$

Here, we used (4.8) on the second line and we used the fact that the effective diffusion coefficient can be written as

$$D_\gamma = \frac{1}{\gamma \beta} \|\partial_p \varphi_\gamma\|^2.$$

to go from the second to the third line. It follows from this calculation that  $D_\gamma \leq \frac{1}{\gamma \beta} \|1 + \partial_q \psi\|^2$ , so that (4.4) follows by taking  $\psi$  in the above estimate to be  $\chi$ , the solution of (4.3), and by using (4.2).

Now we proceed with the bound from below. This time, we use a test function  $\psi$  of the form

$$\psi(p, q) = \begin{cases} \varphi \circ H & \text{for } p \geq 0 \\ -\varphi \circ H & \text{for } p \leq 0 \end{cases}$$

where  $\varphi: \mathbf{R}_+ \rightarrow \mathbf{R}_+$  is a smooth function with  $\varphi(H) = 0$  for  $H \leq E_0$  and such that  $\lim_{H \downarrow E_0} \varphi'(H) \neq 0$ . Plugging this ansatz into equation (4.5), we obtain

$$\beta^{-1} \int_{\mathbf{T} \times \mathbf{R}} \partial_p \varphi_\gamma \partial_p \psi \mu(dp dq) = \int_{\mathbf{T} \times \mathbf{R}} p \psi \mu(dp dq) = -\beta^{-1} \int_{\mathbf{T} \times \mathbf{R}} \partial_p \psi \mu(dp dq).$$

Here, we used integration by parts and the explicit expression for  $\mu$  in order to obtain the second equality. Cauchy-Schwarz now yields:

$$D_\gamma = \frac{1}{\gamma \beta} \|\partial_p \varphi_\gamma\|^2 \geq \frac{\left( \int_{\mathbf{T} \times \mathbf{R}} \partial_p \psi \mu(dp dq) \right)^2}{\gamma \beta \|\partial_p \psi\|^2}.$$

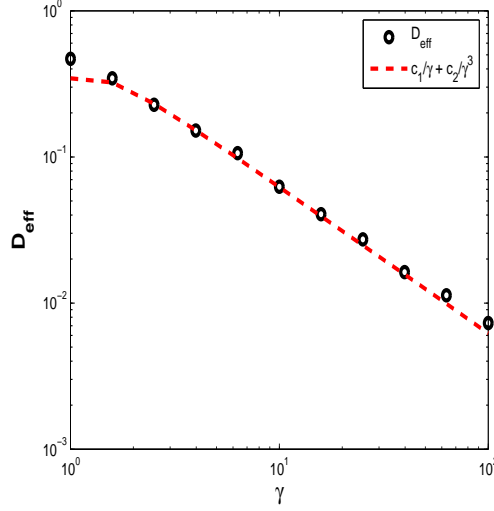
At this point, we notice that, with the notations of Section 2, this is equivalent to

$$D_\gamma \geq \frac{\left( 2Z_\beta^{-1} \int_{E_0}^\infty \varphi'(z) e^{-\beta z} dz \right)^2}{2\gamma \beta Z_\beta^{-1} \int_{E_0}^\infty (\varphi'(z))^2 S(z) e^{-\beta z} dz}.$$

Choosing  $\varphi$  such that  $\varphi'(z) = 1/S(z)$ , we finally obtain

$$D_\gamma \geq \frac{2}{\gamma \beta Z_\beta} \int_{E_0}^\infty \frac{e^{-\beta z}}{S(z)} dz$$

which, combined with (2.8), is the required bound.  $\square$

Figure 3: Large  $\gamma$  asymptotic for the effective diffusivity.

#### 4.1 Large $\gamma$ Asymptotic

It is well known that, when  $\gamma$  is large, solutions to the Langevin equation (1.1) are approximated by solutions to the Smoluchowski equation (4.1), see e.g. [Nel67, Thm. 10.1], [Fre04]. It is therefore not surprising that a result similar to Proposition 3.3 holds in the large  $\gamma$  limit:

$$\lim_{\gamma \rightarrow \infty} \gamma D = \bar{D} = \frac{1}{\beta Z \widehat{Z}},$$

where

$$Z = \int_0^1 e^{-\beta V(q)} dq, \quad \widehat{Z} = \int_0^1 e^{\beta V(q)} dq.$$

In the above we used the fact that  $\bar{D}$  can be calculated explicitly [PS07, Sec. 13.6]. It is also quite straightforward (at least formally) to obtain the next term in the small  $\gamma^{-1}$  expansion for  $D_\gamma$ . We solve perturbatively (3.2) using the technique presented in [HL84, Ch. 8] we obtain

$$D_\gamma = \frac{1}{\beta \gamma Z \widehat{Z}} - \frac{\beta Z_1}{\gamma^3 Z \widehat{Z}^2} + \mathcal{O}\left(\frac{1}{\gamma^5}\right), \quad (4.9)$$

where  $Z$  and  $\widehat{Z}$  are as before, and  $Z_1$  is given by  $Z_1 = \int_0^1 (V'(q))^2 e^{\beta V(q)} dq$ .

In Figure 3, we plot the diffusion coefficient  $D$  for the nonlinear pendulum obtained from direct numerical simulations, together with the approximation (4.9). As expected, the agreement between the result of the Monte-Carlo simulation and the theoretical prediction is very good, even for values of  $\gamma$  that are close to  $\mathcal{O}(1)$ .<sup>1</sup>

<sup>1</sup>In the case where the potential has period  $\ell$ , as opposed to 1, then formula (4.9) has to be multiplied by  $\ell^2$  and all the integrals that define the coefficients that appear in the formula are taken from 0 to  $\ell$ .

## 5 The intermediate regime: the $\alpha \in (0, +\infty)$ case

In this section we consider intermediate length and time scales, between and Freidlin-Wentzell and the central limit theorem ones. In particular, we prove Theorem 1.2, namely that, at intermediate length/time scales the particle position converges weakly to a Brownian motion with the Freidlin-Wentzell effective diffusivity 2.8.

*Proof of Theorem 1.2.* Notice that the stationarity assumption implies that, for every smooth function in  $L^1(\mu)$ , periodic in  $q$ ,

$$\mathbb{E}f(p(t), q(t)) = \int_{\mathbf{T} \times \mathbf{R}} f(p, q) \mu(dp dq).$$

Let  $\varphi_\gamma$  be the solution to the Poisson equation (3.2). We apply Itô's formula to  $\varphi_\gamma(p, q)$  to obtain

$$\begin{aligned} q^\gamma(t) &= \lambda_\gamma q(0) + \lambda_\gamma \int_0^{t/\mu_\gamma} p(s) ds \\ &= \lambda_\gamma q(0) - \lambda_\gamma \gamma^{-1} \left( \varphi_\gamma(p(t/\mu_\gamma), q(t/\mu_\gamma)) - \varphi_\gamma(p(0), q(0)) \right) \\ &\quad + \sqrt{2\gamma^{-1} \lambda_\gamma^2 \beta^{-1}} \int_0^{t/\mu_\gamma} \partial_p \varphi_\gamma(p(s), q(s)) dW(s) \\ &=: \lambda_\gamma q(0) + R^\gamma + M^\gamma, \end{aligned}$$

where  $\lambda_\gamma, \mu_\gamma$  are given in (1.10). We obviously have that  $\lim_{\gamma \rightarrow 0} \mathbb{E}(\lambda_\gamma q(0))^2 = 0$ . Proposition 6.1, the stationarity assumption and our assumption that  $\alpha > 0$ , furthermore imply that

$$\mathbb{E}|R^\gamma|^2 \leq C\gamma^\alpha \rightarrow 0,$$

as  $\gamma \rightarrow 0$ .

Consider now the martingale term  $M^\gamma$ . According to the martingale central limit theorem [EK86], in order to prove that  $M^\gamma$  converges to a Brownian motion, it is sufficient to show that the quadratic variation process  $\langle M^\gamma \rangle$ , converges weakly to a constant times  $t$ . This quadratic variation process is given by:

$$\langle M^\gamma \rangle_t = \frac{2\lambda_\gamma^2}{\gamma\beta} \int_0^{t/\mu_\gamma} |\partial_p \varphi_\gamma(p(s), q(s))|^2 ds.$$

Define

$$f_\gamma(p, q) := \frac{2\lambda_\gamma^2}{\gamma\mu_\gamma\beta} |\partial_p \varphi_\gamma(p, q)|^2 = 2\beta^{-1} |\partial_p \varphi_\gamma|^2$$

and

$$\bar{f}_\gamma := \int_{\mathbf{T} \times \mathbf{R}} f_\gamma(p, q) \mu(dp dq),$$

where  $\mu = Z^{-1} \exp(-\beta H(p, q)) dp dq$ . It follows from Propositions 6.1 and 6.3 that  $\bar{f}_\gamma$  remains bounded between two positive constants as  $\gamma \rightarrow 0$ .

In order to bound the error between  $\langle M^\gamma \rangle_t$  and  $\bar{f}_\gamma t$ , the idea is to subdivide the interval  $[0, t]$  into  $N$  'small' intervals of size  $\tau = t/N$  and to add the individual errors made at each time interval. Denote  $t_k = k\tau$  and  $\varepsilon_k = |\langle M^\gamma \rangle_{t_{k+1}} - \langle M^\gamma \rangle_{t_k} - \bar{f}_\gamma \tau|$ . Then, the fact that  $\langle M^\gamma \rangle$  is an increasing process implies that

$$\sup_{s \in [0, t/\mu_\gamma]} |\langle M^\gamma \rangle_s - \bar{f}_\gamma s| \leq \sum_{k=1}^N \varepsilon_k + \bar{f}_\gamma \tau + \sup_{k=1}^N \varepsilon_k \leq 2 \sum_{k=1}^N \varepsilon_k + \bar{f}_\gamma \tau. \quad (5.1)$$

The individual errors  $\varepsilon_k$  can be bounded in a standard way by

$$\begin{aligned} \mathbb{E}\varepsilon_k^2 &= \mathbb{E}\left(\int_{t_{k-1}}^{t_k} f_\gamma(p(s/\mu_\gamma), q(s/\mu_\gamma)) ds - \bar{f}_\gamma \tau\right)^2 \\ &= \mathbb{E}\left(\int_{t_{k-1}}^{t_k} f_\gamma(p(s/\mu_\gamma), q(s/\mu_\gamma)) ds\right)^2 - \bar{f}_\gamma^2 \tau^2 \\ &= \int_0^\tau \int_0^\tau \int_{\mathbf{T} \times \mathbf{R}} f_\gamma(p, q)(\mathcal{P}_{|r-s|/\mu_\gamma}^\gamma f_\gamma)(p, q) \mu(dp dq) dr ds - \bar{f}_\gamma^2 \tau^2 \\ &\leq \int_0^\tau \int_0^\tau \|f_\gamma\|^2 e^{-C\gamma|r-s|/\mu_\gamma} dr ds \leq \frac{C}{\gamma} \|f_\gamma\|_\mu^2 \tau \mu_\gamma. \end{aligned}$$

Here, we used the stationarity assumption. We also used Theorem 1.6 to bound the action of the semigroup  $\mathcal{P}_t^\gamma$ . Combining this with (5.1) yields

$$\begin{aligned} \mathbb{E}\left(\sup_{s \in [0, t/\mu_\gamma]} |\langle M^\gamma \rangle_s - \bar{f}_\gamma s|\right) &\leq C \|f_\gamma\|_\mu \sqrt{\frac{\mu_\gamma}{\gamma \tau}} + \bar{f}_\gamma \tau \\ &= C \|\partial_p \varphi_\gamma\|_{L^4(\mu)}^2 \gamma^\alpha \tau^{-1/2} + C \|\partial_p \varphi_\gamma\|^2 \tau \leq C(\gamma^{\alpha-1/2} \tau^{-1/2} + \tau). \end{aligned}$$

We now choose  $\tau = \gamma^\zeta$  for some  $\zeta > 0$ , arbitrarily small. Since we assumed  $\alpha > 1/2$ , we conclude that

$$\lim_{\gamma \rightarrow 0} \mathbb{E}\left(\sup_{s \in [0, t/\mu_\gamma]} |\langle M^\gamma \rangle_s - \bar{f}_\gamma s|\right) = 0.$$

Furthermore, it follows from the definition of  $\bar{f}_\gamma$  and from Proposition 3.3 that one has  $\lim_{\gamma \rightarrow 0} \bar{f}_\gamma = 2D^*$ . This immediately implies that, as  $\gamma \rightarrow 0$ ,  $\langle M^\gamma \rangle_t$  converges to  $2D^*t$  in  $L^1(\mu)$  and therefore  $M^\gamma$  converges to a Brownian motion with diffusivity  $D^*$ .  $\square$

The proof of the result stated in Remark 1.5 on the large  $\gamma$  asymptotic is essentially identical to the one presented above: Itô's formula, our assumption of stationarity and the scaling  $\lambda_\gamma = \gamma^{-\alpha}$  lead to

$$\gamma^{-\alpha} q(t\gamma^{1+2\alpha}) = M^\gamma + R^\gamma,$$

where  $\lim_{\gamma \rightarrow \infty} \|R^\gamma\| = 0$  and

$$M^\gamma = 2\gamma^{-1-2\alpha} \beta^{-1} \int_0^{t\gamma^{1+2\alpha}} |\partial_p \varphi_\gamma(p(s), q(s))|^2 ds.$$

The result now follows from the martingale central limit theorem, the subdivision of  $[0, t]$  that was used in the proof above and the fact that, for  $\gamma \gg 1$ , estimate (1.15) becomes

$$\|\partial_p \varphi_\gamma\|_{L^4(\mu)} \leq C,$$

for some constant independent of  $\gamma$ .

## 6 Resolvent bounds

In this section, we obtain the main bounds on the solution  $\varphi_\gamma$  of the Poisson equation (3.2). It will be convenient to work not only in the  $L^2$  space weighted by the invariant



measure  $\mu = \exp(-\beta H(p, q)) dp dq$ , but in the whole scale of spaces  $\mathcal{H}_\delta = L^2(\mu_\delta)$  for  $\delta \in (0, \beta]$ . The main technical difficulty is to obtain bounds in spaces for  $\delta \neq \beta$ , but this seems to be required in order to obtain the bound on the  $L^4$ -norm of  $\partial_p \varphi_\gamma$  required in Section 5. We first focus on bounds for the case  $\delta = \beta$ .

The norm and scalar product in  $\mathcal{H}_\delta$  will be denoted by  $\|\cdot\|_\delta$  and  $\langle \cdot, \cdot \rangle_\delta$  respectively. The subscript is omitted in the case  $\delta = \beta$ . We also denote by  $\mu_\delta$  the probability measure on  $\mathbf{T} \times \mathbf{R}$  proportional to  $\exp(-\delta H(p, q)) dp dq$  and by  $\nu_\delta$  the probability measure on  $\mathbf{R}$  proportional to  $\exp(-\delta p^2/2) dp$ .

### 6.1 Bounds in $\mathcal{H}_\beta$

We have the following preliminary bound:

**Proposition 6.1.** *Let  $\varphi_\gamma$  denote the solution of (3.2) and assume that  $V(q) \in C_{per}^\infty(\mathbf{T})$ . Then,  $\varphi_\gamma$  satisfies the bound*

$$\|\partial_p \varphi_\gamma\| \leq C, \quad (6.1)$$

for some constant  $C$  independent of  $\gamma$ .

*Proof.* Existence and uniqueness of solutions to (3.2) is proved for example in [PV85], see also [HP04, Thm. 3.3]. The smoothness of the solution follows from the hypoellipticity of the operator  $L^\gamma$ . Estimate (6.1) follows from the Poincaré inequality for Gaussian measures in the following way: we multiply (3.2) by  $\varphi_\gamma$  and integrate by parts on the left hand side to obtain

$$\beta^{-1} \|\partial_p \varphi_\gamma\|^2 = \langle p, \bar{\varphi} + \tilde{\varphi} \rangle,$$

where we defined

$$\bar{\varphi}_\gamma(q) = \int \varphi_\gamma(p, q) \nu_\beta(dp), \quad \tilde{\varphi}_\gamma(p, q) = \varphi_\gamma(p, q) - \bar{\varphi}_\gamma(q).$$

Since, for every  $q$ ,  $\tilde{\varphi}_\gamma$  averages to zero with respect to  $\nu_\beta$ , it satisfies the Poincaré inequality. On the other hand, we have that  $\langle p, \bar{\varphi}_\gamma \rangle = 0$ , since  $\bar{\varphi}_\gamma$  is a function of  $q$  only. Hence, by Cauchy-Schwarz and Poincaré, we have the bound

$$\|\partial_p \varphi_\gamma\|^2 = \beta \langle p, \tilde{\varphi}_\gamma \rangle \leq \beta \|p\| \|\tilde{\varphi}_\gamma\| \leq C \|\partial_p \tilde{\varphi}_\gamma\| = C \|\partial_p \varphi_\gamma\|,$$

for some constant  $C$  independent of  $\gamma$ . This concludes the proof.  $\square$

We proceed now with the proof of Theorem 1.6 which we restate here for the reader's convenience.

**Theorem 6.2.** *There exist constants  $C$  and  $\alpha$  independent of  $\gamma$  such that*

$$\|e^{L^\gamma t} f\| \leq C e^{-\alpha t} \|f\|, \quad (6.2)$$

holds for every  $t > 0$ , every  $\gamma < 1$ , and every  $f \in L^2(\mu)$  such that  $\int f d\mu = 0$ .

*Proof.* The proof is a variation on the commutator techniques introduced in [Koh69, Koh78] and further developed in [EPRB99, EH00, HN04, HN05, Vil06]. The argument given here is actually mainly inspired by the techniques developed by Villani in [Vil06]. In particular, we make use of his idea of constructing a 'skewed' scalar product in which the coercivity of  $L_\gamma$  becomes apparent. The main difference is that we are going to track carefully the dependence of the various terms on the parameter  $\gamma$ .

We will use the following notations:

$$\begin{aligned} A &= \beta^{-1/2} \partial_p, & A^* &= -\beta^{-1/2} \partial_p + \beta^{1/2} p, \\ B &= p \partial_q - V'(q) \partial_p, & B^* &= -B, \end{aligned}$$

The reason why we are using the symbol  $B$  for the Liouville operator and not  $\mathcal{A}$  as previously is to be consistent with the notations adopted in [Vil06]. With these notations, we have  $L_\gamma = -A^* A + \gamma^{-1} B$ . Here, the adjoints  $A^*$  and  $B^*$  are taken with respect to the scalar product in  $\mathcal{H} = L^2(\mu)$ . We also introduce the operators

$$\begin{aligned} \hat{C} &= [A, B] = \beta^{-1/2} \partial_q, \\ R &= [\hat{C}, B] = -\beta^{-1/2} V''(q) \partial_p = -V''(q) A. \end{aligned}$$

We introduce the symmetric sesquilinear form  $\langle\langle \cdot, \cdot \rangle\rangle$  defined by polarisation from

$$\langle\langle f, f \rangle\rangle = a \langle f, f \rangle + \gamma (b \langle Af, Af \rangle + 2 \operatorname{Re} \langle Af, \hat{C} f \rangle + b \langle \hat{C} f, \hat{C} f \rangle),$$

for some constants  $a$  and  $b$  to be determined later. If we take  $b > 1$ , then this is indeed positive definite and induces a norm equivalent to the norm  $\|\cdot\|_{1,\gamma}$  given by

$$\|f\|_{1,\gamma}^2 = \|f\|^2 + \gamma (\|\partial_p f\|^2 + \|\partial_q f\|^2). \quad (6.3)$$

Following the same manipulations as in [Vil06, Theorem 18], we see that there exists a constant  $c$  independent of  $\gamma$  such that

$$\begin{aligned} \operatorname{Re} \langle f, L_\gamma f \rangle &= -\|Af\|^2, \\ \operatorname{Re} \langle Af, AL_\gamma f \rangle &\leq -\|A^2 f\|^2 + c \|Af\|^2 + \frac{c}{\gamma} \|Af\| \|\hat{C} f\|, \\ \operatorname{Re} \langle Af, \hat{C} L_\gamma f \rangle + \operatorname{Re} \langle AL_\gamma f, \hat{C} f \rangle &\leq -\frac{1}{\gamma} \|\hat{C} f\|^2 + \frac{c}{\gamma} \|Af\|^2 \\ &\quad + c \|A^2 f\| \|\hat{C} Af\| + c \|\hat{C} f\| \|Af\|, \\ \operatorname{Re} \langle \hat{C} f, \hat{C} L_\gamma f \rangle &\leq -\|\hat{C} Af\|^2 + \frac{c}{\gamma} \|Af\| \|\hat{C} f\|. \end{aligned}$$

It is now easy to see that we can choose  $a \gg b \gg 1$  sufficiently large (but still independently of  $\gamma$ !) so that

$$\operatorname{Re} \langle\langle f, L_\gamma f \rangle\rangle \leq -\|Af\|^2 - \|\hat{C} f\|^2 - \gamma (\|A^2 f\|^2 + \|\hat{C} Af\|^2). \quad (6.4)$$

Note now that, provided that  $f$  is centred with respect to  $\mu$ , the Poincaré inequality tells us that there exists a constant  $\kappa$  such that

$$\|Af\|^2 + \|\hat{C} f\|^2 \geq \kappa \|f\|^2,$$

so that (6.4) implies in particular that  $\operatorname{Re} \langle\langle f, L_\gamma f \rangle\rangle \geq \kappa' \langle\langle f, f \rangle\rangle$  for some  $\kappa'$ . This immediately implies that there exist positive constants  $C$  and  $\alpha$  such that

$$\|e^{L_\gamma t} f\|_{1,\gamma} \leq C e^{-\alpha t} \|f\|_{1,\gamma}. \quad (6.5)$$

We will now show that there exists a time  $\tau$  and a constant  $C$ , both independent of  $\gamma$  (provided that  $\gamma$  is sufficiently small) such that

$$\|e^{L_\gamma \tau} f\|_{1,\gamma} \leq C \|f\|. \quad (6.6)$$

Combining this with (6.5) and (6.3) then implies that (6.2) holds.

In order to show (6.6), we combine the previous technique with the usual trick for proving regularisation results for parabolic PDEs. We fix a smooth function  $f$  and we define the quantity

$$2A_f(t) = K\|f_t\|^2 + \gamma(t\|Af_t\|^2 + t^3\|\hat{C}f_t\|^2 + \delta t^2\langle Af_t, \hat{C}f_t \rangle), \quad f_t = \mathcal{P}_t^\gamma f,$$

for some (large) constant  $K$  and some (small) constant  $\delta$  to be determined later. Taking the time derivative of  $A_f$ , we obtain

$$\begin{aligned} \partial_t A_f &\leq -K\|Af_t\|^2 + \gamma\|Af_t\|^2 + t(-\gamma\|A^2f_t\|^2 + c\gamma\|Af_t\|^2 + c\|Af_t\|\|\hat{C}f_t\|) \\ &\quad + 3\gamma t^2\|\hat{C}f_t\|^2 + t^3(-\gamma\|\hat{C}Af_t\|^2 + c\|Af_t\|\|\hat{C}f_t\|) + 2t\gamma\delta\langle Af_t, \hat{C}f_t \rangle \\ &\quad + \delta t^2(-\|\hat{C}f_t\|^2 + c\|Af_t\|^2 + c\gamma\|A^2f_t\|\|\hat{C}Af_t\| + c\gamma\|\hat{C}f_t\|\|Af_t\|) \\ &\leq -\frac{K}{2}\|Af_t\|^2 - \gamma t\|A^2f_t\|^2 - \gamma t^3\|\hat{C}Af_t\|^2 - \delta t^2\|\hat{C}f_t\|^2 \\ &\quad + ct\|Af_t\|\|\hat{C}f_t\| + c\gamma\delta t^2\|A^2f_t\|\|\hat{C}Af_t\|. \end{aligned}$$

(For the second inequality we changed the value of the constant  $c$  and we assumed that  $t \in [0, 1]$ .) Notice now that one can first choose  $\delta$  sufficiently small (but independently of  $\gamma$ ) such that

$$c\gamma\delta t^2\|A^2f_t\|\|\hat{C}Af_t\| \leq \gamma t\|A^2f_t\|^2 + \gamma t^3\|\hat{C}Af_t\|^2.$$

We can then choose  $K$  sufficiently large so that

$$ct\|Af_t\|\|\hat{C}f_t\| \leq \frac{K}{2}\|Af_t\|^2 + \delta t^2\|\hat{C}f_t\|^2.$$

With these choices, we get  $\partial_t A_f \leq 0$ , so that  $A_f(1) \leq A_f(0)$ . This immediately implies the bound (6.6).  $\square$

By simply integrating from 0 to  $\infty$ , this implies that one has the resolvent bound:

$$\|L_\gamma^{-1}f\| \leq C\|f\|, \quad (6.7)$$

holding for every  $f \in \mathcal{H}_\beta$  such that  $\langle 1, f \rangle = 0$ . It turns out that, up to a constant, this bound is actually optimal:

**Proposition 6.3.** *There exists a constant  $C$  independent of  $\gamma$  such that the operator norm of the resolvent satisfies*

$$\|L_\gamma^{-1}\| \geq C.$$

*Proof.* We make use of the fact that the norm of the resolvent can be characterized by

$$\|L_\gamma^{-1}\| = \left( \inf_{f \in \mathcal{D}(L_\gamma): \langle 1, f \rangle = 0} \frac{\|L_\gamma f\|}{\|f\|} \right)^{-1}. \quad (6.8)$$

If we take  $f$  of the form  $f = \varphi \circ H$  for an arbitrary smooth bounded function  $\varphi$  such that  $\langle 1, f \rangle = 0$ , then  $L_\gamma f$  (and therefore also  $\|L_\gamma f\|$ ) is independent of  $\gamma$ . Similarly,  $\|f\|$  is independent of  $\gamma$  so that the infimum appearing in (6.8) is bounded from above by a constant independent of  $\gamma$ , thus proving the claim.  $\square$

We now use these estimates to obtain bounds on the solution  $\varphi_\gamma$  to the Poisson equation  $-L_\gamma \varphi_\gamma = p$ .

**Proposition 6.4.** *There exists a constant  $C$  independent of  $\gamma$  such that*

$$\|\varphi_\gamma\| + \|\partial_p \varphi_\gamma\| + \|\partial_q \varphi_\gamma\| \leq C .$$

*Proof.* We have from (6.4) and the fact that the  $\|\cdot\|_{1,\gamma}$ -norm of  $p$  is bounded independently of  $\gamma$  that

$$\|\partial_p \varphi_\gamma\|^2 + \|\partial_q \varphi_\gamma\|^2 \leq \operatorname{Re}\langle\langle \varphi_\gamma, L\varphi_\gamma \rangle\rangle = \operatorname{Re}\langle\langle \varphi_\gamma, p \rangle\rangle \leq C\|\varphi_\gamma\|_{1,\gamma} \leq C .$$

The last inequality followed from the bound (6.5). One can actually extract slightly more from the above bounds. At this stage, we note that one can write  $B = \gamma(L - A^*A)$ , so that

$$\|B\varphi_\gamma\|^2 = \gamma\langle p, B\varphi_\gamma \rangle - \gamma\langle A\varphi_\gamma, AB\varphi_\gamma \rangle .$$

Since furthermore  $B$  is antisymmetric and  $[A, B] = \partial_q$ , we have

$$\|B\varphi_\gamma\|^2 \leq C\gamma + C\gamma\|\partial_p \varphi_\gamma\|\|\partial_q \varphi_\gamma\| .$$

Collecting this with the previous estimates, we obtain the existence of a constant  $C$  such that  $\|B\varphi_\gamma\| \leq C\sqrt{\gamma}$ , which in turn yields a bound of the type  $\|A^*A\varphi_\gamma\| \leq C/\sqrt{\gamma}$ .  $\square$

## 6.2 Bounds in $\mathcal{H}_\delta$ with $\delta \neq \beta$

We now show that similar bounds hold in every  $\mathcal{H}_\delta$ . The main difficulty is that these spaces are no longer weighted by the invariant measure of the system, so that several simplifications are lost. In particular, the very useful relation  $\operatorname{Re}\langle \varphi, L_\gamma \varphi \rangle = -\beta^{-1}\|\partial_p \varphi\|^2$  does not hold anymore.

Throughout this section, we will write  $L_{\text{sym}}$  for the symmetric part of  $L_\gamma$  in  $\mathcal{H}_\delta$ :  $\langle \varphi, L_\gamma \varphi \rangle_\delta = \langle \varphi, L_{\text{sym}} \varphi \rangle_\delta$ . An explicit calculation shows that one has

$$L_{\text{sym}} = -\beta^{-1}\partial_p^* \partial_p + \frac{\beta - \delta}{2\beta} - \frac{\delta(\beta - \delta)}{2\beta} p^2 ,$$

where we denote by  $\partial_p^* = -\partial_p + \delta p$  the adjoint of  $\partial_p$  in  $\mathcal{H}_\delta$ . Note that one has  $L_{\text{sym}} = -\beta^{-1}\partial_p^* \partial_p$  if and only if  $\delta = \beta$ . A standard calculation shows that  $L_{\text{sym}}$  is unitarily equivalent to the Schrödinger operator corresponding to the harmonic oscillator, so that one can explicitly compute its spectral decomposition. In order to do so, we define

$$\alpha = -\frac{\delta}{2} + \frac{\sqrt{\delta(2\beta - \delta)}}{2} , \quad A = \beta^{-1/2}(\partial_p + \alpha p) , \quad (6.9)$$

and we note that one can write

$$L_{\text{sym}} = -A^*A + \frac{\beta - \sqrt{\delta(2\beta - \delta)}}{2\beta} . \quad (6.10)$$

Furthermore, one has  $[A^*, A] = -(2\alpha + \delta)/\beta$ . This shows that the eigenvalues of  $L_{\text{sym}}$  are given by

$$\lambda_n = \frac{\beta - \sqrt{\delta(2\beta - \delta)}}{2\beta} - n \frac{\sqrt{\delta(2\beta - \delta)}}{\beta} , \quad n = 0, 1, \dots ,$$

and the corresponding eigenfunctions are  $f_n \propto (A^*)^n f_0$  with  $f_0 \propto \exp(-\alpha p^2/2)$ . In the special case  $\delta = \beta$ , one simply has  $\lambda_n = -n$ .

In order to obtain bounds in  $\mathcal{H}_\delta$ , we note that (3.2) yields the relation

$$\|A\varphi_\gamma\|_\delta^2 - \frac{\beta - \sqrt{\delta(2\beta - \delta)}}{2\beta} \|\varphi_\gamma\|_\delta^2 = \langle \varphi_\gamma, p \rangle_\delta .$$

This immediately implies that there exist constants  $C$  and  $N$  independent of  $\gamma$  such that one has

$$\frac{1}{2}(\|A\varphi_\gamma\|_\delta^2 + \|\varphi_\gamma\|_\delta^2) \leq |\langle \varphi_\gamma, p \rangle_\delta| + C \sum_{k=0}^N \int_{\mathbf{T}} \left( \int_{\mathbf{R}} f_k(p) \varphi_\gamma(p, q) e^{-\delta p^2/2} dp \right)^2 dq .$$

On the other hand, all the  $f_k$ 's are of the form  $P_k(p)e^{-\alpha p^2/p}$  for some polynomial  $P_k$  of degree  $k$ . This implies that, for every  $\delta' < 2(\alpha + \delta)$ , there exist constants  $C_1, C_2$  such that one has the bound

$$\|A\varphi_\gamma\|_\delta + \|\varphi_\gamma\|_\delta \leq C_1 + C_2 \|\varphi_\gamma\|_{\delta'} .$$

Since, for  $\delta \geq \beta$ , one has  $\alpha \geq 0$ , one has in particular the bound

$$\|A\varphi_\gamma\|_\delta + \|\varphi_\gamma\|_\delta \leq C(1 + \|\varphi_\gamma\|_{2\delta}) . \quad (6.11)$$

This calculation shows that:

**Proposition 6.5.** *One has  $\varphi_\gamma \in \bigcap_{\delta>0} \mathcal{H}_\delta$  and, for every  $\delta \in (0, \beta]$ , there exists a constant  $C$  independent of  $\gamma$  such that*

$$\|\partial_p \varphi_\gamma\|_\delta^2 + \|\varphi_\gamma\|_\delta^2 \leq C . \quad (6.12)$$

*Proof.* Since one has  $\|\varphi_\gamma\|_\delta \leq C\|\varphi_\gamma\|_{\delta'}$  for  $\delta \geq \delta'$ , we can apply (6.11) recursively to obtain

$$\|A\varphi_\gamma\|_\delta + \|\varphi_\gamma\|_\delta \leq C(1 + \|\varphi_\gamma\|_\beta) \leq C ,$$

where we made use of Proposition 6.1 for the second inequality (the two constants  $C$  are of course different). Since furthermore  $\|p\varphi_\gamma\|_\delta \leq C\|\varphi_\gamma\|_{\delta'}$  for  $\delta \geq \delta'$ , this proves the claim.  $\square$

We are now going to show that it is also possible to obtain an order 1 bound for  $\|\partial_q \varphi_\gamma\|_\delta$ , but as before this is less straightforward. We first start with the following preparatory result:

**Proposition 6.6.** *There exists a constant  $C$  independent of  $\gamma$  such that*

$$\|\partial_p^2 \varphi_\gamma\| + \|\partial_p \partial_q \varphi_\gamma\| + \|\partial_q^2 \varphi_\gamma\| \leq \frac{C}{\sqrt{\gamma}} .$$

*Proof.* The bound for  $\|\partial_p^2 \varphi_\gamma\|$  was obtained in Proposition 6.4. In order to obtain the bound on  $\partial_p \partial_q \varphi_\gamma$ , note that one has  $[L_\gamma, \partial_q] = \gamma^{-1} V''(q) \partial_p$ , so that  $L_\gamma \partial_q \varphi_\gamma = \gamma^{-1} V''(q) \partial_p \varphi_\gamma$ . Therefore, we have

$$\|\partial_p \partial_q \varphi_\gamma\|^2 = \langle \partial_q \varphi_\gamma, L_\gamma \partial_q \varphi_\gamma \rangle = \gamma^{-1} \langle \partial_q \varphi_\gamma, V''(q) \partial_p \varphi_\gamma \rangle \leq \frac{C}{\gamma} \|\partial_q \varphi_\gamma\| \|\partial_p \varphi_\gamma\| ,$$

so that the bound follows from Proposition 6.4. Finally, it follows from (6.4) that we have the bound

$$\|\partial_q^2 \varphi_\gamma\|^2 \leq |\langle \partial_q \varphi_\gamma, L_\gamma \partial_q \varphi_\gamma \rangle| = \gamma^{-1} |\langle \partial_q \varphi_\gamma, V''(q) \partial_p \varphi_\gamma \rangle|$$

$$\begin{aligned}
&\leq \frac{C}{\gamma} \|\partial_q \varphi_\gamma\| \|\partial_p \varphi_\gamma\| + C(\|\partial_p \partial_q \varphi_\gamma\|^2 + \|\partial_p \partial_q \varphi_\gamma\| \|\partial_p^2 \varphi_\gamma\| + \|\partial_q^2 \varphi_\gamma\| \|\partial_p \partial_q \varphi_\gamma\| \\
&\quad + \|\partial_q^2 \varphi_\gamma\| \|\partial_p^2 \varphi_\gamma\| + \|\partial_q^2 \varphi_\gamma\| \|\partial_p \varphi_\gamma\| + \|\partial_p \partial_q \varphi_\gamma\| \|\partial_p \varphi_\gamma\|) \\
&\leq \frac{C}{\gamma} + \frac{1}{2} \|\partial_q^2 \varphi_\gamma\|^2,
\end{aligned}$$

where we made use of all of the the previously obtained bounds in the last step.  $\square$

Our aim now is to mimic the proof of Theorem 1.6, with the space  $\mathcal{H}_\beta$  replaced by  $\mathcal{H}_\delta$  for some arbitrary  $\delta \in (0, \beta]$ . We define  $A$  as in (6.9) and we set as before  $B = p\partial_q - V'(q)\partial_p$ . We furthermore define the operator  $\tilde{B}$  (which is antisymmetric in  $\mathcal{H}_\delta$ ) by

$$\tilde{B} = \frac{\delta - \beta}{\beta} \left( p\partial_p - \frac{\delta}{2} p^2 + \frac{1}{2} \right).$$

With these notations, we can check that  $L_\gamma$  can be written as

$$L_\gamma = -A^*A + \frac{1}{\gamma}B + \tilde{B} + \frac{\beta - \sqrt{\delta(2\beta - \delta)}}{2\beta},$$

where the adjoint of  $A$  is taken in  $\mathcal{H}_\delta$ . This motivates the definition of an operator  $\hat{L}_\gamma$  given by

$$\hat{L}_\gamma = -A^*A + \frac{1}{\gamma}B.$$

Our strategy is then to obtain a bound similar to (6.4) with  $L_\gamma$  replaced by  $\hat{L}_\gamma$  and to use make use of the fact that the difference between  $L_\gamma$  and  $\hat{L}_\gamma$  is sufficiently ‘‘small’’.

**Theorem 6.7.** *For every  $\delta \in (0, \beta]$ , there exists a constant  $C$  such that*

$$\|\partial_p \varphi_\gamma\|_\delta^2 + \|\partial_q \varphi_\gamma\|_\delta^2 + \gamma(\|\partial_p^2 \varphi_\gamma\|_\delta^2 + \|\partial_p \partial_q \varphi_\gamma\|_\delta^2 + \|\partial_q^2 \varphi_\gamma\|_\delta^2) \leq C, \quad (6.13)$$

independently of  $\gamma$ .

**Remark 6.8.** *In terms of  $L^2$ -estimates, these bounds are likely not to be absolutely optimal. In the limit  $\gamma \rightarrow 0$  the solution  $\varphi_\gamma$  of the Poisson equation (3.2) indeed converges to a function of the form*

$$\varphi_{\gamma,0}(p, q) = \begin{cases} \varphi \circ H & \text{for } p \geq 0 \\ -\varphi \circ H & \text{for } p \leq 0 \end{cases}$$

where  $\varphi: \mathbf{R}_+ \rightarrow \mathbf{R}_+$  is a smooth function with  $\varphi_\gamma(H) = 0$  for  $H \leq E_0$  and such that  $\lim_{H \downarrow E_0} \varphi'(H) \neq 0$ . Note that the second derivative of  $\varphi_{\gamma,0}$  is therefore not square-integrable. For small values of  $\gamma$ , it is believed [Sow03, Sow05] that, around  $H = E_0$ , the function  $\varphi_\gamma$  develops a ‘boundary layer’ of width  $\sqrt{\gamma}$  on which, from simple scaling arguments, its second derivative should be of order  $\gamma^{-1/2}$ .

*Proof of Theorem 6.7.* We define as before the operators  $\hat{C}$  and  $R$  by

$$\hat{C} = [A, B] = \beta^{-1/2}(\partial_q + \alpha V'(q)), \quad R = [\hat{C}, B] = -V''(q)A.$$

With these notations, we define similarly as before the scalar product

$$\langle\langle f, f \rangle\rangle_\delta = a\|f\|_\delta^2 + \gamma(b\langle Af, Af \rangle_\delta + 2\text{Re}\langle Af, \hat{C}f \rangle_\delta + b\langle \hat{C}f, \hat{C}f \rangle_\delta),$$

where  $a$  and  $b$  are constants to be determined later. Since the algebraic relations between  $\hat{L}_\gamma$ ,  $A$ ,  $B$ ,  $\hat{C}$ , and  $R$  are exactly the same as above, we can retrace step by step the proof of (6.4) to get

$$\|Af\|_\delta^2 + \|\hat{C}f\|_\delta^2 + \gamma(\|A^2f\|_\delta^2 + \|\hat{C}Af\|_\delta^2) \leq -\operatorname{Re}\langle f, \hat{L}_\gamma f \rangle_\delta. \quad (6.14)$$

Since furthermore we know from Proposition 6.5 that  $\|\varphi_\gamma\|_\delta$  and (and therefore also  $\|p^n \varphi_\gamma\|_\delta$  for every  $n$ ) are bounded by constants independent of  $\gamma$ , this implies the existence of a constant  $C$  such that

$$\begin{aligned} \|\partial_p \varphi_\gamma\|_\delta^2 + \|\partial_q \varphi_\gamma\|_\delta^2 + \gamma(\|\partial_p^2 \varphi_\gamma\|_\delta^2 + \|\partial_p \partial_q \varphi_\gamma\|_\delta^2) \\ \leq C(1 + \langle \varphi_\gamma, \varphi_\gamma \rangle_\delta + |\langle \varphi_\gamma, p \partial_p \varphi_\gamma \rangle_\delta|). \end{aligned}$$

However, it is a straightforward calculation to check that, from Proposition 6.5 and the definition of  $\langle \cdot, \cdot \rangle_\delta$ , one has

$$|\langle \varphi_\gamma, p \partial_p \varphi_\gamma \rangle_\delta| \leq \frac{1}{2}(\|\partial_p \varphi_\gamma\|_\delta^2 + \gamma(\|\partial_p^2 \varphi_\gamma\|_\delta^2 + \|\partial_p \partial_q \varphi_\gamma\|_\delta^2)) + C(1 + \langle \varphi_\gamma, \varphi_\gamma \rangle_\delta),$$

so that we get the bound

$$\|\partial_p \varphi_\gamma\|_\delta^2 + \|\partial_q \varphi_\gamma\|_\delta^2 + \gamma(\|\partial_p^2 \varphi_\gamma\|_\delta^2 + \|\partial_p \partial_q \varphi_\gamma\|_\delta^2) \leq C(1 + \langle \varphi_\gamma, \varphi_\gamma \rangle_\delta).$$

We can actually even get slightly better than that, in the same way as in Proposition 6.6. Using (6.14) and the commutation relation  $[\hat{L}_\gamma, \partial_q] = \gamma^{-1} V''(q) \partial_p$ , we have:

$$\|\partial_q^2 \varphi_\gamma\|_\delta^2 \leq C + |\langle \partial_q \varphi_\gamma, \hat{L}_\gamma \partial_q \varphi_\gamma \rangle_\delta| \leq C + C|\gamma^{-1} \langle \partial_q \varphi_\gamma, V''(q) \partial_p \varphi_\gamma \rangle_\delta|,$$

so that we finally get the existence of a constant  $C$  such that

$$\|\partial_p \varphi_\gamma\|_\delta^2 + \|\partial_q \varphi_\gamma\|_\delta^2 + \gamma(\|\partial_p^2 \varphi_\gamma\|_\delta^2 + \|\partial_p \partial_q \varphi_\gamma\|_\delta^2 + \|\partial_q^2 \varphi_\gamma\|_\delta^2) \leq C(1 + \langle \varphi_\gamma, \varphi_\gamma \rangle_\delta). \quad (6.15)$$

Our aim now is to show that, for every  $\delta \in (0, \beta]$ , there exists a constant  $C$  such that  $\langle \varphi_\gamma, \varphi_\gamma \rangle_\delta \leq C$ , independently of  $\gamma$ , which will then conclude the proof of the theorem. This will be performed thanks to a bootstrapping argument similar to the one we used already in the proof of Proposition 6.5. One has, for some constant  $c > 0$ ,

$$\begin{aligned} c \langle \varphi_\gamma, \varphi_\gamma \rangle_\delta &\leq \|\varphi_\gamma\|_\delta^2 + \gamma(\|\partial_p \varphi_\gamma\|_\delta^2 + \|\partial_q \varphi_\gamma\|_\delta^2) \\ &\leq \|\varphi_\gamma\|_\delta^2 + \gamma \int_{\mathbf{T}} \int_{\mathbf{R}} ((\partial_p \varphi_\gamma)^2 + (\partial_q \varphi_\gamma)^2) \mu_\delta(dp dq) \\ &\leq \|\varphi_\gamma\|_\delta^2 + \gamma \int_{\mathbf{T}} \int_{\mathbf{R}} (|\varphi_\gamma \partial_p^2 \varphi_\gamma| + |\varphi_\gamma \partial_q^2 \varphi_\gamma| \\ &\quad + \delta |p \varphi_\gamma \partial_p \varphi_\gamma| + \delta |V'(q) \varphi_\gamma \partial_q \varphi_\gamma|) \mu_\delta(dp dq) \end{aligned}$$

Writing  $2\delta = \delta_1 + \delta_2$  with  $\delta_i > 0$  and applying Cauchy-Schwarz, we obtain from this the existence of positive constants  $c$  and  $C$  such that

$$\begin{aligned} c \langle \varphi_\gamma, \varphi_\gamma \rangle_\delta &\leq \|\varphi_\gamma\|_\delta^2 + C\gamma(\|\varphi_\gamma\|_{\delta_1} + \|p \varphi_\gamma\|_{\delta_1}) \\ &\quad \times (\|\partial_p^2 \varphi_\gamma\|_{\delta_2} + \|\partial_q^2 \varphi_\gamma\|_{\delta_2} + \|\partial_p \varphi_\gamma\|_{\delta_2} + \|\partial_q \varphi_\gamma\|_{\delta_2}). \end{aligned}$$

It therefore follows from (6.15) and Proposition 6.5 that there is a constant (depending on the choice of  $\delta_i$ ) such that

$$\langle \varphi_\gamma, \varphi_\gamma \rangle_\delta \leq C(1 + \langle \varphi_\gamma, \varphi_\gamma \rangle_{\delta_2}).$$

Since  $\delta_2$  can be chosen larger than  $\delta$  (actually up to, but not including  $2\delta$ ), we can apply this inequality recursively to bound  $\langle\langle \varphi_\gamma, \varphi_\gamma \rangle\rangle_\delta$  by  $\langle\langle \varphi_\gamma, \varphi_\gamma \rangle\rangle_\beta$  which in turn has already been bounded in Propositions 6.5 and 6.6.  $\square$

As a simple corollary, we have the following bound on  $\partial_p \varphi_\gamma$  which is used in the proof of Theorem 1.2:

**Corollary 6.9.** *The function  $\partial_p \varphi_\gamma$  belongs to  $L^4(\mu_\delta)$  for every  $\delta \in (0, \beta]$  and every  $\gamma > 0$ . Its norm in  $L^4(\mu_\delta)$  is of order  $\mathcal{O}(\gamma^{-1/4})$ .*

*Proof.* Denoting by  $\Delta$  the Laplacian on  $\mathbf{R}^2$ , it follows from the fractional Sobolev inequalities that

$$\begin{aligned} \left( \int |\partial_p \varphi_\gamma|^4 \mu_\delta(dp dq) \right)^{1/2} &\leq \int \left( (1 - \Delta)^{1/4} \partial_p \varphi_\gamma e^{-\delta H(p,q)/4} dp dq \right)^2 dp dq \\ &\leq \int \left( (1 - \Delta)^{1/2} \partial_p \varphi_\gamma e^{-\delta H(p,q)/4} \right) \partial_p \varphi_\gamma e^{-\delta H(p,q)/4} dp dq \\ &\leq C \|\partial_p \varphi_\gamma\|_{\delta/2} (\|\partial_p \varphi_\gamma\|_{\delta/2} + \|\partial_p^2 \varphi_\gamma\|_{\delta/2} + \|\partial_q \partial_p \varphi_\gamma\|_{\delta/2} + \|p \partial_p \varphi_\gamma\|_{\delta/2}) \\ &\leq C \left( 1 + \gamma^{-1/2} \right), \end{aligned}$$

were we used Theorem 6.7.  $\square$

**Remark 6.10.** *In a similar way, one can obtain, for every  $p \in [1, \infty)$ , bounds of order  $\mathcal{O}(1)$  for  $\varphi_\gamma \in L^p(\mu_\delta)$ . Unfortunately, using the Sobolev bounds obtained for  $\varphi_\gamma$  in this section, it is not possible to obtain bounds of order  $\mathcal{O}(1)$  for  $\partial_p \varphi_\gamma$  in  $L^p(\mu_\delta)$ , even though we conjecture that such bounds hold true.*

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