A SEMICLASSICAL APPROACH TO THE KRAMERS–SMOLUCHOWSKI EQUATION

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ABSTRACT. We consider the Kramers–Smoluchowski equation at a low temperature regime and show how semiclassical techniques developed for the study of the Witten Laplacian and Fokker–Planck equation provide quantitative results. This equation comes from molecular dynamics and temperature plays the role of a semiclassical paramater. The presentation is self-contained in the one dimensional case, with pointers to the recent paper [15] for results needed in higher dimensions. One purpose of this note is to provide a simple introduction to semiclassical methods in this context.

1. INTRODUCTION

The Kramers–Smoluchowski equation describes the time evolution of the probability density of a particle undergoing a Brownian motion under the influence of a chemical potential – see [1] for the background and references. Mathematical treatments in the low temperature regime have been provided by Peletier et al [16] using Γ-convergence, by Herrmann–Niethammer [11] using Wasserstein gradient flows and by Evans–Tabrizian [5].

The purpose of this note is to explain how precise quantitative results can be obtained using semiclassical methods developed by, among others, Bovier, Gayrard, Helffer, Hérau, Hitrik, Klein, Nier and Sjöstrand [2, 7, 8, 9, 10] for the study of spectral asymptotics for Witten Laplacians [17] and for Fokker–Planck operators. The semiclassical parameter h is the (low) temperature. This approach is much closer in spirit to the heuristic arguments in the physics literature [6, 13] and the main point is that the Kramers–Smoluchowski equation *is* the heat equation for the Witten Laplacian acting on functions. Here we give a self-contained presentation of the one dimensional case and explain how the recent paper by the first author [15] can be used to obtain results in higher dimensions.

Let $\varphi : \mathbb{R}^d \to \mathbb{R}$ be a smooth function. Consider the corresponding Kramers-Smoluchowski equation:

$$\left\{ \begin{array}{l} \partial_t \rho = \partial_x \cdot (\partial_x \rho + \epsilon^{-2} \rho \partial_x \varphi) \\ \quad \rho_{|t=0} = \rho_0 \end{array} \right. \tag{1.1}$$

where $\epsilon \in (0,1]$ denotes the temperature of the system and will be the small asymptotic parameter. Assume that there exists $C > 0$ and a compact $K \subset \mathbb{R}^d$ such that for all

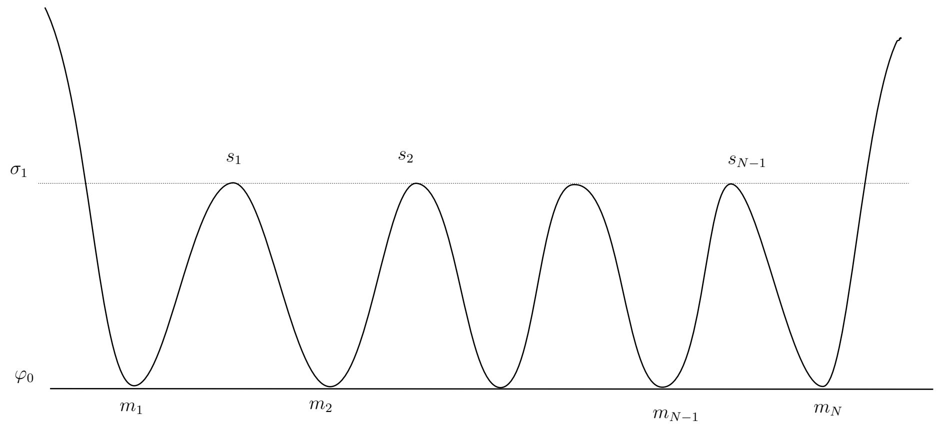

FIGURE 1. A one dimensional potential with interesting Kramers–Smoluchowski dynamics.

$x \in \mathbb{R}^d \setminus K$, we have

$$|\partial\varphi(x)| \geq \frac{1}{C}, \quad |\partial^2_{x_i x_j}\varphi| \leq C|\partial\varphi|^2, \quad \varphi(x) \geq C|x|. \tag{1.2}$$

Suppose additionally that φ is a Morse function, that is, φ has isolated and non-degenerate critical points. Then, thanks to the above assumptions the set $\mathcal{U}$ of critical points of φ is finite. For $p = 0, \ldots, d$, we denote by $\mathcal{U}^{(p)}$ the set of critical points of index p. Let us denote

$$\varphi_0 = \inf_{x\in\mathbb{R}^d} \varphi(x) = \inf_{\mathbf{m}\in\mathcal{U}^{(0)}} \varphi(\mathbf{m}) \quad \text{and} \quad \sigma_1 = \sup_{\mathbf{s}\in\mathcal{U}^{(1)}} \varphi(\mathbf{s}) \tag{1.3}$$

Thanks to (1.2), the sublevel set of σ_1 is decomposed in finitely many connected components $E_1, \ldots, E_N$:

$$\{x \in \mathbb{R}^d, \, \varphi(x) < \sigma_1\} = \bigsqcup_{n=1}^{N} E_n. \tag{1.4}$$

We assume that

$$\inf_{x\in E_n} \varphi(x) = \varphi_0, \quad n = 1, \ldots, N, \quad \varphi(\mathbf{s}) = \sigma_1, \quad \mathbf{s} \in \mathcal{U}^{(1)}. \tag{1.5}$$

which corresponds to the situation where φ admits N wells of the same height. In order to avoid heavy notations, we also assume that for $n = 1, \ldots, N$ the minimum of φ on E_n is attained in a single point that we denote by $\mathbf{m}_n$.

The associated *Arrhenius number*, $S = \sigma_1 - \varphi_0$, governs the long time dynamics of (1.1). That is made quantitative in Theorems 1 below. More general assumptions can be made as will be clear from the proofs. We restrict ourselves to the case in which the asymptotics are cleanest.

To state the simplest result let us assume that $d = 1$ and that the values of φ at local minima and local maxima (saddle points) are all equal to φ_0 and σ_1, respectively, and that values of second derivatives also agree. The potential then looks like the one shown in Fig.1. For $\kappa > 0$ We define

$$A_0 = \frac{\kappa}{\pi}\begin{pmatrix} 1 & -1 & 0 & 0 & \dots & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & \dots & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & \dots & 0 \\ \vdots & 0 & -1 & 2 & \ddots & \ddots & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & -1 & 0 \\ 0 & \vdots & \ddots & \ddots & \ddots & -1 & 2 & -1 \\ 0 & 0 & \dots & \dots & \dots & 0 & -1 & 1 \end{pmatrix}. \tag{1.6}$$

This matrix is positive semi-definite with a simple eigenvalue at 0.

The following result is a generalization of Theorem 2.5 in [5]:

Theorem 1. *Suppose that $d = 1$ and φ satisfies (1.2) and (1.5). We also assume that the second derivatives at maxima and minima are all given by $-\nu$ and μ respectively. If*

$$\rho_0 = \left(\frac{\mu}{2\pi\epsilon^2}\right)^{\frac{1}{2}} \left(\sum_{n=1}^{N} \beta_n \, 1\!\!1_{E_n} + r_\epsilon\right) e^{-\varphi/\epsilon^2}, \quad \lim_{\epsilon\to 0} \|r_\epsilon\|_{L^\infty} = 0, \quad \beta \in \mathbb{R}^N, \tag{1.7}$$

then the solution to (1.1) satisfy, uniformly for $\tau \geq 0$,

$$\rho(2\epsilon^2 e^{S/\epsilon^2}\tau, x) \ \to \ \sum_{n=1}^{N} \alpha_n(\tau)\delta_{\mathbf{m}_n}(x), \quad \epsilon \to 0, \tag{1.8}$$

in the sense of distributions in x, where $S = \sigma_1 - \varphi_0$ and where $\alpha(\tau) = (\alpha_1, \dots, \alpha_n)(\tau)$ solves

$$\partial_\tau \alpha = -A_0\alpha, \quad \alpha(0) = \beta, \tag{1.9}$$

with A_0 given by (1.6) and $\kappa = \mu^{\frac{1}{2}}\nu^{\frac{1}{2}}$.

A higher dimensional version of this result is given in Theorem 3 in §3. Using methods of [5] and [2], it was already proved by Seo–Tabrizian [12, Theorem 1.2]. The matrix A_0 becomes a graph Laplacian for a graph obtained by taking minima as vertices and saddle points as edges. The same graph Laplacian was constructed by Landim et al [14] in the context of a discrete model of the Kramers–Smoluchowski equation.

Here, Theorem 1 is a consequence of a more precise asymptotic formula given in Theorem 2 formulated using the Witten Laplacian. Provided that certain topological assumptions are satisfied (see [15, §1.1, §1.2]) an analogue of Theorem 1 in higher dimensions is immediate – see §3 for geometrically interesting examples.

The need for the new results of [15] comes from the fact that in the papers on the low lying eigenvalues of the Witten Laplacian [2, 7, 8, 9, 10] the authors make assumptions on the relative positions of minima and of saddle points. These assumptions mean that the Arrhenius numbers are distinct and hence potentials for which the Kramers–Smoluchowski dynamics ,(3.6) is interesting are excluded. With this motivation the general case was studied in [15] and to explain how the results of that paper can be used in higher dimensions we give a self-contained presentation in dimension one.

A development of the methods presented in this note would also allow having additional variables as done in [5]. Since our goal is to explain general ideas in a simple setting we do not address this issue here.

We remark that the specially prepared initial data (1.7) is needed to get results valid for all times and that E_n's in the statement could be replaced by any interval in E_n containing the minimum. Theorem 2 also shows that a weaker result is valid for any L^2 data: suppose that $\rho_0 \in L^2_\varphi := L^2(e^{\varphi(x)/\epsilon^2}dx)$ and that

$$\beta_n := \left(\frac{\mu}{2\pi\epsilon^2}\right)^{\frac14} \int_{E_n} \rho_0(x)dx.$$

Then, uniformly for $\tau \geq 0$,

$$\begin{aligned} &\rho(t,x) = \left(\frac{\mu}{2\pi\epsilon^2}\right)^{\frac14} \sum_{n=1}^{N} \alpha_n((2\epsilon^2)^{-1}e^{-S/\epsilon^2}t)\, 1\!\!1_{E_n}(x)e^{-\varphi/\epsilon^2} + r_\epsilon(t,x), \\ &\|r_\epsilon(t)\|_{L^1(dx)} \leq C(\epsilon^{\frac52} + \epsilon^{\frac12}e^{-t\epsilon^2})\|\rho_0\|_{L^2_\varphi}, \quad L^2_\varphi := L^2(\mathbb{R}, e^{\varphi(x)/\epsilon^2}dx). \end{aligned} \tag{1.10}$$

where α solves (1.9). The proof of (1.10) is given at the end of §2.6.

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2. Dimension one

In this section we assume that the dimension is equal to $d = 1$. That allows to present self-contained proofs which indicate the strategy for higher dimension.

Ordering the sets E_n such that $\mathbf{m}_1 < \mathbf{m}_2 < \ldots < \mathbf{m}_N$ it follows that for all $n = 1, \ldots N-1$ $\bar{E}_n \cap \bar{E}_{n+1} = \{\mathbf{s}_n\}$ is a saddle point and we assume additionally that there exists $\mu_n, \nu_k > 0$ such that for $n = 1, \ldots, N$ and $k = 1, \ldots, N-1$,

$$\varphi''(\mathbf{m}_n) = \mu_n \quad \text{and} \quad \varphi''(\mathbf{s}_k) = -\nu_k. \tag{2.1}$$

Using this notation we define a symmetric $N \times N$ matrix: $A_0 = (a_{ij})_{1\leq i,j\leq N}$, where (with the convention that $\nu_0 = \nu_N = 0$)

$$a_{ii} = \pi^{-1}\mu_j^{\frac12}(\nu_{j-1}^{\frac12} + \nu_j^{\frac12}), \quad a_{i,i+1} = -\pi^{-1}\nu_i^{\frac12}\mu_i^{\frac14}\mu_{i+1}^{\frac14}, \quad 1 \leq i \leq N-1, \tag{2.2}$$

and $a_{i,i+k} = 0$, for $k > 1$, $a_{ij} = a_{ji}$. The matrix A_0 is symmetric positive and the eigenvalue 0 has multiplicity 1. When μ_j's and ν_j's are all equal our matrix takes the particularly simple form (1.6).

First, observe that we can assume without loss of generality that $\varphi_0 = 0$. Define the operator appearing on the right hand side of (1.1) by

$$P := \partial_x \cdot (\partial_x + \epsilon^{-2}\partial_x\varphi)$$

and denote

$$h = 2\epsilon^2.$$

Then, considering $e^{\pm\varphi/h}$ as a multiplication operator,

$$P = \partial_x \circ (\partial_x + 2h^{-1}\partial_x\varphi) = \partial_x \circ e^{-2\varphi/h} \circ \partial_x \circ e^{2\varphi/h}$$

and

$$e^{\varphi/h} \circ P \circ e^{-\varphi/h} = -h^{-2}\Delta_\varphi, \quad \Delta_\varphi := -h^2\Delta + |\partial_x\varphi|^2 - h\Delta\varphi.$$

Hence, ρ is solution of (1.1) if $u(t,x) := e^{\varphi(x)/h}\rho(h^2t,x)$ is a solution of

$$\partial_t u = -\Delta_\varphi u, \quad u_{|t=0} = u_0 := \rho_0 e^{\varphi/h}. \tag{2.3}$$

In order to state our result for this equation, we denote

$$\psi_n(x) := c_n(h)h^{-\frac{1}{4}}\, 1\!\!1_{E_n}(x)e^{-(\varphi-\varphi_0)(x)/h}, \quad n = 1,\ldots,N, \tag{2.4}$$

where $c_n(h)$ is a normalization constant such that $\|\psi_n\|_{L^2} = 1$. The method of steepest descent shows that

$$c_n(h) \sim \sum_{k=0}^{\infty} c_{n,k}h^k, \quad c_{n,0} = (\mu_n/\pi)^{\frac{1}{4}}, \quad n = 1,\ldots N. \tag{2.5}$$

We then define a map $\Psi : \mathbb{R}^N \to L^2$ by

$$\Psi(\beta) := \sum_{n=1}^{N} \beta_n\psi_n, \quad \beta = (\beta_1,\ldots,\beta_N) \in \mathbb{R}^N. \tag{2.6}$$

The following theorem describes the dynamic of the above equation when $h \to 0$.

Theorem 2. *There exists $C > 0$ and $h_0 > 0$ such that for all $\beta \in \mathbb{R}^N$ and all $0 < h < h_0$, we have*

$$\|e^{-t\Delta_\varphi}\Psi(\beta) - \Psi(e^{-t\nu_h A}\beta)\|_{L^2} \leq Ce^{-1/Ch}|\beta|, \quad t \geq 0, \tag{2.7}$$

where $\nu_h = he^{-2S/h}$, $S = \sigma_1 - \varphi_0$, and $A = A(h)$ is a real symmetric positive matrix having a classical expansion $A \sim \sum_{k=0}^{\infty} h^k A_k$ with A_0 given by (2.2). In addition,

$$\|e^{-t\Delta_\varphi}\Psi(\beta) - \Psi(e^{-t\nu_h A_0}\beta)\|_{L^2} \leq Ch|\beta| \tag{2.8}$$

uniformly with respect to $t \geq 0$.

We first show how

Theorem 2 implies Theorem 1. First recall that we assume here $\mu_n = \mu$ for all $n = 1, \dots N$ and $\nu_k = \nu$ for all $k = 1, \dots N-1$. Suppose that ρ is the solution to (1.1) with ρ_0 as in Theorem 1. Then $u(t,x) := e^{\varphi(x)/h}\rho(h^2t, x)$ is a solution of (2.3), that is $u(t) = e^{-t\Delta_\varphi}u_0$ with

$$\begin{aligned} u_0 = \rho_0 e^{\varphi/2\epsilon^2} &= \left(\frac{\mu}{2\pi\epsilon^2}\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \beta_n 1\!\!1_{E_n} + r_\epsilon\right) e^{-\varphi/2\epsilon^2} \\ &= \left(\frac{\mu}{\pi h}\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \beta_n 1\!\!1_{E_n} + r_h\right) e^{-\varphi/h} \end{aligned} \tag{2.9}$$

Since, $c_n(h) = (\mu/\pi)^{\frac{1}{4}} + \mathcal{O}(h)$ it follows that

$$u_0 = (\mu/\pi h)^{\frac{1}{4}}\Psi(\beta) + \tilde{r}_h, \quad \tilde{r}_h = \left(\mathcal{O}(h^{\frac{1}{2}}) + h^{-\frac{1}{2}}r_h\right)e^{-\varphi/h}.$$

Since $h^{-\frac{1}{2}}e^{-\varphi/h} = \mathcal{O}_{L^1}(1)$, we have $\tilde{r}_h \to 0$ in L^1 when $h \to 0$. Hence, it follows from the by-product in Theorem 2 that

$$\begin{aligned} \rho(h^2t, x) &= e^{-\varphi(x)/h}u(t,x) = e^{-\varphi(x)/h}e^{-t\Delta_\varphi}\left((\mu/\pi h)^{\frac{1}{4}}\Psi(\beta) + \tilde{r}_h\right) \\ &= e^{-\varphi(x)/h}\left((\mu/\pi h)^{\frac{1}{4}}\Psi(e^{-t\nu_h A_0}\beta) + e^{-t\Delta_\varphi}\tilde{r}_h + \mathcal{O}_{L^2}(h)\right) \end{aligned}$$

With the new time variable $s = t\nu_h$, we obtain

$$\rho(she^{2S/h}, x) = e^{-\varphi(x)/h}\left((\mu/\pi h)^{\frac{1}{4}}\Psi(e^{-sA_0}\beta) + e^{-t\Delta_\varphi}\tilde{r}_h + \mathcal{O}_{L^2}(h)\right) \tag{2.10}$$

and denoting $\alpha(s) = e^{-sA_0}\beta$, we get

$$e^{-\varphi(x)/h}(\mu/\pi h)^{\frac{1}{4}}\Psi(e^{-sA_0}\beta) = (\mu/\pi)^{\frac{1}{4}}\sum_{n=1}^N \alpha_n(t)h^{-\frac{1}{2}}c_n(h)\chi_n(x)e^{-2\varphi(x)/h}.$$

On the other hand, $h^{-\frac{1}{2}}\chi_n(x)e^{-2\varphi(x)/h} \longrightarrow (\pi/\mu)^{\frac{1}{2}}\delta_{x=m_n}$, as $h \to 0$, in the sense of distributions. Since, $c_n(h) = (\mu/\pi)^{\frac{1}{4}} + \mathcal{O}(h)$, it follows that

$$e^{-\varphi/h}(\mu/\pi h)^{\frac{1}{4}}\Psi(e^{-sA_0}\beta) \longrightarrow \sum_{n=1}^N \alpha_n(t)\delta_{x=m_n} \tag{2.11}$$

when $h \to 0$. Moreover, since $e^{-t\Delta_\varphi}$ is bounded by 1 on L^2, then

$$\|h^{-\frac{1}{2}}e^{-\varphi/h}e^{-t\Delta_\varphi}(r_h e^{-\varphi/h})\|_{L^1} \le \|r_h\|_{L^\infty}\|h^{-\frac{1}{4}}e^{-\varphi/h}\|_{L^2}^2 \le C\|r_h\|_{L^\infty}$$

and recalling that $r_h \to 0$ in L^∞, we see that

$$e^{-\varphi(x)/h}(e^{-t\Delta_\varphi}\tilde{r}_h + \mathcal{O}_{L^2}(h)) \longrightarrow 0 \tag{2.12}$$

in the sense of distributions. Inserting (2.11) and (2.12) into (2.10) and recalling that $h = 2\epsilon^2$, we obtain (1). □

2.1. **Witten Laplacian in dimension one.** The Witten Laplacian is particularly simple in dimension one but one can already observe features which play a crucial role in general study. For more information we refer to [4, §11.1] and [7].

We first consider Δ_φ acting on $C_c^\infty(\mathbb{R})$ and recall a supersymmetric structure which is the starting point of our analysis:

$$\Delta_\varphi = d_\varphi^* \circ d_\varphi \tag{2.13}$$

with $d_\varphi = e^{-\varphi/h} \circ h\partial_x \circ e^{\varphi/h} = h\partial_x + \partial_x\varphi$ and $d_\varphi^* = -h\partial_x + \partial_x\varphi = -d_{-\varphi}$. From this square structure, it is clear that Δ_φ is non negative and that we can use the Friedrichs extension to define a self-adjoint operator Δ_φ with domain $D(\Delta_\varphi)$. Moreover, since the embedding $D(\Delta_\varphi) \subset L^2(\mathbb{R})$ is compact, it follows that Δ_φ has compact resolvant and hence its spectrum is made of finite multiplicity eigenvalues with no accumulation point except infinity.

Moreover, since $d_\varphi(e^{-\varphi/h}) = 0$ and $e^{-\varphi/h} \in D(\Delta_\varphi)$ it follows that the eigenvalue 0 is the lowest eigenvalue of Δ_φ. The following proposition gives a preliminary description of the other low lying eigenvalues.

Proposition 1. *There exist $\varepsilon_0, h_0 > 0$ such that for any $h \in (0, h_0]$, Δ_φ has exactly N eigenvalues $0 = \lambda_1 \leq \lambda_2 \ldots \leq \lambda_N$ in the interval $[0, \epsilon_0 h]$. Moreover, for any $\epsilon > 0$ there exists C such that*

$$\lambda_n(h) \leq Ce^{-(S-\epsilon)/h}, \quad S = \sigma_1 - \varphi_0. \tag{2.14}$$

This is proved in [4, Theorem 11.1] with $h^{\frac{3}{2}}$ in place of $\epsilon_0 h$. The proof applies in any dimension and we present it in that greater generality.

Proof. The fact there exists at least N eigenvalues in the interval $[0, Ce^{-(S-\epsilon)/h}]$ is a direct consequence of the existence of N linearly independent quasimodes – see Lemma 2 and (2.30) below.

To show that N is the exact number of eigenvalues in $[0, \epsilon_0 h)$ it suffices to find a N dimensional vector space V and $\varepsilon_0 > 0$ such that the operator Δ_φ is bounded from below by $\varepsilon_0 h$ on $V^\perp$ – see for instance [18, Theorem C.15].

To find V we introduce a family of harmonic oscillators associated to minima $\mathbf{m} \in \mathcal{U}^{(0)}$ and obtained by replacing φ by its harmonic approximation in the expression for Δ_φ:

$$H_\mathbf{m} := -h^2\Delta + |\varphi''(\mathbf{m})(x - \mathbf{m})|^2 - h\Delta\varphi(\mathbf{m}), \quad \mathbf{m} \in \mathcal{U}^{(0)}.$$

The spectrum of this operator is known explicitly, see [7, Sect 2.1] with the simple eigenvalue 0 at the bottom. We denote by $e_\mathbf{m}$ the normalized eigenfunction, $H_\mathbf{m} e_\mathbf{m} = 0$. The other eigenvalues of $H_\mathbf{m}$ are bounded from below by $c_0 h$ for some $c_0 > 0$.

Let $\chi \in C_c^\infty(\mathbb{R}^d; [0,1])$ be equal to 1 near 0 and satisfy $(1-\chi^2)^{\frac{1}{2}} \in C^\infty(\mathbb{R}^d)$. We define $\chi_\mathbf{m}(x) = \chi((x - \mathbf{m})/\sqrt{Mh})$ where $M > 0$ will be chosen later. For h small enough, the functions $\chi_\mathbf{m}$ have disjoint supports and hence the function χ_∞ defined by $1 - \chi_\infty^2 = \sum_{\mathbf{m} \in \mathcal{U}^{(0)}} \chi_\mathbf{m}^2$ is smooth. We now put

$$V = \text{span}\,\{\chi_\mathbf{m} e_\mathbf{m},\ \mathbf{m} \in \mathcal{U}^{(0)}\}, \quad \dim V = N.$$

The proof is completed if we show that there exist $\varepsilon_0, h_0 > 0$ such that

$$\langle \Delta_\varphi u, u\rangle \geq \varepsilon_0 h \|u\|^2, \quad u \in V^\perp \cap D(\Delta_\varphi), \quad 0 < h < h_0. \tag{2.15}$$

To establish (2.15) we use the following localization formula the verification of which is left to the reader (see [4, Theorem 3.2]):

$$\Delta_\varphi = \sum_{\mathbf{m}\in\mathcal{U}^{(0)}\cup\{\infty\}} \chi_{\mathbf{m}} \circ \Delta_\varphi \circ \chi_{\mathbf{m}} - h^2 \sum_{\mathbf{m}\in\mathcal{U}^{(0)}\cup\{\infty\}} |\nabla \chi_{\mathbf{m}}|^2.$$

Since, $\nabla\chi_{\mathbf{m}} = \mathcal{O}((Mh)^{-\frac{1}{2}})$, this implies, for $u \in D(\Delta_\varphi)$, that

$$\langle \Delta_\varphi u, u\rangle = \langle \Delta_\varphi \chi_\infty u, \chi_\infty u\rangle + \sum_{\mathbf{m}\in\mathcal{U}^{(0)}} \langle \Delta_\varphi \chi_{\mathbf{m}} u, \chi_{\mathbf{m}} u\rangle + \mathcal{O}(hM^{-1}\|u\|^2). \tag{2.16}$$

On the support of χ_∞ we have $|\nabla\varphi|^2 - h\Delta\varphi \geq (1 - \mathcal{O}(h))|\nabla\varphi|^2 \geq c_1 Mh$ for some $c_1 > 0$, and hence

$$\langle \Delta_\varphi \chi_\infty u, \chi_\infty u\rangle \geq Mc_1 h\|\chi_\infty u\|^2 \tag{2.17}$$

On the other hand, near any $\mathbf{m} \in \mathcal{U}^{(0)}$, $|\nabla\varphi(x)|^2 = |\varphi''(\mathbf{m})(x-\mathbf{m})|^2 + \mathcal{O}((x-\mathbf{m})^3)$ and $\varphi''(x) = \varphi''(\mathbf{m}) + \mathcal{O}((x-\mathbf{m}))$. Since on the support of $\chi_{\mathbf{m}}$ we have $|x - \mathbf{m}| \leq \sqrt{Mh}$, it follows that

$$\langle \Delta_\varphi \chi_{\mathbf{m}} u, \chi_{\mathbf{m}} u\rangle = \langle H_{\mathbf{m}} \chi_{\mathbf{m}} u, \chi_{\mathbf{m}} u\rangle + \mathcal{O}((Mh)^{\frac{3}{2}}). \tag{2.18}$$

Let us now assume that $u \in D(\Delta_\varphi)$ is orthogonal to $\chi_{\mathbf{m}} e_{\mathbf{m}}$ for all $\mathbf{m}$. Then $\chi_{\mathbf{m}} u$ is orthogonal to $e_{\mathbf{m}}$ the spectral gap $c_0 h$ of $H_{\mathbf{m}}$ and (2.18) show that

$$\langle \Delta_\varphi \chi_{\mathbf{m}} u, \chi_{\mathbf{m}} u\rangle \geq c_0 h\|\chi_{\mathbf{m}} u\|^2 - \mathcal{O}((Mh)^{\frac{3}{2}}\|u\|^2), \quad \mathbf{m} \in \mathcal{U}^{(0)}. \tag{2.19}$$

Combining this with (2.16), (2.17) and (2.19) gives

$$\begin{aligned}\langle \Delta_\varphi u, u\rangle &\geq c_0 h \sum_{\mathbf{m}\in\mathcal{U}^{(0)}\cup\{\infty\}} \|\chi_{\mathbf{m}} u\|^2 + \mathcal{O}(hM^{-1}\|u\|^2) + \mathcal{O}((Mh)^{\frac{3}{2}}\|u\|^2) \\ &\geq c_0 h\|u\|^2 + \mathcal{O}(hM^{-1}\|u\|^2) + \mathcal{O}((Mh)^{\frac{3}{2}}\|u\|^2).\end{aligned}$$

Taking M large enough completes the proof of (2.15). □

We denote by $E^{(0)}$ the subspace spanned by eigenfunctions of these low lying eigenvalues and by

$$\Pi^{(0)} := 1\!\!1_{[0,\varepsilon_0 h]}(\Delta_\varphi) \tag{2.20}$$

the spectral projection onto $E^{(0)}$. This projector is expressed by the standard contour integral.

$$\Pi^{(0)} = \frac{1}{2\pi i}\int_{\partial B(0,\delta\varepsilon_0 h)} (z - \Delta_\varphi)^{-1} dz, \quad 0 < \delta \ll 1. \tag{2.21}$$

In our analysis, we will also need the operator $\Delta_{-\varphi}$, noting that in dimension one $\Delta_{-\varphi}$ is the Witten Laplacian on 1-forms. Since $-\varphi$ has exactly $N-1$ minima (given by the $N-1$ maxima of φ), we deduce from the above discussion that there exists $\varepsilon_1 > 0$ such that $\Delta_{-\varphi}$ has $N-1$ eigenvalues in $[0, \varepsilon_1 h]$ and that these eigenvalues are actually exponentially small. We denote by $E^{(1)}$ the subspace spanned by eigenfunctions of these low lying eigenfunctions of $\Delta_{-\varphi}$ and by $\Pi^{(1)}$ the corresponding projector onto $E^{(1)}$,

$$\Pi^{(1)} = 1\!\!1_{[0,\varepsilon_1 h]}(\Delta_{-\varphi}). \tag{2.22}$$

Similarly to (2.21), we have

$$\Pi^{(1)} = \frac{1}{2\pi i}\int_{\partial B(0,\delta\varepsilon_1 h)} (z-\Delta_{-\varphi})^{-1}dz, \qquad 0<\delta\ll 1. \tag{2.23}$$

2.2. **Supersymmetry.** The key point in the analysis is the following intertwining relations which follows directly from (2.13)

$$\Delta_{-\varphi}\circ d_\varphi = d_\varphi\circ\Delta_\varphi \tag{2.24}$$

and its adjoint relation

$$d_\varphi^*\circ\Delta_{-\varphi} = \Delta_\varphi\circ d_\varphi^*. \tag{2.25}$$

From these relations we deduce that $d_\varphi(E^{(0)})\subset E^{(1)}$ and $d_\varphi^*(E^{(1)})\subset E^{(0)}$. Indeed, suppose that $\Delta_\varphi u = \lambda u$, with $u\neq 0$ and $\lambda\in[0,\varepsilon_0 h]$. Then, we see from (2.24) that

$$\Delta_{-\varphi}(d_\varphi u) = d_\varphi(\Delta_\varphi u) = \lambda d_\varphi u.$$

Therefore, either $d_\varphi u$ is null and obviously belongs to $E^{(1)}$ or $d_\varphi u\neq 0$ and hence $d_\varphi u$ is an eigenvector of $\Delta_{-\varphi}$ associated to $\lambda\in[0,\varepsilon_0 h]$. This proves the first statement. The inclusion $d_\varphi^*(E^{(1)})\subset E^{(0)}$ is obtained by similar arguments.

By definition, the operator Δ_φ maps $E^{(0)}$ into itself and we can consider its restriction to $E^{(0)}$. From the above discussion we know also that $d_\varphi(E^{(0)})\subset E^{(1)}$ and $d_\varphi^*(E^{(1)})\subset E^{(0)}$. Hence we consider $\mathcal{L} = (d_\varphi)_{|E^{(0)}\to E^{(1)}}$ and $\mathcal{L}^* = (d_\varphi^*)_{|E^{(1)}\to E^{(0)}}$. When restricted to $E^{(0)}$, the structure equation (2.13) becomes

$$\mathcal{M} = \mathcal{L}^*\mathcal{L}, \qquad \mathcal{M} := \Delta_\varphi|_{E^{(0)}}, \quad \mathcal{L} := (d_\varphi)|_{E^{(0)}\to E^{(1)}}. \tag{2.26}$$

2.3. **Quasimodes for Δ_φ.** Let $\delta_0 = \inf\{\mathrm{diam}(E_n),\, n=1,\dots,N\}$ and let $\epsilon>0$ be small with respect to δ_0. For all $n=1,\dots,N$, let χ_n be smooth cut-off functions such that

$$\begin{cases} \qquad 0\le\chi_n\le 1, \\ \mathrm{supp}(\chi_n)\subset\{x\in E_n,\, \varphi(x)\le\sigma_1-\epsilon\} \\ \chi_n = 1 \text{ on } \{x\in E_n,\, \varphi(x)\le\sigma_1-2\epsilon\}, \end{cases} \tag{2.27}$$

where $\epsilon>0$ will be chosen small (in particular much smaller than δ_0 in (2.31)). Consider now the family of approximated eigenfunctions defined by

$$f_n^{(0)}(x) = h^{-\frac14}c_n(h)\chi_n(x)e^{-\varphi(x)/h}, \quad \|f_n^{(0)}\|_{L^2}=1, \tag{2.28}$$

where $c_n(h) = \varphi''(m_n)^{\frac14}\pi^{-\frac14}+\mathcal{O}(h)$. We introduce the projection of these quasimodes onto the eigenspace space $E^{(0)}$:

$$g_n^{(0)} = \Pi^{(0)}f_n^{(0)}. \tag{2.29}$$

Lemma 2. *The approximate eigenfunctions defined by* (2.28) *satisfy*

$$\langle f_n^{(0)}, f_m^{(0)} \rangle = \delta_{n,m}, \quad n, m = 1, \ldots, N,$$

and

$$d_\varphi f_n^{(0)} = \mathcal{O}_{L^2}(e^{-(S-\epsilon)/h}), \qquad g_n^{(0)} - f_n^{(0)} = \mathcal{O}_{L^2}(e^{-(S-\epsilon')/h})$$

for any $\epsilon' > \epsilon$.

Proof. The first statement is a direct consequence of the support properties of the cut-off functions χ_n and the choice of the normalizing constant. To see the second estimate, recall that $d_\varphi e^{-\varphi/h} = 0$. Hence

$$d_\varphi f_n^{(0)}(x) = h^{\frac{3}{4}} c_n(h) \chi_n'(x) e^{-\varphi(x)/h}$$

Moreover, thanks to (2.27), there exists $c > 0$ such that for $\epsilon > 0$ small enough we have $\varphi(x) \geq S - \epsilon$ for $x \in \operatorname{supp}(\chi_n')$. Combining these two facts gives estimates on $f_n^{(0)}$.

Comparisons with $g_n^{(0)}$ comes from an estimate for $\Delta_\varphi f_n^{(0)}$. We have

$$\Delta_\varphi f_n^{(0)} = d_\varphi^* d_\varphi f_n^{(0)} = h^{\frac{3}{4}} c_n(h) d_\varphi^*(\chi_n' e^{-\varphi/h}) = h^{\frac{3}{4}} c_n(h)(-h\chi_n'' + 2\partial_x \varphi \chi_n') e^{-\varphi/h}$$

The same argument as before shows that

$$\Delta_\varphi f_n^{(0)} = \mathcal{O}_{L^2}(e^{-(S-\epsilon)/h}). \tag{2.30}$$

To use this we recall (2.21) so that by the Cauchy formula,

$$\begin{aligned} g_k^{(0)} - f_k^{(0)} = \Pi^{(0)} f_k^{(0)} - f_k^{(0)} &= \frac{1}{2\pi i} \int_\gamma (z - \Delta_\varphi)^{-1} f_k^{(0)} dz - \frac{1}{2\pi i} \int_\gamma z^{-1} f_k^{(0)} dz \\ &= \frac{1}{2\pi i} \int_\gamma (z - \Delta_\varphi)^{-1} z^{-1} \Delta_\varphi f_k^{(0)} dz, \quad \gamma = \partial B(0, \delta h), \quad 0 < \delta \ll 1. \end{aligned}$$

Since Δ_φ is selfadjoint and $\sigma(\Delta_\varphi) \cap [0, \epsilon_0 h] \subset [0, e^{-1/Ch}]$, we have for $\alpha > 0$ small enough

$$\|(z - \Delta_\varphi)^{-1}\| = \mathcal{O}(h^{-1}),$$

uniformly for $z \in \gamma$. Using (2.30), we get $\|(z - \Delta_\varphi)^{-1} z^{-1} \Delta_\varphi f_k^{(0)}\| = \mathcal{O}(h^{-2} e^{-(S-\epsilon)/h})$, and, after integration, $\|g_k^{(0)} - f_k^{(0)}\| = \mathcal{O}(h^{-1} e^{-(S-\epsilon)/h}) = \mathcal{O}(e^{-(S-\epsilon')/h})$, for any $\epsilon' > \epsilon$. □

2.4. **Quasimodes for $\Delta_{-\varphi}$.** Since, φ and $-\varphi$ share similar properties, the construction of the preceding section produces quasimodes for $\Delta_{-\varphi}$. Eventually we will only need quasimodes localized near the saddle points s_k. Hence, let $\theta_k \in C_c^\infty(\mathbb{R}; [0, 1])$ satisfy

$$\operatorname{supp} \theta_k \subset \{|x - s_k| \leq \delta_0\}, \quad \theta_k = 1 \text{ on } \{|x - s_k| \leq \frac{\delta_0}{2}\}. \tag{2.31}$$

We take ϵ in the definition (2.27) small enought then for all $k = 1, \ldots N - 1$, we have

$$\theta_k \chi_k' = \chi_{k,+}' \text{ and } \theta_k \chi_{k+1}' = \chi_{k+1,-}' \tag{2.32}$$

where $\chi_{k,\pm}$ are the smooth functions defined by

$$\chi_{k,+}(x) = \begin{cases} \chi_k(x) & \text{if } x \geq m_k, \\ 1 & \text{if } x < m_k, \end{cases} \qquad \chi_{k,-}(x) = \begin{cases} \chi_k(x) & \text{if } x \leq m_k, \\ 1 & \text{if } x > m_k. \end{cases}$$

Moreover, we also have $\theta_k\theta_l = 0$ for all $k \neq l$. The family of quasimodes associated to these cut-off function is given by

$$f_k^{(1)}(x) = h^{-\frac{1}{4}} d_k(h)\theta_k(x) e^{(\varphi(x)-S)/h}, \quad \|f_k^{(1)}\|_{L^2} = 1, \tag{2.33}$$

where $d_k(h) = |\varphi''(s_k)|^{\frac{1}{4}}\pi^{-\frac{1}{4}} + \mathcal{O}(h)$ is the normalizing constant. Again, we introduce the projection of these quasimodes onto the eigenspace $E^{(1)}$:

$$g_k^{(1)}(x) = \Pi^{(1)} f_k^{(1)} \tag{2.34}$$

Lemma 3. *There exists $\alpha > 0$ independant of ϵ such that the following hold true*

$$\langle f_k^{(1)}, f_l^{(1)}\rangle = \delta_{k,l}, \quad k, l = 1, \dots, N-1,$$

$$d_\varphi^* f_k^{(1)} = \mathcal{O}_{L^2}(e^{-\alpha/h}), \quad g_k^{(1)} - f_k^{(1)} = \mathcal{O}_{L^2}(e^{-\alpha/h})$$

Proof. The proof follows the same lines as the proof of Lemma 2. □

2.5. **Computation of the operator $\mathcal{L}$.** In this section represent $\mathcal{L}$ in a suitable basis. For that we first observe that the bases $(g_n^{(0)})$ and $(g_k^{(1)})$ are quasi-orthonormal. Indeed, thanks to Lemmas 2 and 3, we have

$$\langle g_n^{(0)}, g_m^{(0)}\rangle = \delta_{n,m} + \mathcal{O}(e^{-\alpha/h}), \quad n, m = 1, \dots, N$$

and

$$\langle g_k^{(1)}, g_l^{(1)}\rangle = \delta_{k,l} + \mathcal{O}(e^{-\alpha/h}), \quad k, l = 1, \dots, N-1.$$

for some $\alpha > 0$. We then obtain orthonormal bases of $E^{(0)}$ and $E^{(1)}$:

$$\begin{aligned} (g_n^{(0)})_{1\leq n\leq N} &\xrightarrow{\text{Gramm–Schmidt process}} (e_n^{(0)})_{1\leq n\leq N}, \\ (g_k^{(1)})_{1\leq k\leq N-1} &\xrightarrow{\text{Gramm–Schmidt process}} (e_k^{(1)})_{1\leq n\leq N-1}. \end{aligned} \tag{2.35}$$

It follows from the approximate orthonormality above that the change of basis matrix P_j from $(g_n^{(j)})$ to $(e_n^{(j)})$ satisfy

$$P_j = I + \mathcal{O}(e^{-\alpha/h}) \tag{2.36}$$

for $j = 0, 1$. To describe the matrix of $\mathcal{L}$ in the bases $(e_n^{(0)})$ and $(e_k^{(1)})$ we introduce a $N-1 \times N$ matrix $\hat{L} = (\hat{\ell}_{ij})$ defined by

$$\hat{\ell}_{ij} = \langle f_i^{(1)}, d_\varphi f_j^{(0)}\rangle. \tag{2.37}$$

We claim that the matrices L and $\hat{L}$ are very close. To see that we give a precise expansion of $\hat{L}$:

Lemma 4. *The matrix $\hat{L}$ defined by (2.37) is given by $\hat{L} = (h/\pi)^{\frac{1}{2}} e^{-S/h} \bar{L}$ where $\bar{L}$ admits a classical expansion $\bar{L} \sim \Sigma_{k=0}^{\infty} h^k L_k$ with*

$$L_0 = \begin{pmatrix} -\nu_1^{\frac14}\mu_1^{\frac14} & \nu_1^{\frac14}\mu_2^{\frac14} & 0 & 0 & \dots & 0 \\ 0 & -\nu_2^{\frac14}\mu_2^{\frac14} & \nu_2^{\frac14}\mu_3^{\frac14} & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & -\nu_{n-1}^{\frac14}\mu_{n-1}^{\frac14} & \nu_{n-1}^{\frac14}\mu_n^{\frac14} \end{pmatrix}. \tag{2.38}$$

Proof. From (2.28) and (2.33), we have

$$\begin{aligned} \hat{\ell}_{ij} = \langle f_i^{(1)}, d_\varphi f_j^{(0)} \rangle &= h^{-\frac12} d_i(h) c_j(h) \int_{\mathbb{R}} \theta_i(x) e^{(\varphi(x)-S)/h} d_\varphi(\chi_j(x) e^{-\varphi(x)/h}) dx \\ &= h^{\frac12} d_i(h) c_j(h) e^{-S/h} \int_{\mathbb{R}} \theta_i(x) \chi_j'(x) dx. \end{aligned}$$

Moreover, since $\operatorname{supp} \theta_i \cap \operatorname{supp} \chi_j = \emptyset$ except for $j = i$ or $j = i+1$, it follows from (2.32) that

$$\int_{\mathbb{R}} \theta_i(x) \chi_j'(x) dx = \delta_{i,j} \int_{\mathbb{R}} \chi_{i,+}'(x) dx + \delta_{i+1,j} \int_{\mathbb{R}} \chi_{i,-}'(x) dx = -\delta_{i,j} + \delta_{i+1,j}. \tag{2.39}$$

On the other hand, we recall that $d_i(h)$ and $c_j(h)$ both have a classical expansion. Together with the above equality, this shows that $\hat{L}$ has the required form and it remains to prove the formula giving L_0. To that end we observe that

$$d_i(h) c_j(h) = \pi^{-\frac12} ((|\varphi''(s_i)| \varphi''(m_j))^{\frac14} + \mathcal{O}(h)) = \mu_j^{\frac14} \nu_i^{\frac14} \pi^{-\frac12} + \mathcal{O}(h)$$

in the notation of (2.1). Combining this with (2.39) we obtain

$$\hat{\ell}_{ij} = h^{\frac12} \pi^{-\frac12} e^{-S/h} \mu_j^{\frac14} \nu_i^{\frac14} (-\delta_{i,j} + \delta_{i+1,j} + \mathcal{O}(h))$$

which gives (2.38). ☐

Lemma 5. *Let L be the matrix of $\mathcal{L}$ in the basis obtained in (2.35). There exists $\alpha' > 0$ such that $L = \hat{L} + \mathcal{O}(e^{-(S+\alpha')/h})$, where $\hat{L}$ is defined by (2.37) and is described in Lemma 4.*

Proof. It follows from (2.36) that

$$L = (I + \mathcal{O}(e^{-\alpha/h})) \tilde{L} (I + \mathcal{O}(e^{-\alpha/h})) \tag{2.40}$$

where $\tilde{L} = (\tilde{\ell}_{i,j})$ with $\tilde{\ell}_{i,j} = \langle g_i^{(1)}, d_\varphi g_j^{(0)} \rangle$. Moreover, (2.24) implies that $\Pi^{(1)} d_\varphi = d_\varphi \Pi^{(0)}$. Using this identity and the fact that $\Pi^{(0)}, \Pi^{(1)}$ are orthogonal projections, we have

$$\begin{aligned} \langle g_i^{(1)}, d_\varphi g_j^{(0)} \rangle = \langle g_i^{(1)}, d_\varphi \Pi^{(0)} f_j^{(0)} \rangle &= \langle g_i^{(1)}, \Pi^{(1)} d_\varphi f_j^{(0)} \rangle = \langle g_i^{(1)}, d_\varphi f_j^{(0)} \rangle \\ &= \langle f_i^{(1)}, d_\varphi f_j^{(0)} \rangle + \langle g_i^{(1)} - f_i^{(1)}, d_\varphi f_j^{(0)} \rangle \end{aligned}$$

But from Lemmas 2, 3 and the Cauchy-Schwarz inequality we get

$$|\langle g_i^{(1)} - f_i^{(1)}, d_\varphi f_j^{(0)} \rangle| \leq C e^{-(\alpha+S-\epsilon')/h}.$$

Since α is independent of ϵ' which can be choosen as small as we want, it follows that there exists $\alpha' > 0$ such that $\tilde{\ell}_{i,j} = \hat{\ell}_{i,j} + \mathcal{O}(e^{-(S+\alpha')/h})$. Combining this estimate, (2.40) and the fact that $\hat{\ell}_{i,j} = \mathcal{O}(e^{-S/h})$, we get the announced result. □

It is now easy to describe $\mathcal{M}$ as a matrix:

Lemma 6. *Let M be the matrix representation of $\mathcal{M}$ in the basis $(e_n^{(0)})$: $M = he^{-2S/h}A$ where A is a symmetric positive with a classical expansion $A \sim \sum_{k=0}^{\infty} h^k A_k$ with A_0 given by* (2.2)

Proof. By definition, $M = L^*L$ and it follows from Lemma 4 and 5 that

$$L^*L = (\hat{L} + \mathcal{O}(e^{-(S+\alpha')/h}))^*(\hat{L} + \mathcal{O}(e^{-(S+\alpha')/h})) = he^{-2S/h}(\bar{L}^*\bar{L} + \mathcal{O}(e^{-\alpha'/h}))$$

Then, $A := h^{-1}e^{2S/h}L^*L$ is clearly positive and admits a classical expansion since $\bar{L}$ does. Moreover, the leading term of this expansion is $\bar{L}_0^*\bar{L}_0$ and a simple computation shows that $\bar{L}_0^*\bar{L}_0 = A_0$, where A_0 is given by (2.2). □

Remark. Innocent as this lemma might seem, the supersymmetric structure, that is writing $-\Delta_\varphi|_{E^{(0)}}$ using d_φ, is very useful here.

Lemma 7. *Let us denote by $\mu_1(h) \leq \ldots \leq \mu_k(h)$ the eigenvalues of $A(h)$. Then,*

$$\mu_0(h) = 0 \text{ and } \mu_k(h) = \mu_k^0 + \mathcal{O}(h), \quad k \geq 2,$$

where $0 = \mu_1^0 < \mu_2^0 \leq \mu_3^0 \leq \ldots \leq \mu_N^0$ denote the eigenvalues of A_0. Moreover, a normalized eigenvector associated to μ_1^0 is $\xi^0 = N^{-\frac{1}{2}}(1, \ldots, 1)$ and there exists a normalized vector $\xi(h) \in \ker(A(h))$, such that

$$\xi(h) = \xi_0 + \mathcal{O}(h). \tag{2.41}$$

Proof. Much of the statements of this lemma are immediate consequence of Lemma 6. Let us just emphasize the fact that 0 belongs to $\sigma(A)$ since $0 \in \sigma(\Delta_\varphi)$. The fact that ξ^0 is in the kernel of A_0 is a simple computation. Eventually, for any $\xi \in \ker(A(h))$, we have

$$\xi - \langle \xi, \xi_0 \rangle \xi_0 = \frac{1}{2i\pi}\Big(\int_\gamma z^{-1}\xi dz - \int_\gamma (A_0 - z)^{-1}\xi dz\Big) = \frac{1}{2i\pi}\int_\gamma (A_0 - z)^{-1} z^{-1} A_0 \xi dz$$

where γ is a small path around 0 in $\mathbb{C}$. Since $A_0\xi = \mathcal{O}(h)$ we obtain (2.41). □

2.6. **Proof of Theorem 2.** Let u be solution of (2.3) with $u_0 = \Psi(\beta)$, $|\beta| \leq 1$ (see (2.4),(2.6) and (2.28) for definitions of ψ_n, Ψ and $f_n^{(0)}$, respectively). Then,

$$\begin{aligned} u &= e^{-t\Delta_\varphi}\Pi^{(0)}u_0 + e^{-t\Delta_\varphi}\widehat{\Pi}^{(0)}u_0 \\ &= e^{-t\mathcal{M}}\Pi^{(0)}u_0 + e^{-t\Delta_\varphi}\widehat{\Pi}^{(0)}u_0, \quad \widehat{\Pi}^{(0)} := I - \Pi^{(0)}. \end{aligned} \tag{2.42}$$

Since $1\!\!1_{E_n} - \chi_n$ is supported near $\{s_{n-1}, s_n\}$, then $\psi_n - f_n^{(0)} = \mathcal{O}_{L^2}(e^{-\alpha/h})$, $n = 1, \ldots, N$, and it follows that

$$u_0 = \bar{u}_0 + \mathcal{O}_{L^2}(e^{-\alpha/h}), \quad \bar{u}_0 := \sum_{n=1}^{N} \beta_n f_n^{(0)}.$$

Then, using Lemma 2 and (2.36), we get $u_0 = \tilde{u}_0 + \mathcal{O}_{L^2}(e^{-\alpha/h})$ with $\tilde{u}_0 := \sum_{n=1}^{N} \beta_n e_n^{(0)}$, where $e_n^{(0)}$ is the orthonormal basis of $E^{(0)}$ given by (2.35). Since $\Pi^{(0)}e_n^{(0)} = e_n^{(0)}$ and $\widehat{\Pi}^{(0)}e_n^{(0)} = 0$, we have

$$u(t) = e^{-t\mathcal{M}}\tilde{u}_0 + \mathcal{O}_{L^2}(e^{-1/Ch}).$$

If M is the matrix of the operator $\mathcal{M}$ in the basis $(e_n^{(0)})$ then

$$u(t) = \sum_{n=1}^{N} (e^{-tM}\beta)_n e_n^{(0)} + \mathcal{O}_{L^2}(e^{-1/Ch}).$$

Going back from $e_n^{(0)}$ to ψ_n as above, we see that

$$u(t) = \sum_{n=1}^{N} (e^{-tM}\beta)_n \psi_n + \mathcal{O}_{L^2}(e^{-1/Ch}) = \Psi(e^{-tM}\beta) + \mathcal{O}_{L^2}(e^{-1/Ch}) \tag{2.43}$$

and the proof is complete. Let us now prove (2.8). Since the linear application $\psi : \mathbb{C}^N \to L^2(dx)$ is bounded uniformly with respect to h, and thanks to (2.7), this reduces to show (after time rescaling) that there exists $C > 0$ such that for all $\beta \in \mathbb{R}^N$,

$$|e^{-\tau A} - e^{-\tau A_0}| \leq Ch, \quad \tau \geq 0 \tag{2.44}$$

Since, by Lemma 7, A and A_0 both have 0 as a simple eigenvalue at 0 with the approximate eigenvector given by $(1, \cdots, 1)$, we see that for any norm on $\mathbb{C}^N$,

$$\begin{aligned} |e^{-\tau A} - e^{-\tau A_0}| &\leq |e^{-\tau A_0}|_{\{(1,\cdots,1)\}^\perp} |I - e^{-\tau\mathcal{O}(h)}|_{\ell^2\to\ell^2} + Ch \\ &\leq Ce^{-c\tau}\tau h + Ch = \mathcal{O}(h). \end{aligned}$$

which is exactly (2.44). □

Proof of (1.10). We have seen in the preceding proof that $e_n^{(0)} - \psi_n = \mathcal{O}_{L^2}(e^{-C/\epsilon^2})$ and since

$$\|\psi_n - (\mu/2\pi\epsilon^2)^{\frac14}\, 1\!\!1_{E_n}\, e^{-\varphi/2\epsilon^2}\|_{L^2} = \mathcal{O}(\epsilon^2),$$

it follows that $\Pi^{(0)}u_0 = \psi(\beta) + \mathcal{O}(\epsilon^2\|u_0\|_{L^2})$ with $\beta \in \mathbb{C}^N$ given by

$$\beta_n = (\tfrac{\mu}{2\pi\epsilon^2})^{\frac14} \int_{E_n} u_0(x)e^{-\varphi(x)/2\epsilon^2}dx = (\tfrac{\mu}{2\pi\epsilon^2})^{\frac14} \int_{E_n} \rho_0(x)dx.$$

From the by product part of Theorem 2 we get (with $h = 2\epsilon^2$)

$$e^{-t\Delta_\varphi}\Pi^{(0)}u_0 = \sum_{n=1}^{N}(e^{-t\nu_h A_0}\beta)_n(\tfrac{\mu}{2\pi\epsilon^2})^{\frac{1}{4}}\,1\!\!1_{E_n}\,e^{-\varphi/2\epsilon^2} + \mathcal{O}_{L^2}(\epsilon^2)\|u_0\|_{L^2}. \tag{2.45}$$

On the other hand, Proposition 1 shows that

$$e^{-t\Delta_\varphi}(I - \Pi^{(0)})u_0 = \mathcal{O}_{L^2}(e^{-t\epsilon^2/C})\|u_0\|_{L^2}. \tag{2.46}$$

Since $\rho(h^2t) = e^{-\varphi/h}u(t)$, (2.45) and (2.46) yield

$$\rho(2\epsilon^2 e^{S/\epsilon^2}\tau) = \sum_{n=1}^{N}(e^{-\tau A_0}\beta)_n(\tfrac{\mu}{2\pi\epsilon^2})^{\frac{1}{4}}\,1\!\!1_{E_n}\,e^{-\varphi/\epsilon^2} + r_\epsilon(\tau) \tag{2.47}$$

with

$$r_\epsilon(\tau) = e^{-\varphi/2\epsilon^2}\Big(\mathcal{O}_{L^2}(e^{-c\tau e^{S/\epsilon^2}}) + \mathcal{O}_{L^2}(\epsilon^2)\Big)\|\rho_0\|_{L^2_\varphi}.$$

By Cauchy-Schwartz it follows that $\|r_\epsilon(\tau)\|_{L^1} \le C(\epsilon^{\frac{5}{2}} + e^{-c\tau e^{S/\epsilon^2}})\|\rho_0\|_{L^2_\varphi}$. □

3. A higher dimensional example

The same principles apply when the wells may have different height and in higher dimensions. In both cases there are interesting combinatorial and topological (when $d > 1$) complications and we refer to [15, §1.1, §1.2] for a presentation and references. To illustrate this we give a higher dimensional result in a simplified setting.

Suppose that $\varphi : \mathbb{R}^d \to \mathbb{R}$ is a smooth Morse function satisfying (1.2) and denote by $\mathcal{U}^{(j)}$ the finite sets of critical points of index j, $n_j := |\mathcal{U}^{(i)}|$. We assume that (1.5) holds and write $S := \sigma_1 - \varphi_0$. In the notation of (1.4) we have $n_0 = N$ and each E_n contains exactly one minimum. Hence we can label the components by the minima:

$$\varphi_0 = \min_{x\in E_n}\varphi(x) = \varphi(\mathbf{m}), \quad \mathbf{m} \in E_n, \quad E(\mathbf{m}) := E_n.$$

Since φ is a Morse function,

$$\begin{gathered}\mathbf{m}, \mathbf{m}' \in \mathcal{U}^{(0)}, \quad \mathbf{m} \neq \mathbf{m}' \implies \bar{E}(\mathbf{m}) \cap \bar{E}(\mathbf{m}') \subset \mathcal{U}^{(1)}, \\ \forall\, \mathbf{s} \in \mathcal{U}^{(1)}\ \exists\,!\,\mathbf{m}, \mathbf{m}' \in \mathcal{U}^{(0)} \quad\ \mathbf{s} \in \bar{E}(\mathbf{m}) \cap \bar{E}(\mathbf{m}').\end{gathered} \tag{3.1}$$

To simplify the presentation we make an addition assumption

$$\mathbf{m}, \mathbf{m}' \in \mathcal{U}^{(0)}, \quad \mathbf{m} \neq \mathbf{m}' \implies |\bar{E}(\mathbf{m}) \cap \bar{E}(\mathbf{m}')| \le 1. \tag{3.2}$$

Under this assumptions, the set $\mathcal{U}^{(0)} \times \mathcal{U}^{(1)}$ defines a graph $\mathcal{G}$. The elements of $\mathcal{U}^{(0)}$ are the vertices of $\mathcal{G}$ and elements of $\mathcal{U}^{(1)}$ are the edges of $\mathcal{G}$: $\mathbf{s} \in \mathcal{U}^{(1)}$ is an edge between $\mathbf{m}$ and $\mathbf{m}'$ in $\mathcal{U}^{(0)}$ if $s \in \bar{E}(\mathbf{m}) \cap E(\mathbf{m}')$ – see Fig.2 for an example.

The same graph has been constructed in [14] for a certain discrete model of the Kramers–Smoluchowski equation.

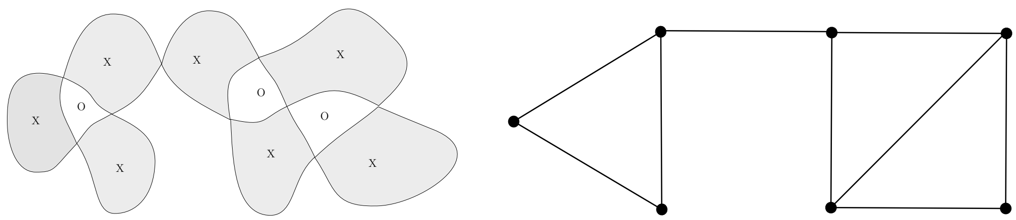

FIGURE 2. *Left:* The sublevel set $\{\varphi < \sigma_1\}$ (dashed region) associated to a potential φ (1.5). The x's represent local minima, the o's, local maxima. *Right:* The graph associated to the potential on the left.

We now introduce the discrete Laplace operator on $\mathcal{G}$, $M_{\mathcal{G}}$ – see [3] for the background and results about $M_{\mathcal{G}}$. If the degree $d(\mathbf{m})$ is defined as the number of edges at the vertex $\mathbf{m}$, $M_{\mathcal{G}}$ is given by the matrix $(a_{\mathbf{m},\mathbf{m}'})_{\mathbf{m},\mathbf{m}'\in\mathcal{U}^{(0)}}$:

$$a_{\mathbf{m},\mathbf{m}'} = \begin{cases} d(\mathbf{m}), & \mathbf{m} = \mathbf{m}' \\ -1 & \mathbf{m} \neq \mathbf{m}', \quad \bar{E}(\mathbf{m}) \cap \bar{E}(\mathbf{m}') \neq \emptyset, \\ \ \ 0 & \text{otherwise} \end{cases} \tag{3.3}$$

Among basic properties of the matrix $M_{\mathcal{G}}$, we recall:

- it has a square structure $M_{\mathcal{G}} = \mathcal{L}^*\mathcal{L}$, where $\mathcal{L}$ is the transpose of the incidence matrix of any oriented version of the graph $\mathcal{G}$. In particular, $M_{\mathcal{G}}$ is symmetric positive.
- thanks to (1.5) and [15, Proposition B.1], the graph $\mathcal{G}$ is connected.
- 0 is a simple eigenvalue of $M_{\mathcal{G}}$

We make one more assumption which is a higher dimensional analogue of the hypothesis in Theorem 1: there exist $\mu, \nu > 0$ such that

$$\begin{aligned} &\det \varphi''(\mathbf{m}) = \mu, \qquad \mathbf{m} \in \mathcal{U}^{(0)}, \\ &\frac{\lambda_1(\mathbf{s})^2}{\det \varphi''(\mathbf{s})} = -\nu, \quad \lambda_1(\mathbf{s}) \in \mathrm{Spec}(\varphi''(\mathbf{s})), \quad \lambda_1(\mathbf{s}) < 0, \quad \mathbf{s} \in \mathcal{U}^{(1)}. \end{aligned} \tag{3.4}$$

Assumptions (3.2) and (3.4) can be easily removed. Without (3.4) the graph $\mathcal{G}$ is replaced by a weighted graph with a weight function depending explicitly of the values of φ'' at critical points. Removing (3.2) leads to multigraphs in which there may be several edges between two vertices. This can be also handled easily.

Assumption (1.5) however is more fundamental and removing it results in major complications. We refer to [15] for results in that situation. Here we restrict ourselves to making the following

Remark. Under the assumption (1.5) the proof presented in the one dimensional case applies with relatively simple modifications. The serious difference lies in the description of $E^{(1)}$, the eigenspace of Δ_φ on one forms, in terms of exponentially accurate quasimodes (in one dimension it was easily done using Lemma 3). That description is however provided by Helffer–Sjöstrand in the self contained Section 2.2 of [9] – see Theorem 2.5 there. The computation of (2.37) becomes more involved and is based on the method of stationary phase – see Helffer–Klein–Nier [8, Proof of Proposition 6.4].

The analogue of Theorem 1 is

Theorem 3. *Suppose that* φ *satisfies* (1.2),(1.5),(3.2) *and* (3.4). *If*

$$\rho_0 = \left(\frac{\mu}{2\pi\epsilon^2}\right)^{\frac{1}{2}} \left(\sum_{n=1}^{N} \beta_n \, 1\!\!1_{E_n} + r_\epsilon\right) e^{-\varphi/\epsilon^2}, \quad \lim_{\epsilon\to 0} \|r_\epsilon\|_{L^\infty} = 0, \quad \beta \in \mathbb{R}^N, \tag{3.5}$$

then the solution to (1.1) *satisfy, uniformly for* $\tau \geq 0$,

$$\rho(2\epsilon^2 e^{S/\epsilon^2}\tau, x) \ \to \ \sum_{n=1}^{N} \alpha_n(\tau)\delta_{m_n}(x), \quad \epsilon \to 0, \tag{3.6}$$

in the sense of distributions in x, *where* $\alpha(t) = (\alpha_1, \ldots, \alpha_n)(\tau)$ *solves*

$$\partial_\tau \alpha = -\kappa M_{\mathcal{G}} \alpha, \quad \alpha(0) = \beta, \tag{3.7}$$

with $M_{\mathcal{G}}$ *is given by* (3.3) *and* $\kappa = \pi^{-1}\mu^{\frac{1}{2}}\nu^{\frac{1}{2}}$ *with* μ *and* ν *in* (3.4).

We also have the analogue of (1.10) for any initial data.

As in the one dimensional case this theorem is a consequence of a more precise theorem formulated using the localized states

$$\psi_n(x) = c_n(h) h^{-\frac{d}{4}} \, 1\!\!1_{E_n}(x) e^{-(\varphi-\varphi_0)(x)/h}, \tag{3.8}$$

where $c_n(h)$ is a normalization constant such that $\|\psi_n\|_{L^2} = 1$. We then define a map $\Psi : \mathbb{R}^{n_0} \to L^2(\mathbb{R}^d)$ by

$$\Psi(\beta) = \sum_{n=1}^{N} \beta_n \psi_n, \quad \beta = (\beta_1, \ldots, \beta_N) \in \mathbb{R}^N. \tag{3.9}$$

We have the following analogue of Theorem 2.

Theorem 4. *Suppose* φ *satisfies* (1.2),(1.5),(3.2) *and* (3.4). *There exists* $C > 0$ *and* $h_0 > 0$ *such that for all* $\beta \in \mathbb{R}^{n_0}$ *and all* $0 < h < h_0$, *we have*

$$\|e^{-t\Delta_\varphi}\Psi(\beta) - \Psi(e^{-t\kappa\nu_h A}\beta)\|_{L^2} \leq Ce^{-1/Ch}, \quad t \geq 0,$$

where $\nu_h = he^{-2S/h}$, $\kappa = \pi^{-1}\mu^{\frac{1}{2}}\nu^{\frac{1}{2}}$ *and* $A = A(h)$ *is a real symmetric positive matrix having a classical expansion* $A \sim \sum_{k=0}^{\infty} h^k A_k$ *and* $A_0 = M_{\mathcal{G}}$ *with* $M_{\mathcal{G}}$ *the Laplace matrix defined by* (3.3).

Let us conclude by one example [15, §6.3] for which the graph $\mathcal{G}$ is elementary. We assume that $d = 2$, φ has a maximum at $x = 0$, there are N minima, m_n, N saddle

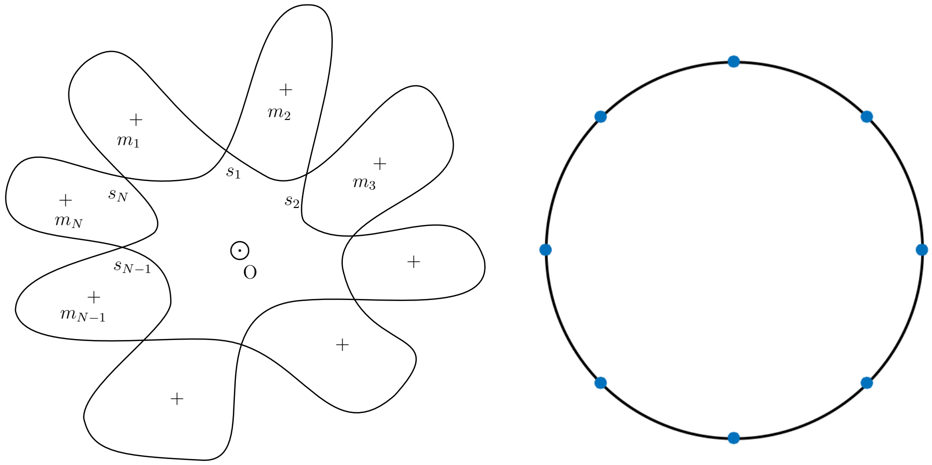

FIGURE 3. A two dimensional potential which is a cyclic analogue of the potential shown in Fig.1: the corresponding matrix describing the Kramer–Smoluchowski evolution is given by (3.10). It should compared to the matrix (1.6) for the potential in Fig.1. The corresponding cyclic graph is shown on the right.

points, s_n, and that (1.5) holds – see Fig.3. We assume also that

$$\det \varphi''(\mathbf{m}_n) = \mu > 0, \quad \frac{\lambda_1(\mathbf{s}_n)}{\lambda_2(\mathbf{s}_n)} = -\nu < 0,$$

where for $\mathbf{s} \in \mathcal{U}^{(1)}$, $\lambda_1(\mathbf{s}) > 0 > \lambda_2(\mathbf{s})$ denote the two eigenvalues of $\varphi''(\mathbf{s})$.

Then assumptions of Theorem 4 are satisfied. The graph $\mathcal{G}$ associated to φ is the cyclic graph with N vertices and the corresponding Laplacian is given by

$$\mathcal{A}_{\mathcal{G}} = \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & \dots & \dots & -1 \\ -1 & 2 & -1 & 0 & \dots & \dots & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & \dots & 0 \\ \vdots & 0 & -1 & 2 & \ddots & \ddots & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & -1 & 0 \\ 0 & \vdots & \ddots & \ddots & \ddots & -1 & 2 & -1 \\ -1 & 0 & \dots & \dots & \dots & 0 & -1 & 2 \end{pmatrix}. \tag{3.10}$$

REFERENCES

1. N. Berglund, *Kramers' law: validity, derivations and generalisations*, Markov Process. Related Fields **19** (2013), no. 3, 459–490.
2. A. Bovier, V. Gayrard, and M. Klein, *Metastability in reversible diffusion processes. II. Precise asymptotics for small eigenvalues*, J. Eur. Math. Soc. **7** (2005), no. 1, 69–99.
3. D. M. Cvetković, M. Doob, and H. Sachs, *Spectra of graphs*, third ed., Johann Ambrosius Barth, Heidelberg, 1995, Theory and applications.

4. H. Cycon, R. Froese, W. Kirsch, and B. Simon, *Schrödinger operators with application to quantum mechanics and global geometry*, study ed., Texts and Monographs in Physics, Springer-Verlag, 1987.
5. L. C. Evans and P. Tabrizian, *Asymptotics for scaled Kramers–Smoluchowski equations*, SIAM J. Math. Anal. **48** (2016), no. 4, 2944–2961.
6. A.H. Eyring, *The activated complex in chemical reactions*, J. Chem. Phys. (1935), no. 3, 107–115.
7. B. Helffer, *Semi-classical analysis for the Schrödinger operator and applications*, Lecture Notes in Mathematics, vol. 1336, Springer-Verlag, 1988.
8. B. Helffer, M. Klein, and F. Nier, *Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach*, Mat. Contemp. **26** (2004), 41–85.
9. B. Helffer and J. Sjöstrand, *Puits multiples en mécanique semi-classique. IV. Étude du complexe de Witten*, Comm. Partial Differential Equations **10** (1985), no. 3, 245–340.
10. F. Hérau, M. Hitrik, and J. Sjöstrand, *Tunnel effect and symmetries for Kramers-Fokker-Planck type operators*, J. Inst. Math. Jussieu **10** (2011), no. 3, 567–634.
11. M. Herrmann and B. Niethammer, *Kramers' formula for chemical reactions in the context of Wasserstein gradient flows*, Commun. Math. Sci. **9** (2011), no. 2, 623–635.
12. S. Insuk and P. Tabrizian, *Kramers–Smoluchowski equation for general potentials, preprint.*
13. H. A. Kramers, *Brownian motion in a field of force and the diffusion model of chemical reactions*, Physica **7** (1940), 284–304.
14. C. Landim, R. Misturini, and K. Tsunoda, *Metastability of reversible random walks in potential fields*, J. Stat. Phys. **160** (2015), no. 6, 1449–1482.
15. L. Michel, *On small eigenvalues of Witten Laplacian*, arXiv:1702.01837.
16. M. A. Peletier, G. Savaré, and M. Veneroni, *Chemical reactions as* Γ*-limit of diffusion*, SIAM Rev. **54** (2012), no. 2, 327–352.
17. E. Witten, *Supersymmetry and Morse theory*, J. Differential Geom. **17** (1982), no. 4, 661–692 (1983).
18. M. Zworski, *Semiclassical analysis*, Graduate Studies in Mathematics, vol. 138, American Mathematical Society, 2012.

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