

Repartition of the quasi-stationary distribution and first exit point density for a double-well potential

Dorian Le Peutrec, Boris Nectoux

▶ To cite this version:

Dorian Le Peutrec, Boris Nectoux. Repartition of the quasi-stationary distribution and first exit point density for a double-well potential. SIAM Journal on Mathematical Analysis, 2020, 52 (1), pp.581-604. 10.1137/19M1246432 . hal-02017327v2

HAL Id: hal-02017327 https://hal.science/hal-02017327v2

Submitted on 13 Nov 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Repartition of the quasi-stationary distribution and first exit point density for a double-well potential

Dorian Le Peutrec^{*} and Boris Nectoux ^{\dagger}

Abstract

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a smooth function and $(X_t)_{t \ge 0}$ be the stochastic process solution to the overdamped Langevin dynamics

$$dX_t = -\nabla f(X_t)dt + \sqrt{h} \ dB_t.$$

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain and assume that $f|_{\overline{\Omega}}$ is a doublewell potential with degenerate barriers. In this work, we study in the small temperature regime, i.e. when $h \to 0^+$, the asymptotic repartition of the quasi-stationary distribution of $(X_t)_{t\geq 0}$ in Ω within the two wells of $f|_{\overline{\Omega}}$. We show that this distribution generically concentrates in precisely one well of $f|_{\overline{\Omega}}$ when $h \to 0^+$ but can nevertheless concentrate in both wells when $f|_{\overline{\Omega}}$ admits sufficient symmetries. This phenomenon corresponds to the so-called tunneling effect in semiclassical analysis. We also investigate in this setting the asymptotic behaviour when $h \to 0^+$ of the first exit point distribution from Ω of $(X_t)_{t\geq 0}$ when X_0 is distributed according to the quasi-stationary distribution.

Key words: overdamped Langevin process, double-well, metastability, tunneling effect, semiclassical analysis, quasi-stationary distribution. AMS classification (2010): 35P15, 35P20, 47F05, 35Q82.

1 Setting and results

1.1 Quasi-stationary distribution and purpose of this work

Let $(X_t)_{t\geq 0}$ be the stochastic process solution to the overdamped Langevin dynamics in \mathbb{R}^d :

$$dX_t = -\nabla f(X_t)dt + \sqrt{h} \ dB_t, \tag{1}$$

where $f : \mathbb{R}^d \to \mathbb{R}$ is the potential (chosen C^{∞} in all this work), h > 0 is the temperature and $(B_t)_{t\geq 0}$ is a standard *d*-dimensional Brownian motion. Let Ω be a C^{∞} bounded open and connected subset of \mathbb{R}^d and introduce

$$\tau_{\Omega} = \inf\{t \ge 0 \,|\, X_t \notin \Omega\}$$

^{*}Laboratoire de Mathématiques d'Orsay, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France. E-mail: dorian.lepeutrec@math.u-psud.fr

[†]Institut für Analysis und Scientific Computing, E101-TU Wien, Wiedner Hauptstr. 8, 1040 Wien, Austria. E-mail: boris.nectoux@asc.tuwien.ac.at

the first exit time from Ω . A quasi-stationary distribution for the process (1) on Ω is a probability measure μ_h on Ω such that, when X_0 is distributed according to μ_h , what we will denote in the following by $X_0 \sim \mu_h$, it holds for any time t > 0 and any Borel set $A \subset \Omega$,

$$\mathbb{P}(X_t \in A \mid t < \tau_{\Omega}) = \mu_h(A).$$

From [5, 10, 17, 22], there exists a probability measure ν_h supported in Ω such that for any probability measure μ_0 on Ω : when $X_0 \sim \mu_0$, one has for any borel set $A \subset \Omega$,

$$\lim_{t \to +\infty} \mathbb{P}(X_t \in A \,|\, t < \tau_{\Omega}) = \nu_h(A).$$
(2)

It follows from (2) that ν_h is the unique quasi-stationary distribution for the process (1) on Ω .

In molecular dynamics, the quasi-stationary distribution ν_h is used to quantify the metastability of the subdomain Ω of \mathbb{R}^d as follows: for a probability measure μ_0 supported in Ω , the domain Ω is said to be metastable for the initial condition μ_0 if, when $X_0 \sim \mu_0$, the convergence in (2) is much quicker than the average exit time from Ω . When Ω is metastable, it is thus relevant to study the exit event ($\tau_{\Omega}, X_{\tau_{\Omega}}$) of the process (1) from Ω starting from ν_h , i.e. when $X_0 \sim \nu_h$. This is used in several algorithms aiming at accelarating the sampling of the exit even from a metastable domain, see for instance [1,17,21,24]. The study of the metastability is a very active field of science research which is at the heart of the numerical challenges observed in molecular dynamics. We refer in particular to [19] for an overview on this topic.

In this work, we study the repartition when $h \to 0$ of the quasi-stationary distribution ν_h within the wells of a double-well Morse potential f with degenerate barriers (see the assumption [**H-Well**] below). We show in particular that ν_h generically concentrates in one well (see Theorem 1 below) but can also concentrate in both wells when the function f is (nearly) even (see Theorems 2 and 3 below). According to the analysis led in [7] (see also the preprint [6] which concatenates the results of [7] and of [18]), the second phenomenon can only appear when the potential function f admits degenerate deepest barriers. It is particularly unstable (see Remark 4 below) and arises from a strong tunneling effect between the wells. The asymptotic behaviour of the law of $X_{\tau_{\Omega}}$ when $h \to 0$ is also investigated in order to discuss the metastability of Ω for deterministic initial conditions within the wells.

1.2 Connections with the existing literature

As it will be clearly stated below in the first part of Section 1.4, the quasidistribution ν_h is completely characterized by the ground state of the Dirichlet realization of the infinitesimal generator $L_{f,h}^{(0)}$ of the diffusion (1),

$$L_{f,h}^{(0)} = -\frac{h}{2}\Delta + \nabla f \cdot \nabla = \frac{1}{2h} e^{-\frac{f}{h}} \Delta_{f,h}^{(0)} e^{\frac{f}{h}},$$

where $\Delta_{f,h}^{(0)} = -h^2 \Delta + |\nabla f|^2 - h \Delta f$ is the usual Witten Laplacian acting on functions. In this respect, the techniques used in this work originate from the semiclassical literature dealing with the obtention of sharp asymptotics on the

low spectrum of $\Delta_{f,h}^{(0)}$ in the limit $h \to 0$ and we refer in particular in this direction to [12] in the case without boundary and to [13] in the case of Dirichlet boundary conditions (see also the prior related works [3, 4] using potentialtheoretic methods and which motivated [12, 13]). However, these references focus on the low spectrum of $\Delta_{f,h}^{(0)}$ and not really on the concentration of the corresponding eigenfunctions. In addition, though they consider multiple-well Morse potentials, they do not consider the case of degenerate barriers. The case of general Morse potentials f, allowing in particular degenerate barriers, has nevertheless been recently treated in the case without boundary in [20] (see also [2] for related results) using the techniques of [12, 13].

More closely related to the present work, the already mentioned paper [7] involving both authors generalizes in particular the results of [13] to more general multiple-well Morse potentials but actually focuses on where the quasistationary distribution (or equivalently the ground state) concentrates in Ω and where the exit point distribution concentrates on $\partial\Omega$. Moreover, our results heavily rely on intermediate results proven in [7] (see Propositions 2 and 4 in Section 2.1.2). However, the degenerate situation considered in the present paper is excluded in [7], where the principal barrier of f is assumed to be non degenerate (see indeed [7, Assumption (A1)]).

1.3 Double-well potential

We assume more generally from now on that $\overline{\Omega} = \Omega \cup \partial \Omega$ is a C^{∞} oriented compact and connected Riemannian manifold of dimension d with boundary $\partial \Omega$. The basic assumption in this work is the following:

[H-Well]: The function f belongs to $C^{\infty}(\overline{\Omega}, \mathbb{R})$, $|\nabla f| \neq 0$ on $\partial\Omega$, and $f:\overline{\Omega} \to \mathbb{R}$ and $f|_{\partial\Omega}$ are Morse functions. Moreover, the function f has only two local minima x_1 and x_2 in Ω which satisfy

$$\underset{\overline{\Omega}}{\operatorname{arg\,min}} f = \underset{\Omega}{\operatorname{arg\,min}} f = \{x_1, x_2\}.$$

Finally, the open set $\{x \in \overline{\Omega}, f(x) < \min_{\partial\Omega} f\}$ has precisely two connected components, denoted by C_1 and C_2 , such that for all $j \in \{1, 2\}$,

$$x_j \in \mathsf{C}_j \quad \text{and} \quad \partial \mathsf{C}_j \cap \partial \Omega \neq \emptyset.$$

Under the assumption **[H-Well]**, the potential function f has precisely two wells, namely the open sets C_1 and C_2 . This double-well potential is moreover said to have degenerate barriers since the depths of C_1 and C_2 are the same and equal (see Figure 1)

$$H := \min_{\partial\Omega} f - \min_{\overline{\Omega}} f = \min_{\partial\Omega} f - \min_{\Omega} f > 0.$$
(3)

Let us also recall that a function $g: \overline{\Omega} \to \mathbb{R}$ is a Morse function if all its critical points are non degenerate. This implies in particular that g has a finite number of critical points.

When replacing the assumption $\arg \min_{\Omega} f = \{x_1, x_2\}$ by $\arg \min_{\Omega} f = \{x_1\}$ in **[H-Well]** (i.e. when the barriers are not degenerate), it is proved in [7,



Figure 1: A one dimensional example where [H-Well] is satisfied.

Proposition 9] that the quasi-stationary distribution ν_h concentrates in C₁ when $h \to 0$. This work aims precisely at studying the degenerate case $\arg \min_{\Omega} f =$ $\{x_1, x_2\}$ which introduces some additional technical difficulties, see the next section for some explanation.

Let us assume from now on that the assumption [H-Well] is satisfed. The set of saddle points of f of index 1 in Ω is denoted by U_1^{Ω} . Let us also define

$$\mathsf{U}_1^{\partial\Omega} \ := \ \{z \in \partial\Omega, \ z \text{ is a local minimum of } f|_{\partial\Omega}\} \cap \{z \in \partial\Omega, \ \partial_n f(z) > 0\}$$

and

$$\mathsf{U}_1^{\overline{\Omega}} := \mathsf{U}_1^{\partial\Omega} \cup \mathsf{U}_1^{\Omega} \quad \mathrm{and} \quad \mathsf{m}_1^{\overline{\Omega}} := \mathrm{Card}(\mathsf{U}_1^{\overline{\Omega}}).$$

According to the terminology of [13, Section 5.2], we call the elements of U_1^{Ω} the generalized saddle points for the Witten Laplacian acting on 1-forms with tangential Dirichlet boundary conditions on $\partial \Omega$. Note that f does not have any saddle point on $\partial \Omega$ (since $\nabla f \neq 0$ there) but that extending f by $-\infty$ outside $\overline{\Omega}$ (which is consistent with zero boundary Dirichlet conditions), the elements of $U_1^{\overline{\Omega}}$ are geometrically saddle points (since for such an element z, z is a local minimum of $f|_{\partial\Omega}$ and a local maximum of $f|_D$, where D is the straight line passing through z and orthogonal to $\partial \Omega$ at z).

Notice that from the assumption **[H-Well**], one has for all $i \in \{1, 2\}$:

$$\partial \mathsf{C}_i \cap \partial \Omega \subset \mathsf{U}_1^{\partial \Omega} \cap \operatorname*{arg\,min}_{\partial \Omega} f = (\partial \mathsf{C}_1 \cup \partial \mathsf{C}_2) \cap \partial \Omega$$

Let us define, for $i \in \{1, 2\}, z_{i,1}, ..., z_{i,n_i}$ by

$$\partial \mathsf{C}_i \cap \partial \Omega = \{z_{i,1}, \dots, z_{i,\mathsf{n}_i}\}, \text{ where } \mathsf{n}_i \ge 1 \text{ according to [H-Well]}.$$
(4)

One defines furthermore $z_{3,1}, \ldots, z_{3,n_3}$ by

$$\{z_{3,1},\ldots,z_{3,\mathsf{n}_3}\}=\mathsf{U}_1^{\overline{\Omega}}\setminus\left(\cup_{j=1}^2\partial\mathsf{C}_j\cap\partial\Omega\right),\,$$

where $\mathbf{n}_3 \in \mathbb{N}$ $(\mathbf{n}_3 = 0 \text{ meaning } \mathbf{U}_1^{\overline{\Omega}} \setminus \left(\cup_{j=1}^2 \partial \mathbf{C}_j \cap \partial \Omega \right) = \emptyset$). From [7, Proposi- $\mathsf{J}_1^\Omega \cap \{f = \min_{\partial \Omega}$ tion 15], it holds

$$\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \subset \mathsf{U}_1^{\scriptscriptstyle M} \cap \{f = \min_{a \in \mathcal{A}} f\}$$

and one orders $z_{3,1}, \ldots, z_{3,n_3}$ so that

$$\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 = \{z_{3,1}, \ldots, z_{3,\mathsf{m}_3}\},\$$

where $m_3 \in \{0, \ldots, n_3\}$. Note finally the relation

$$\mathbf{m}_{1}^{\Omega} = \mathbf{n}_{1} + \mathbf{n}_{2} + \mathbf{n}_{3}. \tag{5}$$

See Figures 2 and 3 for a schematic representation of the potential f under [**H-Well**] when $\partial C_1 \cap \partial C_2 = \emptyset$ and when $\partial C_1 \cap \partial C_2 \neq \emptyset$.



Figure 2: Schematic representation of the connected components C_1 and C_2 of $\{f < \min_{\partial\Omega} f\}$ when the assumption [H-Well] is satisfied. In this representation, $\partial C_1 \cap \partial C_2 = \emptyset$, $U_1^{\partial\Omega} = \{z_{1,1}, z_{1,2}, z_{2,1}\}$, $\partial C_1 \cap \partial\Omega = \{z_{1,1}, z_{1,2}\}$, $\partial C_2 \cap \partial\Omega = \{z_{2,1}\}$, $U_1^{\Omega} = \emptyset$ and $\arg\min_{\overline{\Omega}} f = \{x_1, x_2\}$. Thus, $n_1 = 2$, $n_2 = 1$ and $n_3 = m_3 = 0$.



Figure 3: Schematic representation of the connected components C_1 and C_2 of $\{f < \min_{\partial\Omega} f\}$ when the assumption [H-Well] is satisfied. In this representation, $\partial C_1 \cap \partial C_2 = \{z_{3,1}\}, U_1^{\partial\Omega} = \{z_{1,1}, z_{2,1}, z_{3,2}\}, \partial C_1 \cap \partial\Omega = \{z_{1,1}\}, \partial C_2 \cap \partial\Omega = \{z_{2,1}\}, U_1^{\Omega} = \{z_{3,1}\}$ and $\arg\min_{\overline{\Omega}} f = \{x_1, x_2\}$. Thus, $n_1 = 1, n_2 = 1, m_3 = 1$ and $n_3 = 2$.

1.4 Results

Preliminary spectral analysis

Let $L_{f,h}^{(0)}$ be the infinitesimal generator of the diffusion (1),

$$L_{f,h}^{(0)} = \frac{h}{2}\Delta_H^{(0)} + \nabla f \cdot \nabla,$$

where $\Delta_{H}^{(0)}$ is the Hodge Laplacian on $\overline{\Omega}$ and ∇ the gradient associated with the metric tensor on $\overline{\Omega}$. Let moreover $L_{f,h}^{D,(0)}$ be the differential operator $L_{f,h}^{(0)}$ on $L^{2}(\Omega, e^{-\frac{2}{h}f(x)}dx)$ with domain

$$D(L_{f,h}^{D,(0)}) = \left\{ w \in H^2(\Omega, e^{-\frac{2}{h}f(x)}dx), \ w = 0 \text{ on } \partial\Omega \right\}$$

The operator $L_{f,h}^{D,(0)}$ is self-adjoint, positive, and has compact resolvent. Moreover, its smallest eigenvalue $\lambda_1(h)$ is positive, non degenerate, and any eigenfunction associated with $\lambda_1(h)$ has a sign on Ω (see for instance [9, Section 6]). Let u_h be an eigenfunction associated with $\lambda_1(h)$. According to [17], the quasistationary distribution ν_h is then given by

$$d\nu_h := \frac{u_h(x) \ e^{-\frac{2}{h}f(x)}}{\int_{\Omega} u_h \ e^{-\frac{2}{h}f}} dx,$$
(6)

where dx is the Lebesgue measure on Ω . We assume furthermore from now on that

$$u_h > 0 \text{ on } \Omega \text{ and } \int_{\Omega} u_h^2 e^{-\frac{2}{h}f} = 1.$$
 (7)

In view of (6), in order to study the asymptotic behaviour of ν_h when $h \to 0$, we look for an accurate approximation of u_h . This is delicate since exponentially small eigenvalues of the same order are into play. Indeed, according to [7, Theorem 4], under [**H-Well**], it holds

$$\lim_{h \to 0} h \ln \left(\lambda_1(h) \right) = -2(\min_{\partial \Omega} f - \min_{\overline{\Omega}} f) = -2H$$

and there exists C > 1 such that for every h > 0 small enough,

$$1 < \frac{\lambda_2(h)}{\lambda_1(h)} \le C,$$

where $\lambda_2(h)$ denotes the second smallest eigenvalue of $L_{f,h}^{D,(0)}$. This makes in particular difficult to properly estimate u_h by simply projecting a well chosen quasi-mode on $\operatorname{Span}(u_h)$ since the quality of such an approximation is typically bounded from above by the quotient $\frac{\lambda_1(h)}{\lambda_2(h)}$ which does not tend to 0 when $h \to 0$. To overcome this difficulty, the key point relies on the fact that we are able to precisely analyse the restriction of $L_{f,h}^{D,(0)}$ to the eigenspace associated with $\lambda_1(h)$ and $\lambda_2(h)$. Indeed, this eigenspace has dimension two and the remaining eigenvalues of $L_{f,h}^{D,(0)}$ are bounded from below by $\frac{\sqrt{h}}{2}$. More precisely, we have according to [13, Theorem 3.2.3] the

Lemma 1. Let us assume that the hypothesis [*H*-Well] is satisfied. Then, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\dim \operatorname{Ran} \pi_{[0,\frac{\sqrt{h}}{2})} \left(L_{f,h}^{D,(0)} \right) = 2,$$

where $\pi_{[0,\frac{\sqrt{h}}{2})}\left(L_{f,h}^{D,(0)}\right)$ is the orthogonal projector on the vector space associated with the eigenvalues of $L_{f,h}^{D,(0)}$ in $[0,\frac{\sqrt{h}}{2})$.

¹They are actually bounded from below by some positive constant.

Remark 1. As a consequence of Lemma 1, there exists $h_0 > 0$ such that for every $h \in (0, h_0)$, the second smallest eigenvalue $\lambda_2(h)$ of $L_{f,h}^{D,(0)}$ is non degenerate.

Moreover, it follows from the general analysis led in [7] that the matrix L of $L_{f,h}^{D,(0)}\Big|_{\operatorname{Ran}\pi_{[0,\frac{\sqrt{h}}{2})}(L_{f,h}^{D,(0)})}$ satisfies Proposition 1 below. Before stating it, let us introduce the following notation. For $(\gamma(h))_{h>0} \in \mathbb{R}^{\mathbb{R}^{*}_{+}}$, one writes $\gamma(h) = \sqrt{h}$ if there exist C > 0 and $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\frac{1}{C}\sqrt{h} \le \gamma(h) \le C\sqrt{h}.$$
(8)

In addition, for $\alpha > 0$, one says that $(r(h))_{h>0}$ admits a full asymptotic expansion in h^{α} , and one writes $r(h) \sim \sum_{k=0}^{+\infty} a_k h^{\alpha k}$, if there exists a sequence $(a_k)_{k\geq 0} \in \mathbb{R}^{\mathbb{N}}$ such that for any $N \in \mathbb{N}$, it holds in the limit $h \to 0$:

$$r(h) = \sum_{k=0}^{N} a_k h^{\alpha k} + \mathcal{O}\left(h^{\alpha(N+1)}\right).$$
(9)

Proposition 1. Let us assume that the hypothesis [*H*-*Well*] is satisfied. Then, there exists $h_0 > 0$ such that for every $h \in (0, h_0)$, there exists an orthonormal basis $\mathcal{B}_0 = (\varphi_1, \varphi_2)$ of $\operatorname{Ran} \pi_{[0, \frac{\sqrt{h}}{2})} \left(L_{f,h}^{D,(0)} \right)$ such that the matrix L of the restriction of $L_{f,h}^{D,(0)}$ to $\operatorname{Ran} \pi_{[0, \frac{\sqrt{h}}{2})} \left(L_{f,h}^{D,(0)} \right)$ in \mathcal{B}_0 has the form:

$$L = \frac{1}{2} \begin{pmatrix} \alpha_1(h) & \varepsilon(h) \\ \varepsilon(h) & \alpha_2(h) \end{pmatrix} h^{-\frac{1}{2}} e^{-\frac{2}{h}H},$$
(10)

where H is defined in (3),

• $\varepsilon(h)$ satisfies in the limit $h \to 0$:

$$\varepsilon(h) = \begin{cases} \mathcal{O}\left(e^{-\frac{c}{h}}\right) & \text{if } \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 = \emptyset \\ \approx \sqrt{h} & \text{if } \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \neq \emptyset, \end{cases}$$
(11)

for some c > 0 independent of h and where the symbol \equiv is defined in (8),

• there exist two sequences $(\kappa_{1,k})_{k\geq 0} \in \mathbb{R}^{\mathbb{N}}$ and $(\kappa_{2,k})_{k\geq 0} \in \mathbb{R}^{\mathbb{N}}$ such that for $i \in \{1,2\}$, in the limit $h \to 0$:

$$\alpha_{i}(h) \sim \begin{cases} \sum_{k=0}^{+\infty} \kappa_{i,k} h^{k} & \text{if } \partial \mathsf{C}_{1} \cap \partial \mathsf{C}_{2} = \emptyset \\ \sum_{k=0}^{+\infty} \kappa_{i,k} h^{\frac{k}{2}} & \text{if } \partial \mathsf{C}_{1} \cap \partial \mathsf{C}_{2} \neq \emptyset, \end{cases}$$
(12)

where the symbol \sim is defined in (9) and

$$\kappa_{i,0} = \sum_{j=1}^{n_i} \frac{2 \,\partial_n f(z_{i,j})}{\pi^{\frac{1}{2}}} \,\frac{\sqrt{\det \operatorname{Hess} f(x_i)}}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_{i,j})}} \,. \tag{13}$$

Moreover, when $\partial C_1 \cap \partial C_2 \neq \emptyset$, one has for every $i \in \{1, 2\}$,

$$\kappa_{i,1} = \sum_{j=1}^{\mathsf{m}_3} \frac{|\lambda_-(z_{3,j})| \left(\det \operatorname{Hess} f(x_i)\right)^{\frac{1}{2}}}{\pi \left|\det \operatorname{Hess} f(z_{3,j})\right|^{\frac{1}{2}}},\tag{14}$$

where $\lambda_{-}(z)$ is the negative eigenvalue of Hess f(z). Finally, the sequence $(\kappa_{1,k})_{k\geq 1}$ (resp. $(\kappa_{2,k})_{k\geq 1}$) only depends on the values of the derivatives of f at x_1 and on $\partial C_1 \cap (\partial \Omega \cup \partial C_2)$ (resp. of the derivatives of f at x_2 and on $\partial C_2 \cap (\partial \Omega \cup \partial C_1)$).

Proposition 1 will be proven in Section 2.1. It permits to reduce the study of the asymptotic repartition of ν_h within the wells C_1 and C_2 to linear algebra considerations in dimension two. Then, when $X_0 \sim \nu_h$, the study of the asymptotic concentration of the law of $X_{\tau_{\Omega}}$ (which occurs on a subset of $\arg \min_{\partial\Omega} f$, see [7, Definition 1] for a precise definition) follows from the analysis made in [7] and based on the following formula [17]: for any $F \in L^{\infty}(\partial\Omega, \mathbb{R})$, it holds

$$\mathbb{E}^{\nu_h} \left[F(X_{\tau_\Omega}) \right] = -\frac{h}{2\lambda_1(h)} \frac{\int_{\partial\Omega} F \,\partial_n u_h \, e^{-\frac{2}{h}f}}{\int_\Omega u_h e^{-\frac{2}{h}f}},\tag{15}$$

where the notation \mathbb{E}^{ν_h} stands for the expectation when $X_0 \sim \nu_h$.

Results when ν_h concentrates in precisely one well when $h \to 0$ Let us define here the following assumption:

[H1]: The assumption **[H-Well]** is satisfied, there exists $h_0 > 0$ such that

either for all
$$h \in (0, h_0), \alpha_1(h) < \alpha_2(h),$$
 (16)

or for all
$$h \in (0, h_0), \alpha_2(h) < \alpha_1(h),$$
 (17)

and it holds

$$\lim_{h \to 0} \frac{\varepsilon(h)}{\alpha_1(h) - \alpha_2(h)} = 0.$$

Note that the assumption [H1] is generic (given an arbitrary function f satisfying [H-Well]) according to the following:

• when $\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 = \emptyset$ and the asymptotic expansion in h of $\alpha_1(h)$ and $\alpha_2(h)$ in (12) differ (i.e. when $(\kappa_{1,k})_{k\geq 0} \neq (\kappa_{2,k})_{k\geq 0}$), the assumption **[H1]** is satisfied and there exists c > 0 such that when $h \to 0$ (see indeed (11)),

$$\frac{\varepsilon(h)}{\alpha_1(h) - \alpha_2(h)} = \mathcal{O}\left(e^{-\frac{c}{h}}\right),\tag{18}$$

• when $\partial C_1 \cap \partial C_2 \neq \emptyset$ the assumption [H1] is, according to (11) and (12), equivalent to $\kappa_{1,0} \neq \kappa_{2,0}$, where $\kappa_{1,0}$ and $\kappa_{2,0}$ are defined in (13). In this case, when $h \to 0$:

$$\frac{\varepsilon(h)}{\alpha_1(h) - \alpha_2(h)} \approx \mathcal{O}(\sqrt{h}). \tag{19}$$

Our main result under the generic assumption [H1] is the following. It implies in particular that when [H1] holds together with (16), ν_h concentrates in any neighborhood of x_1 (i.e. $\lim_{h\to 0} \nu_h(O_1) = 1$ for any open subset O_1 of Ω containing x_1 , see more precisely (21) below). This can be roughly explained as follows: when [H1] holds, the term $\varepsilon(h)$ can be neglected in the expression of the matrix L given in (10), and (16) breaks the symmetry between the two wells C_1 and C_2 , ensuring more precisely the concentration of ν_h in C_1 .

Theorem 1. Let us assume that the hypotheses [*H*-Well] and [*H1*] together with (16) are satisfied. Let ν_h be the quasi-stationary distribution of the process (1) on Ω (see (6)). Let $O_1 \subset \Omega$ be an open neighborhood of x_1 and $O_2 \subset \Omega$ be an open neighborhood of x_2 such that $O_1 \cap O_2 = \emptyset$. Then, there exists c > 0such that in the limit $h \to 0$:

$$\nu_h(\mathsf{O}_1) + \nu_h(\mathsf{O}_2) = 1 + \mathcal{O}(e^{-\frac{c}{h}}), \tag{20}$$

where for $k \in \{1, 2\}$,

$$\nu_h(\mathsf{O}_k) = \delta_{1,k} + \mathcal{O}\left(\frac{|\varepsilon(h)|}{|\alpha_2(h) - \alpha_1(h)|}\right) + \mathcal{O}\left(e^{-\frac{c}{h}}\right).$$
(21)

Moreover, for any $F \in L^{\infty}(\partial\Omega,\mathbb{R})$ and for any family $(\Sigma_{i,j})_{(i,j)\in\bigcup_{p=1}^{2}\{p\}\times\{1,\ldots,n_{p}\}}$ of disjoint open neighborhoods of $(z_{i,j})_{(i,j)\in\bigcup_{p=1}^{2}\{p\}\times\{1,\ldots,n_{p}\}}$ in $\partial\Omega$, there exists c > 0 such that in the limit $h \to 0$:

$$\mathbb{E}^{\nu_{h}}\left[F\left(X_{\tau_{\Omega}}\right)\right] = \sum_{(i,j)\in\bigcup_{p=1}^{2}\{p\}\times\{1,\dots,\mathsf{n}_{p}\}} \mathbb{E}^{\nu_{h}}\left[\mathbf{1}_{\Sigma_{i,j}}F\left(X_{\tau_{\Omega}}\right)\right] + \mathcal{O}\left(e^{-\frac{c}{h}}\right)$$
(22)

and

$$\sum_{j=1}^{n_2} \mathbb{E}^{\nu_h} \left[\mathbf{1}_{\Sigma_{2,j}} F\left(X_{\tau_\Omega} \right) \right] = \mathcal{O}\left(\frac{|\varepsilon(h)|}{|\alpha_2(h) - \alpha_1(h)|} \right) + \mathcal{O}\left(e^{-\frac{c}{h}} \right).$$
(23)

In addition, when, for some $j \in \{1, ..., n_1\}$, F is C^{∞} around $z_{1,j}$, one has when $h \to 0$:

$$\mathbb{E}^{\nu_{h}}\left[\mathbf{1}_{\Sigma_{1,j}}F\left(X_{\tau_{\Omega}}\right)\right] = F(z_{1,j})\,a_{1,j} + \mathcal{O}\left(\frac{|\varepsilon(h)|}{|\alpha_{2}(h) - \alpha_{1}(h)|}\right) + \mathcal{O}(h),\qquad(24)$$

where, for $i \in \{1, 2\}$ and $j \in \{1, \ldots, n_i\}$, the constant $a_{i,j}$ is defined by

$$a_{i,j} := \frac{\partial_n f(z_{i,j})}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_{i,j})}} \left(\sum_{k=1}^{\mathsf{n}_i} \frac{\partial_n f(z_{i,k})}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_{i,k})}} \right)^{-1}.$$
 (25)

Remark 2. When [*H*-Well] and [*H1*] are satisfied, one also obtains from Proposition 1 sharp asymptotic estimates on the two smallest eigenvalues $0 < \lambda_1(h) < \lambda_2(h)$ of $L_{f,h}^{D,(0)}$ when $h \to 0$, see indeed (54) and (55).

From Theorem 1, when **[H-Well]** holds and **[H1]** is satisfied with (16), the quasi-stationary distribution ν_h concentrates when $h \to 0$ in C_1 and more precisely around any arbitrary small neighborhood of x_1 . Moreover, when $X_0 \sim \nu_h$,

the law of $X_{\tau_{\Omega}}$ concentrates when $h \to 0$ on $\{z_{1,1}, \ldots, z_{1,n_1}\} = \partial \mathsf{C}_1 \cap \partial \Omega$ with an explicit repartition given by (25). Adapting the proof of [6, Proposition 11] (see also [18]) by using (20) and (21), one can also show that when $X_0 = x \in \mathsf{C}_1$, the law of $X_{\tau_{\Omega}}$ concentrates when $h \to 0$ on $\{z_{1,1}, \ldots, z_{1,n_1}\} = \partial \mathsf{C}_1 \cap \partial \Omega$ with the same repartition as when $X_0 \sim \nu_h$. This exhibits a metastable behavior for such initial conditions. Moreover, when $|\nabla f| \neq 0$ on $\partial \mathsf{C}_2$, it follows from [6, Theorem 2] that when $X_0 = x \in \mathsf{C}_2$, the law of $X_{\tau_{\Omega}}$ concentrates when $h \to 0$ on $\{z_{1,2}, \ldots, z_{1,n_2}\} = \partial \mathsf{C}_2 \cap \partial \Omega$ with the repartition given by (25) (with i = 2). This exhibits a non metastable behavior for such initial conditions.

To connect with the literature dealing with semiclassical Schrödinger operators of the form $h^2 \Delta_H^{(0)} + V$ on manifolds without boundary (where V is a potential function independent of h), one can say in this situation that the tunneling effect between the two wells is too weak to mix their respective properties and that these two wells are hence somehow independent, that is, in the terminology of [15,16], weakly resonant or non resonant. We also refer to [11] for an overview on this topic for semiclassical Schrödinger operators (see in particular pp. 41–42 there). Notice lastly that (21) shows that some tunneling effect of order \sqrt{h} appears nevertheless when $\partial C_1 \cap \partial C_2 \neq \emptyset$ (see indeed (19)), contrary to the case $\partial C_1 \cap \partial C_2 = \emptyset$ when $\alpha_1(h)$ and $\alpha_2(h)$ do not have the same asymptotic expansion, see (18). As expected, when $\partial C_1 \cap \partial C_2 \neq \emptyset$, the independence between the two wells in this case is hence generically weaker.

Results when ν_h concentrates in both wells when $h \to 0$ Let us define here the following assumption:

[H2]: The assumption **[H-Well]** is satisfied. Moreover, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$, it holds

$$\varepsilon(h) \neq 0$$
 and $\lim_{h \to 0} \frac{\alpha_1(h) - \alpha_2(h)}{\varepsilon(h)} = 0.$

Let us exhibit situations where the assumption [H2] is satisfied.

• When $\partial C_1 \cap \partial C_2 \neq \emptyset$, the assumption **[H2]** is satisfied if and only if $\kappa_{1,0} = \kappa_{2,0}$ and $\kappa_{1,1} = \kappa_{2,1}$. This equivalence follows from (11) and (12). Therefore, when $\partial C_1 \cap \partial C_2 \neq \emptyset$, using (13) and (14), the assumption **[H2]** is satisfied if and only if

$$\sum_{j=1}^{n_1} \frac{\partial_n f(z_{1,j})}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_{1,j})}} = \sum_{j=1}^{n_2} \frac{\partial_n f(z_{2,j})}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_{2,j})}},$$
(26)

and

$$\det \operatorname{Hess} f(x_1) = \det \operatorname{Hess} f(x_2). \tag{27}$$

Moreover, it holds in this case:

$$\frac{\alpha_1(h) - \alpha_2(h)}{\varepsilon(h)} = \mathcal{O}(\sqrt{h})$$

• Let us assume that f is an even function as defined by (34) below. Then, from Theorem 3 below, the assumption **[H2]** is satisfied (see indeed Remark 7).

Remark 3. When $\partial C_1 \cap \partial C_2 = \emptyset$, we are not able to explicit assumptions on f which imply [**H2**] except in the symmetric situation described in Theorem 3. Note in particular that when $\partial C_1 \cap \partial C_2 = \emptyset$ and [**H2**] holds, one has when $h \to 0$: $\alpha_1(h) = \alpha_2(h) \left(1 + O(e^{-\frac{c}{h}})\right)$ (which follows from [**H2**], (12) and the fact that $\varepsilon(h) = O(e^{-\frac{c}{h}})$, see (11)) and thus:

$$\kappa_{1,k} = \kappa_{2,k} \quad \text{for all } k \in \mathbb{N}. \tag{28}$$

Moreover, it also holds in this case $\lambda_1(h) = \lambda_2(h) \left(1 + \mathcal{O}(e^{-\frac{c}{h}})\right)$ (see (67)).

Remark 4. The assumption [H2] is non generic, that is unstable with respect to perturbations of the potential f in the following sense. For any f satisfying [H2], it follows from (26)–(28) that there exists an arbitrary small perturbation $\delta f: \overline{\Omega} \to \mathbb{R}$ such that $f + \delta f$ satisfies [H1]. Then, according to Theorem 1, the quasi-stationary distribution for the potential $f + \delta f$ concentrates when $h \to 0$ in precisely one of the wells C_1 or C_2 .

The following result shows that when **[H2]** is satisfied, the quasi-stationary distribution ν_h concentrates when $h \to 0$ in the two wells C_1 and C_2 .

Theorem 2. Let us assume that the hypotheses [*H*-*Well*] and [*H2*] are satisfied. Let ν_h be the quasi-stationary distribution of the process (1) on Ω (see (6)). Let $O_1 \subset \Omega$ be an open neighborhood of x_1 and $O_2 \subset \Omega$ be an open neighborhood of x_2 such that $O_1 \cap O_2 = \emptyset$. Then, there exists c > 0 such that in the limit $h \to 0$:

$$\nu_h(\mathsf{O}_1) + \nu_h(\mathsf{O}_2) = 1 + \mathcal{O}\left(e^{-\frac{\nu}{h}}\right),\tag{29}$$

where, for $k \in \{1, 2\}$,

$$\nu_h(\mathsf{O}_k) = b_k + \mathcal{O}\left(\frac{|\alpha_2(h) - \alpha_1(h)|}{|\varepsilon(h)|}\right) + \mathcal{O}(h),\tag{30}$$

where, defining q by $\{q\} = \{1,2\} \setminus \{k\},\$

$$b_k = \frac{\left(\det \operatorname{Hess} f(x_q)\right)^{\frac{1}{4}}}{\left(\det \operatorname{Hess} f(x_1)\right)^{\frac{1}{4}} + \left(\det \operatorname{Hess} f(x_2)\right)^{\frac{1}{4}}}.$$
(31)

Moreover, for any $F \in L^{\infty}(\partial\Omega, \mathbb{R})$ and for any family $(\Sigma_{i,j})_{(i,j)\in\bigcup_{p=1}^{2}\{p\}\times\{1,\ldots,n_{p}\}}$ of disjoint open neighborhoods of $(z_{i,j})_{(i,j)\in\bigcup_{p=1}^{2}\{p\}\times\{1,\ldots,n_{p}\}}$ in $\partial\Omega$, there exists c > 0 such that in the limit $h \to 0$:

$$\mathbb{E}^{\nu_{h}}\left[F\left(X_{\tau_{\Omega}}\right)\right] = \sum_{(i,j)\in\bigcup_{p=1}^{2}\{p\}\times\{1,\dots,\mathsf{n}_{p}\}} \mathbb{E}^{\nu_{h}}\left[\mathbf{1}_{\Sigma_{i,j}}F\left(X_{\tau_{\Omega}}\right)\right] + \mathcal{O}\left(e^{-\frac{c}{h}}\right).$$
(32)

Lastly, when, for some $(i, j) \in \bigcup_{p=1}^{2} \{p\} \times \{1, \dots, n_p\}$, F is C^{∞} around $z_{i,j}$, one has when $h \to 0$:

$$\mathbb{E}^{\nu_{h}}\left[\mathbf{1}_{\Sigma_{i,j}}F\left(X_{\tau_{\Omega}}\right)\right] = F(z_{i,j})\,a_{i,j}\,b_{i} + \mathcal{O}\left(\frac{|\alpha_{2}(h) - \alpha_{1}(h)|}{|\varepsilon(h)|}\right) + \mathcal{O}(h), \quad (33)$$

where b_i is defined in (31) and $a_{i,j}$ is defined in (25).

Remark 5. When [*H*-Well] and [*H2*] are satisfied, one also gives sharp asymptotic estimates on the two smallest eigenvalues $0 < \lambda_1(h) < \lambda_2(h)$ of $L_{fh}^{D,(0)}$ when $h \to 0$, see indeed (67), (68) and (69).

When **[H-Well]** and **[H1]** hold, Theorem 2 implies that the quasi-stationary distribution ν_h concentrates when $h \to 0$ in C_1 and C_2 , and more precisely around any arbitrary small neighborhood of x_1 and x_2 . Note also that when $\partial C_1 \cap \partial C_2 \neq \emptyset$, the coefficient (31) specifying the repartition of ν_h within the wells equals $\frac{1}{2}$ according to (27). Moreover, when $X_0 \sim \nu_h$ the law of X_{τ_Ω} concentrates when $h \to 0$ on $\{z_{1,1}, \ldots, z_{1,n_1}\} \cup \{z_{2,1}, \ldots, z_{2,n_2}\} = (\partial C_1 \cup \partial C_2) \cap \partial \Omega$ with an explicit repartition given by (25). In addition, when $|\nabla f| \neq 0$ on $\partial C_1 \cup \partial C_2$, it follows from [6, Theorem 2] that when $X_0 = x \in C_k$, $k \in \{1, 2\}$, the law of X_{τ_Ω} concentrates when $h \to 0$ on $\{z_{k,1}, \ldots, z_{k,n_k}\} = \partial C_k \cap \partial \Omega$ with the repartition given by (25). This shows that in this case the domain Ω is not metastable for deterministic initial conditions within $C_1 \cup C_2$.

Connecting again with the literature dealing with semiclassical Schrödinger operators of the form $h^2 \Delta_H^{(0)} + V$ on manifolds without boundary, when the assumptions **[H-Well]** and **[H2]** are satisfied, a strong tunneling effect appears when $h \to 0$ and mixes the respective properties of both wells. We refer to [11, pp. 45– 46] for a symmetric case with two wells and to [16] for more general symmetric situations.

Let us conclude this section by specifying the statement of Theorem 2 in a completely symmetric situation. To this end, we recall that an isometry Φ : $\overline{\Omega} \to \overline{\Omega}$ is a C^{∞} diffeomorphism which satisfies, for all $x \in \overline{\Omega}$ and all $v, w \in T_x \overline{\Omega}$: $v \cdot w = D\Phi_x(v) \cdot D\Phi_x(w)$, where \cdot is the scalar product associated with the metric of $\overline{\Omega}$ on the tangent bundle $T\overline{\Omega}$. One says moreover that $f: \overline{\Omega} \to \overline{\Omega}$ is even if there exists an isometry Φ such that

$$\Phi(x_1) = x_2, \ \Phi^2 = I, \quad \text{and} \quad f \circ \Phi = f, \tag{34}$$

where I is the identity map on $\overline{\Omega}$. When f is even, the following improvement of Theorem 2 holds.

Theorem 3. Let us assume that the hypothesis [**H**-Well] is satisfied. Let ν_h be the quasi-stationary distribution of the process $(X_t)_{t\geq 0}$ on Ω (see (6)). Assume that f is an even function as defined by (34). Then, the assumption [**H**2] is satisfied with in particular, for all h small enough:

 $\alpha_1(h) = \alpha_2(h)$, where $\alpha_1(h)$ and $\alpha_2(h)$ are defined by (10).

Furthermore, let $O_1 \subset \Omega$ be an open neighborhood of x_1 and $O_2 \subset \Omega$ be an open neighborhood of x_2 such that $O_1 \cap O_2 = \emptyset$. Then, for $k \in \{1, 2\}$, there exists c > 0 such that in the limit $h \to 0$:

$$\nu_h(\mathsf{O}_k) = \frac{1}{2} + \mathcal{O}\big(e^{-\frac{c}{h}}\big).$$

Moreover, one has $n_1 = n_2$ (see (4)) and the asymptotic estimates (32) and (33).

2 Proof of our main results

2.1 Proof of Proposition 1

2.1.1 The operator $L_{fh}^{D,(1)}$

For $p \in \{0, \ldots, d\}$, one denotes by $\Lambda^p C^{\infty}(\overline{\Omega})$ the space of C^{∞} *p*-forms on $\overline{\Omega}$ and by $\Lambda^p C_T^{\infty}(\overline{\Omega})$ the subset of $\Lambda^p C^{\infty}(\overline{\Omega})$ made of the *p*-forms *v* such that $\mathbf{t}v = 0$ on $\partial\Omega$, where \mathbf{t} denotes the tangential trace on forms. We recall that $\mathbf{t}v = 0$ on $\partial\Omega$ means that the restriction to $\partial\Omega$ of the *p*-form *v* vanishes when applied to tangential vector fields, and we refer e.g. to [23, Equation (2.25)] for a rigorous definition of the tangential trace. For $q \in \mathbb{N}$, one denotes by $\Lambda^p H^q_w(\Omega)$ the weighted Sobolev spaces of *p*-forms with regularity index *q*, for the weight $e^{-\frac{2}{h}f}$ on Ω (where the subscript *w* refers to the fact that the weight function appears in the inner product), and we refer again to [23] for an introduction to weighted Sobolev spaces on manifolds with boundaries. The set $\Lambda^p H^1_{w,T}(\Omega)$ is then defined by

$$\Lambda^p H^1_{w,T}(\Omega) := \left\{ v \in \Lambda^p H^1_w(\Omega), \ \mathbf{t}v = 0 \text{ on } \partial\Omega \right\}.$$

We will denote by $\|.\|_{H^q_w}$ the norm on the weighted space $\Lambda^p H^q_w(\Omega)$ and by $\langle \cdot, \cdot \rangle_{L^2_w}$ the scalar product on $\Lambda^p L^2_w(\Omega)$. Notice that $\Lambda^0 L^2_w(\Omega)$ is the space $L^2(\Omega, e^{-\frac{2}{h}f(x)}dx)$ and $\Lambda^0 H^2_w(\Omega)$ is the space $H^2(\Omega, e^{-\frac{2}{h}f(x)}dx)$ introduced in the definition of $L^{D,(0)}_{f,h}$ in Section 1.4.

In the following, one denotes respectively by $d: \Lambda^p C^{\infty}(\overline{\Omega}) \to \Lambda^{p+1} C^{\infty}(\overline{\Omega})$ and $d^*: \Lambda^{p+1} C^{\infty}(\overline{\Omega}) \to \Lambda^p C^{\infty}(\overline{\Omega})$ the exterior and the co-differential derivatives on $\overline{\Omega}$. Let us introduce the differential operator

$$L_{f,h}^{(1)} = \frac{h}{2}\Delta_{H}^{(1)} + \mathcal{L}_{\nabla f} = \frac{1}{2h}e^{\frac{f}{h}} \left(h^{2}\Delta_{H}^{(1)} + |\nabla f|^{2} + h(\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^{*})\right)e^{-\frac{f}{h}}$$

acting on $\Lambda^1 C^{\infty}(\overline{\Omega})$, where $\Delta_H^{(1)} = (d + d^*)^2$ is the Hodge Laplacian on $\overline{\Omega}$, $\mathcal{L}_{\nabla f}$ is the Lie derivative with respect to the vector field ∇f , and $\mathcal{L}_{\nabla f}^*$ its formal adjoint in $L^2(\Omega)$. The (tangential) Dirichlet realization of $L_{f,h}^{(1)}$ is denoted by $L_{f,h}^{D,(1)}$ and its domain is

$$D\big(L^{D,(1)}_{f,h}\big) = \big\{v \in \Lambda^1 H^2(\Omega), \ \mathbf{t}v = 0 \ \text{and} \ \mathbf{t}d^*e^{-\frac{2}{h}f}v = 0 \ \text{on} \ \partial\Omega\big\}.$$

From [13, Section 2.4], the operator $L_{f,h}^{D,(1)}$ is self-adjoint, positive and has compact resolvent. One has moreover the following result from [13, Theorem 3.2.3].

Lemma 2. Under the assumption [*H*-Well], there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\dim \operatorname{Ran} \pi_{[0,\frac{\sqrt{h}}{2})} \left(L_{f,h}^{D,(1)} \right) = \mathsf{m}_1^{\overline{\Omega}},$$

where $\mathbf{m}_{1}^{\overline{\Omega}}$ is defined in (5) and $\pi_{[0,\frac{\sqrt{h}}{2})}\left(L_{f,h}^{D,(1)}\right)$ is the orthogonal projector on the vector space associated with the eigenvalues of $L_{f,h}^{D,(1)}$ in $[0,\frac{\sqrt{h}}{2})$.

In the following, the exterior differential d will be denoted, with a slight abuse of notation, by ∇ . For ease of notation, one also denotes, for $p \in \{0, 1\}$,

$$\pi_{h}^{(p)} = \pi_{[0,\frac{\sqrt{h}}{2})} \left(L_{f,h}^{D,(p)} \right)$$

From [13, Corollary 2.4.4], the following relation holds on $\Lambda^0 H^1_{w,T}(\Omega)$:

$$\nabla \pi_h^{(0)} = \pi_h^{(1)} \nabla \,. \tag{35}$$

This implies in particular that

$$\nabla : \operatorname{Ran} \pi_h^{(0)} \to \operatorname{Ran} \pi_h^{(1)} \tag{36}$$

and then, when $[\mathbf{H}\text{-}\mathbf{Well}]$ holds, according to Lemma 1, that for every h small enough,

$$\nabla u_h \in \operatorname{Ran} \pi_h^{(1)}.\tag{37}$$

We refer to [7, Section 3.1.2] for more details concerning this section.

2.1.2 Proof of Proposition 1

In the following, we assume that **[H-Well]** holds.

The finite dimensional vector spaces $\operatorname{Ran} \pi_h^{(0)}$ and $\operatorname{Ran} \pi_h^{(1)}$ are endowed with the scalar product $\langle ., . \rangle_{L^2_w}$ of $L^2_w(\Omega)$ introduced in Section 2.1.1. Moreover, the set $\{i_j\}_{(i,j)\in\bigcup_{p=1}^3 \{p\}\times\{1,...,n_p\}}$ is ordered using the lexicographical order, i.e.

$$\{i_j\}_{(i,j)\in\bigcup_{p=1}^3\{p\}\times\{1,\ldots,n_p\}}=\{1_1,\ldots,1_{n_1},2_1,\ldots,2_{n_2},3_1\ldots,3_{m_3},3_{m_3+1},\ldots,3_{n_3}\},$$

where we recall $\mathbf{n}_1 = \text{Card} (\partial \mathsf{C}_1 \cap \partial \Omega), \mathbf{n}_2 = \text{Card} (\partial \mathsf{C}_2 \cap \partial \Omega), \mathbf{m}_3 = \text{Card} (\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2)$ and $\mathbf{n}_3 = \text{Card} (\mathsf{U}_1^{\overline{\Omega}} \setminus (\cup_{k=1}^2 \partial \mathsf{C}_k \cap \partial \Omega)) = \mathsf{m}_1^{\overline{\Omega}} - \mathsf{n}_1 - \mathsf{n}_2$ are defined in Section 1.3.

Let us now define

$$\widetilde{u}_{1} := \frac{\chi_{1}}{\left\|\chi_{1}\right\|_{L^{2}_{w}}} \in \Lambda^{0} H^{1}_{w,T}\left(\Omega\right) \text{ and } \widetilde{u}_{2} := \frac{\chi_{2}}{\left\|\chi_{2}\right\|_{L^{2}_{w}}} \in \Lambda^{0} H^{1}_{w,T}\left(\Omega\right)$$
(38)

where, for $i \in \{1, 2\}$, $0 \not\equiv \chi_i \in C^{\infty}(\Omega, \mathbb{R}^+)$ is compactly supported in Ω , χ_1 and χ_2 have disjoint supports, and for some small $\alpha > 0$ and $\beta > 0$,

$$\operatorname{supp} \chi_i \subset \left(\mathsf{C}_i + B(0,\alpha)\right) \cap \Omega \text{ and } \chi_i = 1 \text{ on } \mathsf{C}_i \cap \{f < \min_{\partial \Omega} f - \beta\}.$$

Let us also consider a family of L^2_w -unitary 1-forms

$$(\psi_{i_j})_{(i,j)\in\bigcup_{p=1}^3\{p\}\times\{1,\dots,\mathsf{n}_p\}}$$
(39)

such that, for $(i, j) \in \bigcup_{p=1}^{3} \{p\} \times \{1, \dots, \mathsf{n}_{p}\}, \ \widetilde{\psi}_{i_{j}} \in \Lambda^{1} H^{1}_{w, T}(\Omega) \cap \Lambda^{1} C^{\infty}(\overline{\Omega}),$ and for some small $\delta > 0$, supp $\widetilde{\psi}_{i_{j}} \subset B(z_{i, j}, \delta) \cap \overline{\Omega}.$ It then holds, for every $(k,q) \in \{1,2\}, (i,j) \in \bigcup_{p=1}^{3} \{p\} \times \{1,\ldots,n_p\}$, and $(i',j') \in \bigcup_{p=1}^{3} \{p\} \times \{1,\ldots,n_p\}$ (for $\delta > 0$ small enough):

$$\langle \widetilde{u}_k, \widetilde{u}_q \rangle_{L^2_w} = \delta_{k,q} \text{ and } \langle \widetilde{\psi}_{i_j}, \widetilde{\psi}_{i'_{j'}} \rangle_{L^2_w} = \delta_{i,i'} \delta_{j,j'}.$$
 (40)

Taking, for every $(i, j) \in \bigcup_{p=1}^{3} \{p\} \times \{1, \ldots, n_p\}, \widetilde{\psi}_{i_j}$ as a (normalized) truncated principal eigen-1-form of a local Witten Laplacian defined around $z_{i,j}$ with Dirichlet boundary conditions ², we obtain the following proposition (see [7, Section 3.2.2 and Definition 42] and references therein for details). It gathers the statements of [7, Propositions 43 and 47] which are the starting points of our analysis.

Proposition 2. Let us assume that the function f satisfies [*H*-Well]. Then, the families $(\tilde{u}_1, \tilde{u}_2)$ and $(\tilde{\psi}_{i_j})_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1, \dots, n_p\}}$ defined in (38), (39) can be chosen so that the following estimates hold when $h \to 0$ (where H is defined in (3)):

- 1. There exists c > 0 such that:
 - a) for every $k \in \{1, 2\}$, it holds

$$\left\| (1 - \pi_h^{(0)}) \widetilde{u}_k \right\|_{L^2_w}^2 \leq h^{\frac{1}{2}} \left\| \nabla \widetilde{u}_k \right\|_{L^2_w}^2 \leq e^{-\frac{2}{h}(H - \frac{c}{2})},$$

b) for every $i \in \{1, 2, 3\}$ and $j \in \{1, ..., n_i\}$, it holds

$$\|(1-\pi_h^{(1)})\widetilde{\psi}_{i_j}\|_{H^1_w}^2 = \mathcal{O}(e^{-\frac{2c}{h}}).$$

2. For every $k \in \{1, 2\}$ and $(i, j) \in \bigcup_{p=1}^{3} \{p\} \times \{1, \dots, n_p\}$, there exists a real constant $\varepsilon_{i,j,k} \in \{-1, 1\}$ independent of h such that it holds

$$\langle \nabla \widetilde{u}_k, \widetilde{\psi}_{i_j} \rangle_{L^2_w} = \begin{cases} -C_{i,j,k} \ h^{-\frac{3}{4}} e^{-\frac{H}{h}} \left(1 + \mathcal{O}(h)\right) & \text{when } z_{i,j} \in \partial \mathsf{C}_k \cap \partial \Omega\\ \varepsilon_{i,j,k} C_{i,j,k} \ h^{-\frac{1}{2}} e^{-\frac{H}{h}} \left(1 + \mathcal{O}(h)\right) & \text{when } z_{i,j} \in \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2\\ 0 & \text{else}, \end{cases}$$

where the remainder terms $\mathcal{O}(h)$ admit a full asymptotic expansion in h, and

$$C_{i,j,k} = \begin{cases} \pi^{-\frac{1}{4}} \sqrt{2 \partial_n f(z_{i,j})} \frac{\left(\det \operatorname{Hess} f(x_k)\right)^{\frac{1}{4}}}{\left(\det \operatorname{Hess} f|_{\partial\Omega}(z_{i,j})\right)^{\frac{1}{4}}} & \text{if } z_{i,j} \in \partial \mathsf{C}_k \cap \partial \Omega\\ \pi^{-\frac{1}{2}} \sqrt{|\lambda_-(z_{i,j})|} \frac{\left(\det \operatorname{Hess} f(x_k)\right)^{\frac{1}{4}}}{\left|\det \operatorname{Hess} f(z_{i,j})\right|^{\frac{1}{4}}} & \text{if } z_{i,j} \in \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2, \end{cases}$$

$$(41)$$

where $\lambda_{-}(z_{i,j})$ denotes the negative eigenvalue of Hess $f(z_{i,j})$.

Remark 6. In the second item in Proposition 2, notice that it follows from the notation introduced in Section 1.3 that for every $k \in \{1,2\}$ and $(i,j) \in \bigcup_{p=1}^{3} \{p\} \times \{1,\ldots,n_p\}$, one has:

²Actually, when $z_{i,j} \in \partial\Omega$ and \mathcal{V} denotes its corresponding neighborhood in $\overline{\Omega}$, (full) Dirichlet boundary conditions are considered on $\partial \mathcal{V} \cap \Omega$ while only tangential Dirichlet boundary conditions are considered on $\partial \mathcal{V} \cap \partial\Omega$.

- $z_{i,j} \in \partial C_k \cap \partial \Omega$ if and only if i = k (and thus $j \in \{1, \dots, n_k\}$),
- $z_{i,j} \in \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2$ if and only if i = 3 (and thus $j \in \{1, \ldots, \mathsf{m}_3\}$).

As a consequence of (40) and the first item in Proposition 2, there exists c > 0 such that it holds in the limit $h \to 0$:

$$G_0 := \left(\left\langle \pi_h^{(0)} \widetilde{u}_k, \pi_h^{(0)} \widetilde{u}_q \right\rangle_{L^2_w} \right)_{k,q \in \{1,2\}} = I_2 + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \tag{42}$$

and

$$G_{1} := \left(\left\langle \pi_{h}^{(1)} \widetilde{\psi}_{i_{j}}, \pi_{h}^{(1)} \widetilde{\psi}_{i_{j'}'} \right\rangle_{L^{2}_{w}} \right)_{\substack{(i,j) \in \bigcup_{p=1}^{3} \{p\} \times \{1, \dots, \mathsf{n}_{p}\} \\ (i',j') \in \bigcup_{p=1}^{3} \{p\} \times \{1, \dots, \mathsf{n}_{p}\}} = I_{\mathsf{m}_{1}^{\overline{\Omega}}} + \mathcal{O}(e^{-\frac{c}{h}}).$$
(43)

It then follows from Lemmata 1 and 2 that, for every h > 0 small enough, the family $(\pi_h^{(0)} \tilde{u}_k)_{k \in \{1,2\}}$ is a basis of $\operatorname{Ran} \pi_h^{(0)}$ and that $(\pi_h^{(1)} \tilde{\psi}_{i_j})_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1, \dots, n_p\}}$ is a basis of $\operatorname{Ran} \pi_h^{(1)}$.

Let us now define the $\mathsf{m}_{1}^{\overline{\Omega}} \times 2$ matrix

$$S := \left(\left\langle \nabla \pi_h^{(0)} \widetilde{u}_k, \pi_h^{(1)} \widetilde{\psi}_{i_j} \right\rangle_{L^2_w} \right)_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1, \dots, \mathsf{n}_p\}, \, k \in \{1, 2\}}.$$
 (44)

According to the two items in Propositions 2, and using the identity

$$\left\langle \nabla \pi_h^{(0)} \widetilde{u}_k, \pi_h^{(1)} \widetilde{\psi}_{i_j} \right\rangle_{L^2_w} = \left\langle \nabla \widetilde{u}_k, \widetilde{\psi}_{i_j} \right\rangle_{L^2_w} - \left\langle \nabla \widetilde{u}_k, \left(1 - \pi_h^{(1)}\right) \widetilde{\psi}_{i_j} \right\rangle_{L^2_w}$$

which follows from (35), there exists c > 0 such that the coefficients of S satisfy when $h \to 0$:

$$S_{i_j,k} = \begin{cases} \left\langle \nabla \widetilde{u}_k, \widetilde{\psi}_{i_j} \right\rangle_{L^2_w} \left(1 + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \right) & \text{if } z_{i,j} \in \partial \mathsf{C}_k \cap \partial \Omega \\ \left\langle \nabla \widetilde{u}_k, \widetilde{\psi}_{i_j} \right\rangle_{L^2_w} \left(1 + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \right) & \text{if } z_{i,j} \in \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \\ \mathcal{O}\left(e^{-\frac{1}{h}(H+c)}\right) & \text{else.} \end{cases}$$
(45)

Let us denote by $\widetilde{\Upsilon}$ and $\widetilde{\Psi}$ the following families written as row vectors,

$$\widetilde{\Upsilon} := (\pi_h^{(0)} \widetilde{u}_1, \pi_h^{(0)} \widetilde{u}_2) \quad \text{and} \quad \widetilde{\Psi} := (\pi_h^{(1)} \widetilde{\psi}_{i_j})_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1, \dots, \mathsf{n}_p\}},$$

and define

$$\mathcal{B}_{0} = (\varphi_{1}, \varphi_{2}) := \widetilde{\Upsilon} G_{0}^{-\frac{1}{2}} \text{ and } \mathcal{B}_{1} = (\psi_{i_{j}})_{(i,j) \in \bigcup_{p=1}^{3} \{p\} \times \{1, \dots, \mathsf{n}_{p}\}} := \widetilde{\Psi} G_{1}^{-\frac{1}{2}},$$
(46)

where G_0 and G_1 are defined in (42) and (43). For every h > 0 small enough, the families \mathcal{B}_0 and \mathcal{B}_1 are then respectively orthonormal bases of $\operatorname{Ran} \pi_h^{(0)}$ and of $\operatorname{Ran} \pi_h^{(1)}$.

The matrix L of $L_{f,h}^{D,(0)}|_{\operatorname{Ran} \pi_h^{(0)}}$ in the basis \mathcal{B}_0 is given by

$$L = G_0^{-\frac{1}{2}} \left(\left\langle L_{f,h} \pi_h^{(0)} \widetilde{u}_k, \pi_h^{(0)} \widetilde{u}_q \right\rangle_{L^2_w} \right)_{1 \le k,q \le 2} G_0^{-\frac{1}{2}}.$$
 (47)

This matrix is sometimes called the *interaction matrix* in the literature dealing with the study of semiclassical Schrödinger operators (see e.g. [14] or [8]).

Moreover, the matrix M of ∇ : Ran $\pi_h^{(0)} \to \operatorname{Ran} \pi_h^{(1)}$ (see (36)) in the bases \mathcal{B}_0 and \mathcal{B}_1 is given by

$$M = G_1^{-\frac{1}{2}} S G_0^{-\frac{1}{2}}, (48)$$

where S is defined in (44). Since $L_{f,h}^{D,(0)}|_{\operatorname{Ran} \pi_h^{(0)}} = \frac{h}{2} \nabla^* \nabla$, the matrix M satisfies

$$L = \frac{h}{2}M^*M.$$
(49)

In order to prove Proposition 1, it is then sufficient to get asymptotic estimates on the coefficients of the matrix M. This is the purpose of the next proposition.

Proposition 3. Let us assume that the hypothesis [*H*-Well] is satisfied. Let $(\tilde{u}_k)_{k \in \{1,2\}}$ be defined by (38). Let $(\varphi_k)_{k \in \{1,2\}}$ and $(\psi_{i_j})_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1,...,n_p\}}$ be defined by (46). Then, for all $k \in \{1,2\}$, there exists c > 0 such that when $h \to 0$:

$$\begin{split} i) \ for \ every \ j \in \{1, \dots, \mathsf{n}_k\}, \\ \langle \nabla \varphi_k, \psi_{k_j} \rangle_{L^2_w} &= \langle \nabla \widetilde{u}_k, \widetilde{\psi}_{k_j} \rangle_{L^2_w} \left(1 + \mathcal{O}(e^{-\frac{c}{h}})\right) = -C_{k,j,k} \ h^{-\frac{3}{4}} \ e^{-\frac{H}{h}} \left(1 + \mathcal{O}(h)\right), \\ ii) \ for \ every \ j \in \{1, \dots, \mathsf{n}_p\} \ with \ p \in \{1, 2\} \setminus \{k\}, \\ &\quad \langle \nabla \varphi_k, \psi_{p_j} \rangle_{L^2_w} = \mathcal{O}\left(e^{-\frac{1}{h}(H+c)}\right), \end{split}$$

iii) for every $j \in \{1, ..., m_3\}$,

$$\langle \nabla \varphi_k, \psi_{3_j} \rangle_{L^2_w} = \langle \nabla \widetilde{u}_k, \widetilde{\psi}_{3_j} \rangle_{L^2_w} \left(1 + \mathcal{O}(e^{-\frac{c}{h}}) \right) = \varepsilon_{3,j,k} \, C_{3,j,k} \, h^{-\frac{1}{2}} \, e^{-\frac{H}{h}} \left(1 + \mathcal{O}(h) \right),$$

iv) and for all $j \in \{m_3 + 1, ..., n_3\}$,

$$\langle \nabla \varphi_k, \psi_{3_j} \rangle_{L^2_w} = \mathcal{O}\left(e^{-\frac{1}{h}(H+c)}\right),$$

where we recall that $H = \min_{\partial\Omega} f - \min_{\overline{\Omega}} f$ (see (3)), the coefficients $C_{i,j,k}$ are defined in (41), and the terms $\mathcal{O}(h)$ admit a full asymptotic expansion in h.

Proof. The results of Proposition 3 follow from (42)–(45), (48), and item 2 in Proposition 2 (see also Remark 6).

Proposition 1 is a consequence of Proposition 3 and of (49). They indeed imply the existence of some c > 0 such that when $h \to 0$, the coefficients $\varepsilon(h)$, $\alpha_1(h)$, and $\alpha_2(h)$ defined by (10) satisfy

$$\varepsilon(h) = \begin{cases} \mathcal{O}\left(e^{-\frac{c}{h}}\right) & \text{if } \partial \mathsf{C}_1 \cap \partial C_2 = \emptyset\\ \sum_{j=1}^{\mathsf{m}_3} \varepsilon_{3,j,1} \, \varepsilon_{3,j,2} \, C_{3,j,1} \, C_{3,j,2} \, \sqrt{h} \left(1 + \mathcal{O}(h)\right) & \text{if } \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \neq \emptyset, \end{cases}$$
(50)

and, for $k \in \{1, 2\}$,

$$\alpha_k(h) = \begin{cases} \sum_{j=1}^{n_k} C_{k,j,k}^2 (1 + \mathcal{O}(h)) & \text{if } \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 = \emptyset \\ \sum_{j=1}^{n_k} C_{k,j,k}^2 (1 + \mathcal{O}(h)) + \sum_{j=1}^{\mathsf{m}_3} C_{3,j,k}^2 \sqrt{h} (1 + \mathcal{O}(h)) & \text{if } \partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \neq \emptyset. \end{cases}$$

where the $C_{i,j,k}$'s are defined in (41) and the remainder terms $\mathcal{O}(h)$ admit a full asymptotic expansion in h. The relations (11)–(14) follow.

Let us conclude this section by noticing the following consequences of Proposition 1 which will needed in upcoming computations.

1. From (10), it holds for $i \in \{1, 2\}$ and every h small enough:

$$\lambda_i(h) = \frac{\alpha_1(h) + \alpha_2(h) + (-1)^i \sqrt{(\alpha_2(h) - \alpha_1(h))^2 + 4\varepsilon(h)^2}}{4\sqrt{h}} e^{-2\frac{H}{h}}, \qquad (51)$$

where $0 < \lambda_1(h) < \lambda_2(h)$ denote the two smallest eigenvalues of $L_{f,h}^{D,(0)}$. It then follows from (51), (50), and (12) that $4\sqrt{h}\lambda_1(h) e^{2\frac{H}{h}}$ and $4\sqrt{h}\lambda_2(h) e^{2\frac{H}{h}}$ admit a full asymptotic expansion in h when $\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 = \emptyset$ and in \sqrt{h} when $\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \neq \emptyset$.

2. From (10), since u_h is the principal eigenfunction of $L_{f,h}^{D,(0)}$ satisfying (7), one has for any h > 0 small enough:

– either $\varepsilon(h) = 0$, in which case one has necessarily $\alpha_1(h) \neq \alpha_2(h)$ (since $0 < \lambda_1(h) < \lambda_2(h)$) and then

$$u_h = \pm \varphi_i$$

where the functions φ_1 and φ_2 are defined by (46) and $i \in \{1, 2\}$ is such that $\alpha_i(h) = \min(\alpha_1(h), \alpha_2(h)),$

- or $\varepsilon(h) \neq 0$, in which case (51) and an elementary computation lead to

$$u_h = \pm \left(\frac{1}{\sqrt{1+\beta(h)^2}}\,\varphi_1 + \frac{\beta(h)}{\sqrt{1+\beta(h)^2}}\,\varphi_2\right),\tag{52}$$

where $\beta(h)$ is defined by

$$\beta(h) = -\frac{2\varepsilon(h)}{\alpha_2(h) - \alpha_1(h) + \sqrt{(\alpha_2(h) - \alpha_1(h))^2 + 4\varepsilon(h)^2}}.$$
(53)

We conclude this section by stating the following proposition which will also be needed to study the asymptotic behaviour when $h \to 0$ of the law of $X_{\tau_{\Omega}}$ when $X_0 \sim \nu_h$. It is the statement of [7, Proposition 65] in our specific setting.

Proposition 4. Let us assume that the hypothesis [**H-Well**] is satisfied. Let $(\psi_{i_j})_{(i,j)\in\bigcup_{p=1}^3\{p\}\times\{1,\ldots,\mathsf{n}_p\}}$ be defined by (46). Let Σ be an open subset of $\partial\Omega$ and $F \in L^{\infty}(\partial\Omega,\mathbb{R})$. One then has for every $(i,j)\in\bigcup_{p=1}^3\{p\}\times\{1,\ldots,\mathsf{n}_p\}$, when $h \to 0$,

$$\int_{\Sigma} F \,\psi_{i_j} \cdot n \, e^{-\frac{2}{\hbar}f} = \begin{cases} \mathcal{O}\big(h^{\frac{d-3}{4}}e^{-\frac{1}{\hbar}\min_{\partial\Omega}f}\big) & \text{if } i \in \{1,2\} \text{ and } z_{i,j} \in \overline{\Sigma} \\ \mathcal{O}\big(e^{-\frac{1}{\hbar}(\min_{\partial\Omega}f+c)}\big) & \text{if } i = 3 \text{ or } z_{i,j} \notin \overline{\Sigma}, \end{cases}$$

where the constant c > 0 is independent of h. Moreover, when $(i, j) \in \bigcup_{p=1}^{2} \{p\} \times \{1, \ldots, n_p\}, z_{i,j} \in \Sigma$, and F is C^{∞} around $z_{i,j}$, it holds

$$\int_{\Sigma} F \psi_{i_j} \cdot n \ e^{-\frac{2}{h}f} = \pi^{\frac{d-1}{4}} \frac{\sqrt{2 \partial_n f(z_{i,j})}}{\left(\det \operatorname{Hess} f|_{\partial\Omega}(z_{i,j})\right)^{\frac{1}{4}}} h^{\frac{d-3}{4}} \ e^{-\frac{1}{h} \min_{\partial\Omega} f} \left(F(z_{i,j}) + \mathcal{O}(h)\right)$$

where the above remainder term $\mathcal{O}(h)$ admits a full asymptotic expansion in h.

2.2 Proof of Theorem 1

In this Section, one proves Theorem 1. To this end, let us assume that the hypotheses **[H-Well]** and **[H1]**, with (16), are satisfied. Then, from (51), (11), and (12), one has in the limit $h \to 0$:

• when $\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 = \emptyset$, it holds $\varepsilon(h) = \mathcal{O}(e^{-\frac{c}{h}})$ for some c > 0 and then, for every $i \in \{1, 2\}$,

$$2\sqrt{h} e^{\frac{2}{h}H} \lambda_i(h) = \alpha_i(h) + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \sim \sum_{k=0}^{+\infty} \kappa_{i,k} h^k , \qquad (54)$$

• when $\partial \mathsf{C}_1 \cap \partial \mathsf{C}_2 \neq \emptyset$, it holds $\varepsilon(h) = \sqrt{h}$ and then, for every $i \in \{1, 2\}$,

$$2\sqrt{h} e^{\frac{2}{h}H} \lambda_i(h) = \alpha_i(h) + \mathcal{O}(h) = \kappa_{i,0} \left(1 + \mathcal{O}(\sqrt{h})\right), \tag{55}$$

where, the remainder term $\mathcal{O}(\sqrt{h})$ in (55) admits a full asymptotic expansion in \sqrt{h} .

Moreover, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$u_h = \pm \left(\frac{1}{\sqrt{1+\beta(h)^2}}\,\varphi_1 + \frac{\beta(h)}{\sqrt{1+\beta(h)^2}}\,\varphi_2\right),\tag{56}$$

where $\beta(h)$ is defined in (53) and (φ_1, φ_2) is defined in (46) (notice that (56) holds in $H^1_w(\Omega)$). Indeed, this is simply the relation (52) when $\varepsilon(h) \neq 0$. In addition, when $\varepsilon(h) = 0$ and $\alpha_2(h) > \alpha_1(h)$ (the latter relation follows from (16)), it holds $u_h = \pm \varphi_1$, that is precisely the relation (56) since in this case $\beta(h)$ is well defined and $\beta(h) = 0$ (see indeed (53)).

Since **[H1]** implies that $\lim_{h\to 0} \frac{\varepsilon(h)}{\alpha_1(h)-\alpha_2(h)} = 0$, one moreover obtains from (53) that in the limit $h \to 0$:

$$\beta(h) = \mathcal{O}\left(\frac{|\varepsilon(h)|}{\alpha_2(h) - \alpha_1(h)}\right).$$
(57)

From (56), (57) together with $u_h > 0$ on Ω , $\tilde{u}_1 \ge 0$ on Ω , (42), and (46), one has, for every h small enough: $\langle u_h, \tilde{u}_1 \rangle_{L^2_{u}} = 1 + o(1)$ and then

$$u_{h} = \left(1 + \mathcal{O}\left(\beta(h)^{2}\right)\right)\varphi_{1} + \mathcal{O}\left(|\beta(h)|\right)\varphi_{2}.$$
(58)

Therefore, using (42), (46), and (57), there exists c > 0 such that for every h small enough:

$$u_h = \left(1 + \mathcal{O}\left(\beta(h)^2\right)\right) \widetilde{u}_1 + \mathcal{O}\left(|\beta(h)|\right) \widetilde{u}_2 + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \text{ in } L^2_w(\Omega).$$
(59)

From (59), one deduces the following proposition which implies, using in addition (6) and (57), the asymptotic estimates (20) and (21) in Theorem 1.

Proposition 5. Let us assume that the hypotheses [*H*-Well] and [*H1*] together with (16) are satisfied. Let u_h be the principal eigenfunction of $L_{f,h}^{D,(0)}$ satisfying (7) and $(\tilde{u}_1, \tilde{u}_2)$ be the functions introduced in (38). Then, for every open set $O \subset \Omega$ and for every h > 0 small enough: *i)* When $O \cap \{x_1, x_2\} = \{x_1\}$, one has

$$\int_{O} u_h \ e^{-\frac{2}{h}f} = \left(1 + \mathcal{O}\left(\beta(h)^2\right) + \mathcal{O}\left(e^{-\frac{c}{h}}\right)\right) \int_{O} \widetilde{u}_1 \ e^{-\frac{2}{h}f}$$
$$= \frac{(h\pi)^{\frac{d}{4}}}{\left(\det \operatorname{Hess} f(x_1)\right)^{\frac{1}{4}}} e^{-\frac{1}{h}\min_{\overline{\Omega}}f} \ \left(1 + \mathcal{O}\left(\beta(h)^2\right) + \mathcal{O}(h)\right),$$

where c > 0 is independent of h and $\beta(h)$ satisfies (57).

ii) When $O \cap \{x_1, x_2\} = \{x_2\}$, *it holds*

$$\int_{O} u_h \ e^{-\frac{2}{h}f} = h^{\frac{d}{4}} \ e^{-\frac{1}{h}\min_{\overline{\Omega}}f} \ \mathcal{O}\left(|\beta(h)| + e^{-\frac{c}{h}}\right)$$

where we recall $\beta(h)$ satisfies (57) and c > 0 is independent of h.

iii) When $O \cap \{x_1, x_2\} = \emptyset$, it holds

$$\int_{O} u_h \ e^{-\frac{2}{h}f} = \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\overline{\Omega}} f + c)}\right), \ \text{where } c > 0 \text{ is independent of } h.$$

Proof. The relation (59) leads to

$$\int_{O} u_h \ e^{-\frac{2}{h}f} = \left(1 + \mathcal{O}\left(\beta(h)^2\right)\right) \int_{O} \widetilde{u}_1 \ e^{-\frac{2}{h}f} + \mathcal{O}\left(|\beta(h)|\right) \int_{O} \widetilde{u}_2 \ e^{-\frac{2}{h}f} + \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\overline{\Omega}} f + c)}\right),$$

where c > 0 is independent of h. In addition, one has, for $i \in \{1, 2\}$, $\tilde{u}_i = \frac{\chi_i}{\|\chi_i\|_{L^2_w}}$ from (38) and it follows from the Laplace method that there exists c > 0 such that for any $k \in \{1, 2\}$, when $h \to 0$,

$$\int_{O} \chi_{i}^{k} e^{-\frac{2}{h}f} = \begin{cases} \frac{(h\pi)^{\frac{d}{2}}}{\left(\det \operatorname{Hess} f(x_{i})\right)^{\frac{1}{2}}} e^{-\frac{2}{h}\min_{\overline{\Omega}}f} \left(1 + \mathcal{O}(h)\right) & \text{if } x_{i} \in \mathsf{O} \\ \mathcal{O}\left(e^{-\frac{2}{h}(\min_{\overline{\Omega}}f+c)}\right) & \text{if } x_{i} \notin \mathsf{O}. \end{cases}$$
(60)

The statement of Proposition 5 follows easily.

We also deduce from (58) and Proposition 3 together with (57) the following estimates.

Proposition 6. Let us assume that the hypotheses [**H**-Well] and [**H1**] together with (16) are satisfied. Let u_h be the principal eigenfunction of $L_{f,h}^{D,(0)}$ satisfying (7). Let also $(\tilde{u}_k)_{k \in \{1,2\}}$ and $(\tilde{\psi}_{i_j})_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1,...,n_p\}}$ be as in Proposition 2, and $(\psi_{i_j})_{(i,j) \in \bigcup_{p=1}^3 \{p\} \times \{1,...,n_p\}}$ be defined by (46). Then, there exists c > 0 such that in the limit $h \to 0$:

i) For every $j \in \{1, ..., n_1\}$,

$$\langle \nabla u_h, \psi_{1_j} \rangle_{L^2_w} = -C_{1,j,1}h^{-\frac{3}{4}}e^{-\frac{H}{h}}(1+\mathcal{O}(\beta(h)^2)+\mathcal{O}(h)),$$

where $C_{1,j,1}$ is defined in (41) and $\beta(h)$ satisfies (57).

ii) For every $j \in \{1, ..., m_3\}$,

$$\left\langle \nabla u_h, \psi_{3_j} \right\rangle_{L^2_w} = \mathcal{O}\left(h^{-\frac{1}{2}} e^{-\frac{H}{h}}\right),$$

iii) When i = 2 and $j \in \{1, ..., n_2\}$ or, i = 3 and $j \in \{m_3 + 1, ..., n_3\}$,

$$\left\langle \nabla u_h, \psi_{i_j} \right\rangle_{L^2_w} = h^{-\frac{3}{4}} e^{-\frac{H}{h}} \mathcal{O}\left(|\beta(h)| + e^{-\frac{c}{h}} \right).$$

We are now in position to prove Theorem 1.

End of the proof Theorem 1. To conclude the proof Theorem 1, it remains to prove (22), (23) and (24). Let assume that **[H-Well]** and **[H1]** hold with (16) and let us consider $F \in L^{\infty}(\partial\Omega, \mathbb{R})$. Let us recall that from (15), one has

$$\mathbb{E}^{\nu_h} \left[F(X_{\tau_\Omega}) \right] = -\frac{h}{2\lambda_1(h)} \frac{\int_{\partial\Omega} F \,\partial_n u_h \, e^{-\frac{2}{h}f}}{\int_{\Omega} u_h \, e^{-\frac{2}{h}f}}$$

Sharp asymptotic estimates when $h \to 0$ of $\lambda_1(h)$ and $\int_{\Omega} u_h e^{-\frac{2}{h}f}$ are respectively given in (54), (55) and in Proposition 5. Therefore, to prove (22), (23) and (24), it only remains to estimate when $h \to 0$, for an open subset Σ of $\partial\Omega$, the term $\int_{\Sigma} F \partial_n u_h e^{-\frac{2}{h}f}$.

Since the family $(\psi_{i_j})_{(i,j)\in\bigcup_{p=1}^3\{p\}\times\{1,\ldots,n_p\}}$ introduced in (46) is an orthonormal basis of $\operatorname{Ran} \pi_h^{(1)}$, it holds when $h \to 0$, from the Parseval identity and from Propositions 4 and 6,

$$\int_{\Sigma} F \,\partial_n u_h \, e^{-\frac{2}{h}f} = \sum_{(i,j)\in\bigcup_{p=1}^3 \{p\}\times\{1,\dots,\mathsf{n}_p\}} \left\langle \nabla u_h, \psi_{i_j} \right\rangle_{L^2_w} \int_{\Sigma} F \,\psi_{i_j} \cdot n \, e^{-\frac{2}{h}f} \quad (61)$$
$$= \sum_{(i,j)\in\bigcup_{p=1}^2 \{p\}\times\{1,\dots,\mathsf{n}_p\}} \left\langle \nabla u_h, \psi_{i_j} \right\rangle_{L^2_w} \int_{\Sigma} F \,\psi_{i_j} \cdot n \, e^{-\frac{2}{h}f} \\+ \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\partial\Omega} f + H + c)}\right), \quad (62)$$

for some c > 0 independent of h. When $\overline{\Sigma}$ does not contain any of the $z_{i,j}$'s for $(i,j) \in \bigcup_{p=1}^{2} \{p\} \times \{1, \ldots, \mathsf{n}_{p}\}$, one has, using again Propositions 4 and 6:

$$\int_{\Sigma} F \,\partial_n u_h e^{-\frac{2}{h}f} = \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\partial\Omega}f + H + c)}\right),\tag{63}$$

where c > 0 is independent of h.

Assume now that $\overline{\Sigma}$ does not contain any of the $z_{1,j}$'s for $j \in \{1, \ldots, n_1\}$. One then has in the limit $h \to 0$, using Propositions 4 and 6 and defining $H' := \min_{\partial \Omega} f + H:$

$$\int_{\Sigma} F \,\partial_n u_h \, e^{-\frac{2}{h}f} = \sum_{j=1}^{n_1} \mathcal{O}\left(h^{-\frac{3}{4}}e^{-\frac{H}{h}}\right) \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\partial\Omega}f+c)}\right) + \mathcal{O}\left(e^{-\frac{1}{h}(H'+c)}\right)$$
$$+ \sum_{j=1}^{n_2} \mathcal{O}\left(h^{-\frac{3}{4}}\left|\beta(h)\right|e^{-\frac{H}{h}}\right) \mathcal{O}\left(h^{\frac{d-3}{4}}e^{-\frac{1}{h}\min_{\partial\Omega}f}\right)$$
$$= \mathcal{O}\left(e^{-\frac{1}{h}(H'+c)}\right) + \mathcal{O}\left(h^{\frac{d-6}{4}}\left|\beta(h)\right|e^{-\frac{H'}{h}}\right), \tag{64}$$

where c > 0 is independent of h.

Finally, let us assume that $\Sigma \cap \{z_{1,1}, \ldots, z_{1,n_1}\} = \{z_{1,j}\}$ and F is C^{∞} around $z_{1,j}$. One then has, using (41), Propositions 4 and 6:

$$\int_{\Sigma} F \,\partial_n u_h \, e^{-\frac{2}{h}f} = \left\langle \nabla u_h, \psi_{1_j} \right\rangle_{L^2_w} \int_{\Sigma} F \,\psi_{1_j} \cdot n \, e^{-\frac{2}{h}f} + h^{\frac{d-6}{4}} e^{-\frac{H'}{h}} \,\mathcal{O}\left(|\beta(h)| + e^{-\frac{c}{h}}\right)$$
$$= -\frac{2 \,\pi^{\frac{d-2}{4}} \,\partial_n f(z_{1,j}) \left(\det \operatorname{Hess} f(x_1)\right)^{\frac{1}{4}}}{\left(\det \operatorname{Hess} f|_{\partial\Omega}(z_{1,j})\right)^{\frac{1}{2}}} \,h^{\frac{d-6}{4}} \, e^{-\frac{H'}{h}}$$
$$\times \left(F(z_{1,j}) + \mathcal{O}\left(|\beta(h)| + h\right)\right). \tag{65}$$

The estimates (22), (23) and (24), follows from (15) and (63)–(65), using in addition (57), (54), (55), and Proposition 5. This concludes the proof of Theorem 1.

2.3 Proofs of Theorems 2 and 3

Let us assume in this section that the hypotheses **[H-Well]** and **[H2]** are satisfied. We recall that **[H2]** means that there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\varepsilon(h) \neq 0 \text{ and } \lim_{h \to 0} \frac{\alpha_1(h) - \alpha_2(h)}{\varepsilon(h)} = 0.$$
 (66)

We then deduce from (51) the following:

• when $\partial C_1 \cap \partial C_2 = \emptyset$, using in addition (12) and the fact that $\varepsilon(h) = \mathcal{O}(e^{-\frac{c}{h}})$ for some c > 0 (see (11)), it holds when $h \to 0$:

$$\lambda_1(h) = \lambda_2(h) \left(1 + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \right), \tag{67}$$

and

$$2\sqrt{h} e^{\frac{2}{h}H} \lambda_1(h) \sim \sum_{k=0}^{+\infty} \kappa_{1,k} h^k, \tag{68}$$

• when $\partial C_1 \cap \partial C_2 \neq \emptyset$, using in addition (12), the fact that $\varepsilon(h) \approx \sqrt{h}$ (see (11)) and $\kappa_{1,0} = \kappa_{2,0}$ (see (26), (27) and (13)) it holds for $i \in \{1,2\}$ when $h \to 0$:

$$\lambda_i(h) = \kappa_{1,0} \frac{e^{-\frac{2}{h}H}}{2\sqrt{h}} \left(1 + \mathcal{O}(\sqrt{h})\right),\tag{69}$$

where, the remainder term $\mathcal{O}(\sqrt{h})$ in (69) admits a full asymptotic expansion in \sqrt{h} .

Remark 7. When there exists an isometry $\Phi : \overline{\Omega} \to \overline{\Omega}$ satisfying (34), i.e. such that $\Phi(x_1) = x_2$, $f \circ \Phi = f$, and $\Phi^2 = I$, it necessarily holds $\mathbf{n}_1 = \mathbf{n}_2$ and $\Phi(\{z_{1,1}, \ldots, z_{1,\mathbf{n}_1}\}) = \{z_{2,1}, \ldots, z_{2,\mathbf{n}_2}\}$. For every h > 0 small enough, it follows moreover from the simplicity of the eigenvalues $\lambda_1(h)$ and $\lambda_2(h)$ (see Remark 1) and from the positivity of u_h in Ω that $u_h \circ \Phi = u_h$ and $u_{2,h} \circ \Phi = -u_{2,h}$, where $u_{2,h}$ denotes any eigenvector of $L_{f,h}^{D,(0)}$ associated with $\lambda_2(h)$. In addition, one can choose χ_1 and χ_2 such that $\chi_2 = \chi_1 \circ \Phi$ in (38). This leads, for h small enough, to $\pi_h^{(0)} \widetilde{u}_1 + \pi_h^{(0)} \widetilde{u}_2 \in \text{Span}(u_h), \pi_h^{(0)} \widetilde{u}_1 - \pi_h^{(0)} \widetilde{u}_2 \in \text{Span}(u_{2,h})$ and hence to

$$\langle \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(0)} \widetilde{u}_1 \rangle_{L^2_w} = \langle \pi_h^{(0)} \widetilde{u}_2, \pi_h^{(0)} \widetilde{u}_2 \rangle_{L^2_w}$$

$$\langle L_{f,h}^{D,(0)} \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(0)} \widetilde{u}_1 \rangle_{L^2_w} = \langle L_{f,h}^{D,(0)} \pi_h^{(0)} \widetilde{u}_2, \pi_h^{(0)} \widetilde{u}_2 \rangle_{L^2_w}.$$

It then follows from (42), (47), and (10) that for h small enough, $\alpha_1(h) = \alpha_2(h)$ and hence, using $\lambda_1(h) \neq \lambda_2(h)$, that $\varepsilon(h) \neq 0$. The relation (66) is thus in particular satisfied in this situation.

Moreover, there exists h > 0 such that for all $h \in (0, h_0)$,

$$u_h = \pm \left(\frac{1}{\sqrt{1+\beta(h)^2}}\,\varphi_1 + \frac{\beta(h)}{\sqrt{1+\beta(h)^2}}\,\varphi_2\right),\tag{70}$$

where $\beta(h)$ is defined in (53) and (φ_1, φ_2) is defined in (46). This is indeed simply (52) since $\varepsilon(h) \neq 0$ according to (66). Using (66) and (53), one obtains moreover that when $h \to 0$:

$$\beta(h) = -\frac{|\varepsilon(h)|}{\varepsilon(h)} + \mathcal{O}\left(\frac{|\alpha_2(h) - \alpha_1(h)|}{|\varepsilon(h)|}\right).$$
(71)

From (70), (71) together with $u_h > 0$ on Ω , $\tilde{u}_1, \tilde{u}_2 \ge 0$ on Ω , (42), and (46), one has, for every h small enough, $\langle u_h, \tilde{u}_1 \rangle_{L^2_w} = \frac{1}{\sqrt{2}} + o(1)$ and $0 < \langle u_h, \tilde{u}_2 \rangle_{L^2_w} = -\frac{|\varepsilon(h)|}{\sqrt{2}\varepsilon(h)} + o(1)$. It follows that for every h small enough: $\varepsilon(h) < 0$,

$$\beta(h) = 1 + \mu(h), \text{ where } \mu(h) = \mathcal{O}\left(\frac{|\alpha_2(h) - \alpha_1(h)|}{|\varepsilon(h)|}\right) \to 0 \text{ when } h \to 0,$$
(72)

and

$$u_{h} = \frac{1}{\sqrt{2}} \left(1 + \mathcal{O}\left(|\mu(h)| \right) \right) \varphi_{1} + \frac{1}{\sqrt{2}} \left(1 + \mathcal{O}\left(|\mu(h)| \right) \right) \varphi_{2}.$$
(73)

Moreover, using (42), (46), and (72), the equality (73) implies that there exists c > 0 such that for every h small enough,

$$u_{h} = \frac{1}{\sqrt{2}} \left(1 + \mathcal{O}\left(|\mu(h)|\right) + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \right) \widetilde{u}_{1} + \frac{1}{\sqrt{2}} \left(1 + \mathcal{O}\left(|\mu(h)|\right) + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \right) \widetilde{u}_{2} + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \text{ in } L^{2}_{w}(\Omega).$$

$$(74)$$

From (73), one deduces the following proposition which implies, using in addition (6) and (72), the asymptotic estimates (29) and (30) in Theorem 2.

Proposition 7. Let us assume that the hypotheses [**H**-Well] and [**H**2] are satisfied. Let u_h be the principal eigenfunction of $L_{f,h}^{D,(0)}$ satisfying (7) and let $(\tilde{u}_j)_{j\in\{1,2\}}$ be the functions introduced in (38). Then, for any open subset O of Ω and for h > 0 small enough:

i) When, for some $i \in \{1, 2\}$, $\mathsf{O} \cap \{x_1, x_2\} = \{x_i\}$, it holds

$$\int_{\mathcal{O}} u_h \ e^{-\frac{2}{h}f} = \frac{1}{\sqrt{2}} \left(1 + \mathcal{O}(|\mu(h)|) + \mathcal{O}\left(e^{-\frac{c}{h}}\right) \right) \int_{\mathcal{O}} \widetilde{u}_i \ e^{-\frac{2}{h}f}$$
$$= \frac{1}{\sqrt{2}} \frac{(h\pi)^{\frac{d}{4}}}{\left(\det \operatorname{Hess} f(x_i)\right)^{\frac{1}{4}}} e^{-\frac{1}{h}\min_{\overline{\Omega}}f} \left(1 + \mathcal{O}(|\mu(h)|) + \mathcal{O}(h) \right),$$

where c > 0 is independent of h and $\mu(h)$ satisfies (72).

ii) When $O \cap \{x_1, x_2\} = \emptyset$, one has

$$\int_{O} u_h \ e^{-\frac{2}{h}f} = \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\overline{\Omega}}f+c)}\right), \ \text{where } c > 0 \text{ is independent of } h.$$

Proof. The proof of Proposition 7 is similar to that one of Proposition 5 using (74) instead of (59).

Remark 8. Let us assume as in Remark 7 that there exists an isometry Φ : $\overline{\Omega} \to \overline{\Omega}$ satisfying (34) and denote by $O_1 \subset \Omega$ and $O_2 \subset \Omega$ two disjoint open sets such that $x_i \in O_i$ for $i \in \{1, 2\}$. Using Proposition 7 and the fact that, for every h small enough, $\tilde{u}_1 \circ \Phi = \tilde{u}_2$, $\alpha_1(h) = \alpha_2(h)$ and hence $\mu(h) = 0$, it holds for $i \in \{1, 2\}$:

$$\int_{\Omega} u_h \ e^{-\frac{2}{h}f} = \left(1 + \mathcal{O}(e^{-\frac{c}{h}})\right) \int_{\mathsf{O}_1 \cup \mathsf{O}_2} u_h \ e^{-\frac{2}{h}f}$$
$$= \left(\sqrt{2} + \mathcal{O}(e^{-\frac{c}{h}})\right) \int_{\mathsf{O}_i} \widetilde{u}_i \ e^{-\frac{2}{h}f}.$$

This implies the first part of Theorem 3.

From (73) and Proposition 3, one deduces the following estimates.

Proposition 8. Let us assume that the hypotheses [**H**-Well] and [**H**2] are satisfied. Let u_h be the principal eigenfunction of $L_{f,h}^{D,(0)}$ satisfying (7). Let moreover $(\widetilde{u}_j)_{j \in \{1,2\}}$ and $(\widetilde{\psi}_{i_j})_{(i,j) \in \bigcup_{p=1}^2 \{p\} \times \{1,\ldots,n_p\}}$ be as in Proposition 2, and $(\psi_{i_j})_{(i,j) \in \bigcup_{p=1}^2 \{p\} \times \{1,\ldots,n_p\}}$ be defined by (46). Then, there exists c > 0 such that in the limit $h \to 0$:

i) For every $k \in \{1, 2\}$ and $j \in \{1, ..., n_k\}$,

$$\left\langle \nabla u_h, \psi_{k_j} \right\rangle_{L^2_w} = -\frac{C_{k,j,k}}{\sqrt{2}} h^{-\frac{3}{4}} e^{-\frac{H}{h}} \left(1 + \mathcal{O}(|\mu(h)|) + \mathcal{O}(h) \right),$$

where $C_{k,j,k}$ is defined in (41) and $\mu(h)$ satisfies (72).

ii) For every $j \in \{1, ..., m_3\}$,

$$\left\langle \nabla u_h, \psi_{3_j} \right\rangle_{L^2_w} = \mathcal{O}\left(h^{-\frac{1}{2}} e^{-\frac{H}{h}}\right).$$

iii) For every $j \in \{m_3 + 1, \dots, n_3\}$,

$$\left\langle \nabla u_h, \psi_{3_j} \right\rangle_{L^2_w} = \mathcal{O}\left(e^{-\frac{1}{h}(H+c)}\right)$$

End of the proofs Theorems 2 and 3. Let us assume that the hypotheses [H-Well] and [H2] are satisfied. It remains to prove the asymptotic estimates (32) and (33). We proceed as we did at the end of Section 2.2 to prove (22), (23), and (24). Let us then consider $F \in L^{\infty}(\partial\Omega, \mathbb{R})$.

Let us first assume that $\overline{\Sigma}$ does not contain any of the $z_{i,j}$'s for $(i, j) \in \bigcup_{p=1}^{2} \{p\} \times \{1, \ldots, n_p\}$. Then, using (61) together with Propositions 4 and 8, one has in the limit $h \to 0$:

$$\int_{\Sigma} F \,\partial_n u_h e^{-\frac{2}{h}f} = \mathcal{O}\left(e^{-\frac{1}{h}(\min_{\partial\Omega} f + H + c)}\right),\tag{75}$$

for some c > 0 independent of h.

Let us now assume that $\Sigma \cap \{z_{i,j}, (i,j) \in \bigcup_{p=1}^{2} \{p\} \times \{1, \dots, \mathsf{n}_{p}\}\} = \{z_{p,\ell}\}$ and that F is C^{∞} around $z_{p,\ell}$. Then, using again (61) together with Propositions 4 and 8, one has when $h \to 0$, defining $H' := \min_{\partial \Omega} f + H$,

$$\int_{\Sigma} F \,\partial_{n} u_{h} \,e^{-\frac{2}{h}f} = \left\langle \nabla u_{h}, \psi_{p_{\ell}} \right\rangle_{L^{2}_{w}} \int_{\Sigma} F \,\psi_{p_{\ell}} \cdot n \,e^{-\frac{2}{h}f} + \mathcal{O}\left(h^{\frac{d-6}{4}}e^{-\frac{1}{h}(H'+c)}\right) \\
= -\sqrt{2} \,\partial_{n} f(z_{p,\ell}) \,\frac{\left(\det \operatorname{Hess} f(x_{p})\right)^{\frac{1}{4}}}{\left(\det \operatorname{Hess} f|_{\partial\Omega}(z_{p,\ell})\right)^{\frac{1}{2}}} \,\pi^{\frac{d-2}{4}} \,h^{\frac{d-6}{4}} \,e^{-\frac{H'}{h}} \\
\times \left(F(z_{p,\ell}) + \mathcal{O}(|\mu(h)|) + \mathcal{O}(h)\right), \tag{76}$$

where c > 0 is independent of h and $\mu(h)$ satisfies (72). The asymptotic estimates (32) and (33) are then straightforward consequences of (15) and (75), (76), using in addition (68), (69), and Proposition 7. This concludes the proof of Theorems 2 and 3.

References

- D. Aristoff and T. Lelièvre. Mathematical analysis of temperature accelerated dynamics. *Multiscale Model. Simul.*, 12(1):290–317, 2014.
- [2] N. Berglund and S. Dutercq. The Eyring-Kramers law for Markovian jump processes with symmetries. J. Theoret. Probab., 29(4):1240–1279, 2016.
- [3] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein. Metastability in reversible diffusion processes. I. Sharp asymptotics for capacities and exit times. J. Eur. Math. Soc. (JEMS), 6(4):399–424, 2004.
- [4] A. Bovier, V. Gayrard, and M. Klein. Metastability in reversible diffusion processes. II. Precise asymptotics for small eigenvalues. J. Eur. Math. Soc. (JEMS), 7(1):69–99, 2005.
- [5] N. Champagnat and D. Villemonais. General criteria for the study of quasistationarity, 2017. ArXiv version : 1712.08092.
- [6] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, 2019. Arxiv version : 1902.03270.

- [7] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 1. J. Math. Pures Appl, 2019. In press: https://doi.org/10.1016/j.matpur.2019.06.003.
- [8] M. Dimassi and J. Sjostrand. Spectral asymptotics in the semi-classical limit. Number 268. Cambridge university press, 1999.
- [9] L.C. Evans. Partial differential equations, volume 19 of Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, second edition, 2010.
- [10] G. Gong, M. Qian, and Z. Zhao. Killed diffusions and their conditioning. Probability Theory and Related Fields, 80(1):151–167, 1988.
- [11] B. Helffer. Semiclassical analysis for the Schrödinger operator and applications, volume 1336 of Lecture Notes in Math. Springer-Verlag, Berlin, 1988.
- [12] B. Helffer, M. Klein, and F. Nier. Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach. *Mat. Contemp.*, 26:41–85, 2004.
- [13] B. Helffer and F. Nier. Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach: the case with boundary. *Mém. Soc. Math. Fr. (N.S.)*, (105):vi+89, 2006.
- [14] B. Helffer and J. Sjostrand. Multiple wells in the semi-classical limit. I. Communications in Partial Differential Equations, 9(4):337–408, 1984.
- [15] B. Helffer and J. Sjöstrand. Multiple wells in the semi-classical limit III - Interaction through non-resonant wells. *Mathematische Nachrichten*, 124(1):263–313, 1985.
- [16] B. Helffer and J. Sjöstrand. Puits multiples en limite semi-classique. II. Interaction moléculaire. Symétries. Perturbation. In Annales de l'IHP Physique théorique, volume 42, pages 127–212, 1985.
- [17] C. Le Bris, T. Lelièvre, M. Luskin, and D. Perez. A mathematical formalization of the parallel replica dynamics. *Monte Carlo Methods and Applications*, 18(2):119–146, 2012.
- [18] T. Lelièvre, D. Le Peutrec, and B. Nectoux. The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 2, 2019. In preparation.
- [19] T. Lelièvre and G. Stoltz. Partial differential equations and stochastic methods in molecular dynamics. Acta Numerica, 25:681–880, 2016.
- [20] L. Michel. About small eigenvalues of the Witten Laplacian. Pure Appl. Anal., 1(2):149–206, 2019.
- [21] D. Perez, E.D. Cubuk, A. Waterland, E. Kaxiras, and A.F. Voter. Longtime dynamics through parallel trajectory splicing. *Journal of chemical* theory and computation, 12(1):18–28, 2015.

- [22] R.G. Pinsky. On the convergence of diffusion processes conditioned to remain in a bounded region for large time to limiting positive recurrent diffusion processes. *The Annals of Probability*, 13(2):363–378, 1985.
- [23] G. Schwarz. Hodge decomposition a method for solving boundary value problems, volume 1607 of Lecture Notes in Math. Springer-Verlag, Berlin, 1995.
- [24] M.R. Sorensen and A.F. Voter. Temperature-accelerated dynamics for simulation of infrequent events. J. Chem. Phys., 112(21):9599–9606, 2000.