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► **To cite this version:**

Giacomo Di Gesù, Mauro Mariani. Full metastable asymptotic of the fisher information. SIAM Journal on Mathematical Analysis, 2017, 10.1137/16M1077805 . hal-01400800

HAL Id: hal-01400800

<https://hal.science/hal-01400800>

Submitted on 22 Nov 2016

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FULL METASTABLE ASYMPTOTIC OF THE FISHER INFORMATION

GIACOMO DI GESÙ AND MAURO MARIANI

ABSTRACT. We establish an expansion by Γ -convergence of the Fisher information relative to the reference measure $e^{-\beta V} dx$, where V is a generic multiwell potential and $\beta \rightarrow \infty$. The expansion reveals a hierarchy of multiple scales reflecting the metastable behavior of the underlying overdamped Langevin dynamics: distinct scales emerge and become relevant depending on whether one considers probability measures concentrated on local minima of V , probability measures concentrated on critical points of V , or generic probability measures on \mathbb{R}^d . We thus fully describe the asymptotic behavior of minima of the Fisher information over regular sets of probabilities. The analysis mostly relies on spectral properties of diffusion operators and the related semiclassical Witten Laplacian and covers also the case of a compact smooth manifold as underlying space.

1. INTRODUCTION

The Fisher information of a probability measure μ relative to a reference measure m on a smooth manifold is given by the expression

$$\mathcal{I}(\mu|m) := \frac{1}{2} \int \frac{|\nabla \varrho|^2}{\varrho} dm = 2 \int |\nabla \sqrt{\varrho}|^2 dm, \quad (1.1)$$

assuming that $\varrho := \frac{d\mu}{dm}$ exists and is sufficiently regular (see the precise Definition 3.1 below). This is a classical and ubiquitous object measuring the discrepancy between two measures and appearing in various fields as Statistics, Information Theory and Statistical Mechanics.

In the context of Statistical mechanics the reference measure usually appears in the form $m_\beta = e^{-\beta V} dx$, where V is a suitable potential describing the interaction in the model, β is a positive parameter, proportional to the inverse temperature and dx is the volume measure corresponding to the absence of interaction. The main interest often lies in the dynamical properties of the associated heat flow evolution featuring m_β as stationary measure. Under suitable regularity assumptions on V it may be described by the Fokker-Planck equation

$$\partial_t u = \Delta u + \beta \operatorname{div}(u \nabla V) \quad (1.2)$$

or, on a pathwise level, by the overdamped Langevin equation

$$\dot{X}_t = -\nabla V(X_t) + \sqrt{2\beta^{-1}} \dot{W}_t, \quad (1.3)$$

where W_t is Brownian motion. The Fisher information may enter the description and analysis of a Statistical Mechanics model in various ways: through functional

2010 *Mathematics Subject Classification.* 35P20, 28D20, 49J45, 60F10.

Key words and phrases. Fisher Information, Metastability, Γ -convergence, Semiclassical spectral theory, Witten Laplacian.

inequalities, prominently the Log-Sobolev and HWI inequality (see e.g. [1] and references therein and in particular [18] for the $\beta \rightarrow \infty$ regime considered here); as rate functional in Large deviation principles describing fluctuations of the empirical occupation measure of (1.3) when $t \rightarrow \infty$, [5]; or also as a tool to give an alternative construction of the dynamics (1.2) as gradient flow with respect to the relative entropy functional [12] (see also the discussion at the end of this introduction).

1.1. The low temperature regime and metastability. In this paper we study the asymptotic behaviour of the Fisher information relative to $m_\beta = e^{-\beta V} dx$ in the low temperature regime, that is $\beta \rightarrow \infty$. When the potential V admits several local minima, in this regime energy traps are created which slowdown the dynamics (1.3) around these minima and produce metastability effects.

In the heuristic picture, there are several relevant time scales that feature a non-trivial dynamics: on short time scales, i.e. when $t = t(\beta)$ grows slowly as a function of β , the system essentially follows the deterministic gradient flow with respect to the potential V . In particular, all critical points of V are absorbing for the limiting dynamics. On a longer time scale (see below), the process just lives on critical points; however on this scale stable critical points (that is, local minima of V) are absorbing for the dynamics (once visited, the system sticks there).

When observed on even larger time scales, typically exponentially large in β [9, Chap. 6.], even among the local minima distinctions become observable: on the long run, rare but sufficiently large fluctuations may occur that allow the process to climb the mountain pass which leads to another local minimum. This tunneling or metastable transition among local minima favors the passage from a minimum point to a deeper, energetically more convenient minimum point. Thus, on the long run, the deeper the local minimum, the more time the process will spend around it.

The reversible diffusion model (1.3) is a paradigmatic model for metastable phenomena, that show up in the dynamical behavior of a large variety of complex real world systems, and can be regarded as a mark of dynamical phase transitions. It is often a detailed theoretical and numerical analysis of metastability that allows for a proper upscaling of microscopic models - defined at the atomic or molecular level - to macroscopic descriptions catching experimental observations in materials science, biology and chemistry. We refer to Kramers' influential [14], to [10] and to [2, 16, 7] for recent brief reviews on some of the mathematical techniques used in the analysis of metastability.

One expects the metastable behavior to be encoded somehow in the asymptotic behavior of the Fisher information. We discuss below why Γ -convergence is the natural tool to characterize this asymptotic behavior, in particular in the context of metastability and convergence of multi-scale reversible dynamics. However, for the sake of readability, we first shortly describe our main result in Section 1.2 below, then informally explain how Γ -convergence can be used as a solid theoretical framework for metastability in Section 1.3, in particular in the context of large deviations of the occupation measure. We quickly review the applications of Γ -convergence in multi-scale gradient flows in Section 1.4 (see also [19] where Γ -convergence is exploited to upscale an essentially one-dimensional metastable Fokker-Planck equation). We recall the definition of Γ -convergence in Section 2.2 below, and refer to [4] for a systematic treatment.

1.2. Informal description of the main result. In this paper a full expansion in the sense of Γ -convergence of the Fisher information is established, which indeed features the complete cascade of metastable scales as informally described above. Using standard techniques, it is not hard to see that, under mild assumptions on the potential V , the rescaled Fisher information

$$I_\beta := \frac{1}{\beta^2} \mathcal{I}(\cdot | e^{-\beta V} dx) \tag{1.4}$$

Γ -converges (in the weak topology of probabilities) as $\beta \rightarrow \infty$ to the linear functional

$$I(\mu) := \frac{1}{2} \int d\mu(x) |\nabla V|^2(x).$$

On the dynamical level this corresponds to the convergence of the diffusion (1.2)-(1.3) to the deterministic transport along the gradient of V . Note that $Z_\beta^{-1} e^{-\beta V} dx$ is the unique minimizer of I_β , provided $Z_\beta = \exp(-\beta V) < \infty$. On the other hand, if V admits several critical points, $I(\mu)$ vanishes on any probability that is concentrated on such points.

This suggests that one may obtain a non-trivial Γ -limit also when multiplying I_β by a suitable diverging constant, so that, according to the heuristic picture described above, the new limiting functional vanishes only on probability measures concentrated on local minima. This is indeed the case, and βI_β also Γ -converges to a functional J with the mentioned properties (see Theorem 2.3 for its explicit characterization).

To capture the exponential scales associated with tunneling between local minima we iterate the same procedure: assuming that there is a unique global minimum point x_0 of V and labelling by $\{x_1, \dots, x_n\}$ the other local minimum points of V , we investigate for each $k = 1, \dots, n$ the Γ -limit of $\beta e^{\beta W_k} I_\beta$, where W_k is the mountain pass barrier which separates x_k from a deeper minimum (see Section 2 for precise definitions). Under generic assumptions, we prove that for each $k = 1, \dots, n$ also $\beta e^{\beta W_k} I_\beta$ Γ -converges to some J_k , which can again be explicitly characterized (see Theorem 2.3) and involves the prefactors already appearing in the famous Kramers formula for metastable critical times [14] (see also the Γ -convergence result in [19]). Since $J_k(\mu) = 0$ for all k 's iff $\mu = \delta_{x_0}$, this amounts to a full expansion of I_β by Γ -convergence (see [4, Chap. 1.10] and Section 2 of this paper). In other terms, as far as infima over closed and open sets are concerned (that is, in the sense of Γ -convergence)

$$I_\beta(\mu) \sim I(\mu) + \frac{1}{\beta} J(\mu) + \sum_{k=1}^n \frac{1}{\beta} e^{-\beta W_k} J_k(\mu). \tag{1.5}$$

As a consequence of (1.5) and the Donsker-Varadhan Large Deviations Principle [5] we infer that, in the sense of large deviations, it holds (see Corollary 2.5)

$$\mathbb{P} \left(\frac{1}{T} \int_0^T ds f(X_s) \sim \int d\mu(x) f(x), \forall f \right) \sim e^{-\beta T \left(I(\mu) + \frac{1}{\beta} J(\mu) + \sum_{k=1}^n \frac{e^{-\beta W_k}}{\beta} J_k(\mu) \right)}. \tag{1.6}$$

That is, we characterize the sharp asymptotic of the l.h.s. for every $\mu \in \mathcal{P}(\mathbb{R}^d)$.

To prove our main result (1.5) we take a spectral point of view and exploit results which were mainly developed in the context of the semiclassical spectral analysis of Schrödinger operators. Indeed, as highlighted by the expression on the

right hand side of (1.1), the Fisher information can be seen as a Dirichlet form on $L^2(dm)$ and thus be studied from a spectral point of view by considering the corresponding selfadjoint operator. When $m_\beta = e^{-\beta V} dx$ the latter is given by the diffusion operator

$$L_\beta = \Delta - \beta \nabla V \cdot \nabla. \quad (1.7)$$

It is well-known that a unitary transformation, sometimes called ground state transformation, turns the generator into a Schrödinger operator acting now on the flat space $L^2(dx)$. More precisely,

$$-e^{-\frac{1}{2}\beta V} L_\beta e^{\frac{1}{2}\beta V} = -\Delta + \frac{\beta^2}{4} |\nabla V|^2 - \frac{\beta}{2} \Delta V. \quad (1.8)$$

The latter operator is a specific Schrödinger operator. This operator coincides with the restriction on the level of functions of the Witten Laplacian, an operator acting on the full algebra of differential forms, considered by Witten in his celebrated paper [23]. Note that the small noise limit $\beta \rightarrow 0$ turns now into a problem in semiclassical analysis of Schrödinger operators. In this paper we use two important results, established in this framework: the approximation of the low-lying spectrum of Schrödinger operators via harmonic oscillators sitting at the bottom of the wells [21], and the fine analysis of the splitting of the exponentially small eigenvalues provided in [11]. For simplicity we restrict here to the case of \mathbb{R}^d or of a compact Riemannian manifold as state space, but our arguments could be adapted without much difficulty to the case of a bounded domain with reflecting (Neumann) boundary conditions, as considered e.g. in [19], by using [15] instead of [11].

1.3. Metastable dynamical systems. Here we informally describe some motivations to approach metastability via Γ -convergence of the Fisher information. By the Birkhoff ergodic theorem, time-averages of an observable of an ergodic (deterministic or random) dynamical system converge in the long time limit to the average of the same observable with respect to the invariant measure m of the system. Assume that we have a family of ergodic systems indexed by some parameter β , that for the sake of simplicity we may take as real number. Under very weak and general conditions, see e.g. [13], dynamical systems also satisfy a large deviation principle, that we informally write for each *fixed* β as

$$\mathbb{P}_\beta \left(\frac{1}{T} \int_0^T ds f(X_s) \sim \int d\mu(x) f(x), \forall f \right) \simeq \exp(-TE_\beta(\mu)), \quad T \gg 1, \quad (1.9)$$

where the *rate* $E_\beta(\mu) \geq 0$ is a positive real valued function defined on probability measures¹. For each fixed β , we assume that the system has good ergodic properties, i.e. $E_\beta(\mu) = 0$ iff $\mu = m_\beta$ is the invariant measure², so that (1.9) can be interpreted as a quantitative version of the Birkhoff theorem.

Suppose now that, informally speaking, a limiting behavior takes place as we move the parameter β to some limit, say $\beta \rightarrow \infty$. Then the invariant measure is

¹Notice that (1.9) makes sense both for random and deterministic systems, as in the latter case the initial distribution induces a probability measure on the trajectories of the system. In other words, for the deterministic systems, the l.h.s. of (1.9) should be interpreted as the measure of initial data such that $\int_0^T f(X_s) ds \sim \int d\mu(x) f(x)$.

²For the sake of simplicity we are assuming that at time 0 we start with distribution m_β . This assumption is usually not needed in the random case, but crucial for deterministic systems.

expected to converge to some limiting measure, $m_\beta \rightarrow m$. Similarly one expects concentration of time averages to take place in the parameter β as well, namely

$$\mathbb{P}_\beta \left(\frac{1}{T} \int_0^T ds f(X_s) \sim \int d\mu(x) f(x), \forall f \right) \simeq \exp(-T a_\beta I(\mu)), \quad T \gg 1, \beta \gg 1 \quad (1.10)$$

where a_β is a sequence of real numbers converging to $+\infty$. It is a general fact, see e.g. [17], that the functional I in (1.10) is nothing but the Γ -limit of $\frac{1}{a_\beta} E_\beta$. If ergodic properties of the system hold uniformly in β , one would expect that $I(\mu) = 0$ iff $\mu = m = \lim_\beta m_\beta$.

On the other hand, we say that the system exhibits a *metastable behavior* (on the scale (a_β)) in the limit $\beta \rightarrow \infty$, if the function $I(\mu) = \Gamma\text{-lim}_\beta \frac{1}{a_\beta} E_\beta$, vanishes on a set strictly larger than $\{m\}$. In other words, if there is a 'small-but-not-so-small' probability that, for T large and β large, the time average of observables does not behave as the spacial average w.r.t. the limiting invariant measure. In such a case, (1.10) states in particular that one needs to consider time scales much longer than a_β to observe convergence of the system to the invariant measure. If the system features a metastable behavior, (1.10) is not completely satisfactory. Indeed, one knows a priori that the l.h.s. should vanish if $\mu \neq m$ (as we sent $T \rightarrow \infty$ before β , and assumed $m_\beta \rightarrow m$), but the r.h.s. does not catch the sharp asymptotic if $I(\mu) = 0$ (and $\mu \neq m$). In other words, if $\mu \neq m$ and $I(\mu) = 0$ (1.10) just states that the l.h.s. vanishes on a slower scale than $\exp(-a_\beta T)$ but does not quantify this scale.

In this case, one would expect a further non-trivial expansion in the r.h.s. of (1.10), say for $T \gg 1, \beta \gg 1$

$$\mathbb{P}_\beta \left(\frac{1}{T} \int_0^T ds f(X_s) \sim \int d\mu(x) f(x), \forall f \right) \simeq \exp \left(-T a_\beta \left(I(\mu) + \frac{1}{b_\beta} J(\mu) \right) \right), \quad (1.11)$$

where $b_\beta \rightarrow \infty$ and $J(\mu)$ is such that $J(m) = 0$, $J(\mu) = \infty$ if $I(\mu) > 0$, and thus $J(\mu)$ gives the asymptotic value of the l.h.s. when $I(\mu) = 0$ and $\mu \neq m$. Actually, it may happen that for such μ 's, the l.h.s. in (1.11) vanishes at different rates, so that a further expansion of the exponent in the r.h.s. is necessary, until the exponential behavior of the l.h.s. at each and every point in $\{I(\mu) = 0\}$ is characterized, and a complete quantitative version of the ergodic convergence of averaged observables is recovered.

The discussion informally carried over above can be made very precise, since both large deviations and Γ -convergence always hold along subsequences, and thus (1.9) can actually be used as a rigorous definition of E_β , and the existence of a non-trivial development by Γ -convergence [4, Chap. 1.10] (or equivalently of multiple large deviations principles³ as in (1.11)) as a general definition of metastability. However we refrain from giving a too abstract formulation of these statements that are not instrumental to our results below.

³This should not be confused with what is called *large and moderate deviations* in the literature, which is not related to metastability. Here the observables are fixed once and for all, and not rescaled. And yet they feature multiple large deviations principles.

1.4. Multiscale gradient flows. The relative entropy $H(\mu)$ of the probability measure μ w.r.t. the reference measure $m = e^{-\beta V} dx$ is defined as

$$H_\beta(\mu) := \int dm \varrho \log \varrho, \quad \mu = \varrho m \quad (1.12)$$

It is a well-known fact [12] that the Fokker–Planck equation

$$\partial_t u = \Delta u + \beta \operatorname{div}(u \nabla V) \quad (1.13)$$

can be written as a gradient flow of the relative entropy H with respect to the 2-Wasserstein distance on probability measures on \mathbb{R}^d . Namely a curve $(\mu_\beta(t))$ of probability measures with bounded second moments on \mathbb{R}^d satisfies (1.13) iff

$$H_\beta(\mu_\beta(0)) \geq H_\beta(\mu_\beta(t)) + \frac{1}{2} \int_0^t \|\partial_s \mu_\beta(s)\|^2 ds + \frac{1}{2} \int_0^t |\nabla_{\mathcal{W}_2} H_\beta|^2(\mu_\beta(s)) ds \quad (1.14)$$

where $\|\cdot\|$ is the tangent norm on the 2-Wasserstein and, most importantly for us, the metric gradient $|\nabla_{\mathcal{W}_2} H_\beta|^2$ coincides with βI_β . Following the approach in [20], and dividing both sides of (1.14) by β , one wants to pass to the limit $\beta \rightarrow \infty$. Then, using the Γ -limit result $I_\beta \rightarrow I$ in Theorem 2.3, one easily gathers that any limit point $(\mu(t))$ of $(\mu_\beta(t))$ satisfies

$$\int V d\mu(0) \geq \int V d\mu(t) + \frac{1}{2} \int_0^t \|\partial_s \mu(s)\|^2 ds + \frac{1}{2} \int_0^t \int |\nabla V|^2 d\mu(s) ds, \quad (1.15)$$

provided the initial data satisfies $\frac{1}{\beta} H_\beta(\mu_\beta(0)) \rightarrow \int V d\mu(0)$. In other words, one recovers the simple fact that the solution u_β to (1.13) satisfies $u_\beta(t/\beta, x) \rightarrow u(t, x)$, where u solves the dual transport equation

$$\partial_t u = \operatorname{div}(u \nabla V). \quad (1.16)$$

Of course, if the initial data concentrates on critical points of V , (1.16) becomes trivial, namely $\partial_t u = 0$. Then the development by Γ -convergence gives the sharp asymptotic of $u_\beta(t/\beta^2)$ exactly in these cases. It turns out that, when the initial condition concentrates on local minima, even this limit is trivial, and still by the Γ -development one can establish the limit of $u_\beta(t/(\beta e^{\beta W_k}), x)$ where the W_k are appropriate constants defined in A.5 below. We do not pursue these problems here, since we plan a detailed study in the non-reversible case (namely when ∇V in (1.16) is replaced by a generic vector field) in a follow-up paper. See [19] for a detailed discussion on a similar model.

1.5. Plan of the paper. In Section 2 we introduce some definitions and state the main result. In Section 3, we shortly review some basic properties of the Fisher information functional. In Section 4 we consider suitable quasimodes associated to the generator L_β . In Section 5 we prove the Γ -convergence and equicoercivity results for the Fisher information. In Section 6 and Section 7 we prove the development by Γ -convergence of the Fisher information respectively under inverse power and exponential rescaling.

2. MAIN RESULT

2.1. Basic notation. Hereafter (M, g) is a smooth d -dimensional Riemannian manifold without boundary and with metric tensor g . We assume that either M is compact or that $M = \mathbb{R}^d$ and g is the canonical Euclidean tensor. Ω is the set

of smooth, compactly supported 1-forms over M . For $\psi \in \Omega$, ψ^2 is understood as $\langle \psi, \psi \rangle_g$, while ∇ , $\nabla \cdot$, Hess and Δ are the covariant gradient, the divergence, the Hessian and the (negative) Laplace-Beltrami operators on M . $\mathcal{P}(M)$ is the set of Borel probability measures on M , and it is naturally equipped with the weak topology of probability measures. If M is compact this is the weakest topology such that the map $\mu \mapsto \int d\mu f$ is continuous for all $f \in C(M)$. If M is not compact, the definition is slightly more involved, as one should require f to be bounded and uniformly continuous with respect to any totally bounded distance on M (this topology is independent on such a distance), see [22, Chap. 3.1]. In any case, $\mathcal{P}(M)$ is a Polish space (that is a completely metrizable, separable topological space), and it's compact if M is compact.

2.2. Γ -convergence. In this section we briefly recall the basic definitions related to Γ -convergence, see [4, Chap. 1]. For X a Polish space (we will always consider $X = \mathcal{P}(M)$) and (H_β) a family of lower semicontinuous functions on X indexed by the directed parameter β (we will always consider $\beta > 0$), one defines

$$\begin{aligned} (\Gamma\text{-}\underline{\lim}_\beta H_\beta)(x) &:= \inf \left\{ \underline{\lim}_\beta H_\beta(x_\beta), \{x_\beta\} \subset X : x_\beta \rightarrow x \right\}, \\ (\Gamma\text{-}\overline{\lim}_\beta H_\beta)(x) &:= \inf \left\{ \overline{\lim}_\beta H_\beta(x_\beta), \{x_\beta\} \subset X : x_\beta \rightarrow x \right\}. \end{aligned} \quad (2.1)$$

Whenever $\Gamma\text{-}\underline{\lim}_\beta H_\beta = \Gamma\text{-}\overline{\lim}_\beta H_\beta =: H$ we say that H_β Γ -converges to H in X . Equivalently, H_β Γ -converges to H iff for each $x \in X$:

- for any sequence $x_\beta \rightarrow x$ it holds $\underline{\lim}_\beta H_\beta(x_\beta) \geq H(x)$;
- there exists a sequence $x_\beta \rightarrow x$ such that $\overline{\lim}_\beta H_\beta(x_\beta) \leq H(x)$.

(H_β) is *equicoercive* if for each $M \in \mathbb{R}$ the set $\{\overline{\lim}_\beta H_\beta \leq M\}$ is precompact in X . If H_β is equicoercive and Γ -converges to H , then $A := \text{argmin}(H)$ contains each limit point of $\text{argmin}(H_\beta)$. Denote by A_0 the set of such limit points. If $A \setminus A_0$ is nonempty, there exists a diverging sequence $(a_\beta^{(1)})$ such that the functional

$$H_\beta^{(1)} := a_\beta^{(1)}(H_\beta - \inf_{x \in X} H_\beta(x)) \quad (2.2)$$

admits a non-trivial (that it having somewhere a value different from 0 and ∞) Γ -liminf. Notice that $H_\beta^{(1)}$ inherits from H_β the property of being equicoercive, and that $(\Gamma\text{-}\overline{\lim}_\beta H_\beta^{(1)})(x) = (\Gamma\text{-}\underline{\lim}_\beta H_\beta^{(1)})(x) = 0$ if $x \in A_0$ and $(\Gamma\text{-}\overline{\lim}_\beta H_\beta^{(1)})(x) = (\Gamma\text{-}\underline{\lim}_\beta H_\beta^{(1)})(x) = +\infty$ if $x \notin A$. If $H_\beta^{(1)}$ admits a Γ -limit $H^{(1)}$ then we say that the development by Γ -convergence

$$H_\beta \sim H + \frac{1}{a_\beta^{(1)}} H^{(1)} \quad (2.3)$$

holds. Iterating the procedure with sequences such that $a_\beta^{(k)}/a_\beta^{(k+1)} \rightarrow 0$, we say that the development by Γ -convergence is *full* if it holds

$$H_\beta \sim H + \sum_k \frac{1}{a_\beta^{(k)}} H^{(k)} \quad (2.4)$$

and for each $x \in A \setminus A_0$ there exists k such that $H^{(k)}(x) \in (0, \infty)$.

Equicoercivity and Γ -convergence of a sequence (H_β) imply an upper bound of infima over open sets, and a lower bound of infima over closed sets, see e.g. [4,

Prop. 1.18], and it is a relevant notion of variational convergence for the problems discussed in the introduction. A full development by Γ -convergence then gives a sharp asymptotic of each of such infima.

2.3. Assumptions on the potential. The *potential* V is a given real-valued function and we consider the following assumptions.

A.1 $V \in C^\infty(M)$ is a Morse function. Namely the Hessian of V is non-degenerate at any critical point of V .

A.2 In the case $M = \mathbb{R}^d$ (M is compact otherwise), it holds for some $\beta_0 \geq 0$

$$\lim_{x \rightarrow \infty} \inf_{\beta \geq \beta_0} \left(\frac{1}{4} |\nabla V|^2 - \frac{1}{2\beta} \Delta V \right)(x) = +\infty. \quad (2.5)$$

A.3 In the case $M = \mathbb{R}^d$ (M is compact otherwise), it holds for some $\beta_0 \geq 0$ and all $\beta \geq \beta_0$

$$Z_\beta := \int e^{-\beta V(x)} dx < +\infty. \quad (2.6)$$

Remark 2.1. If $M = \mathbb{R}^d$, **A.1-A.3** imply that $\lim_{|x| \rightarrow +\infty} V(x) = +\infty$ (see [11, Proposition 2.2]). Thus, in both cases of M compact and $M = \mathbb{R}^d$, the set $\{V \leq c\}$ is compact for all $c \geq \inf_{x \in M} V(x)$.

Remark 2.2. Assumption **A.2** says that, after the ground state transformation of the diffusion generator L_β and division by β^2 (see (1.7),(1.8)), the Schrödinger potential grows to infinity at infinity, uniformly in β .

Let \wp be the set of critical points of V , namely $z \in \wp$ iff $\nabla V(z) = 0$. By **A.1-A.2**, \wp is finite. Let $\wp_0 \subset \wp$ be the set of local minima of V and define $W: \wp_0 \rightarrow (0, \infty]$ as

$$W(x) := \inf_{y \neq x: V(y) \leq V(x)} \inf_{\gamma \in \Gamma(x,y)} \sup_{t \in [0,1]} V(\gamma(t)) - V(x), \quad (2.7)$$

where $\Gamma(x, y)$ is the set of continuous curves connecting x and y in time 1. In other words $W(x)$ is the lowest mountain pass to climb when going from x to a deeper minimum of V .

A.4 For each $x \in \wp_0$ such that $W(x) < +\infty$ there exists a unique point $\hat{x} \in \wp$ such that the two following conditions hold:

- (i) $V(\hat{x}) = V(x) + W(x)$.
- (ii) \hat{x} and x lie in the same connected component of the compact set $\{y \in M : V(y) \leq V(x) + W(x)\}$.

In other words, there is a unique saddle point \hat{x} such that all the optimal curves γ in the variational problem (2.7) pass through \hat{x} .

A.5 $W(x) \neq W(y)$ whenever $x \neq y$, $x, y \in \wp_0$.

By **A.5** we can label $\wp_0 = \{x_0, \dots, x_n\}$ by requiring

$$W_n < \dots < W_1 < W_0 = +\infty, \quad (2.8)$$

where we use the shorthand notation $W_i := W(x_i)$. Note that x_0 is the unique global minimizer of V and \hat{x}_i exists for $i \neq 0$ by **A.4**.

2.4. The Γ -development theorem. For $\beta \geq \beta_0$ define the reference measure m_β on M as

$$dm_\beta(x) = e^{-\beta V(x)} dx, \quad (2.9)$$

where dx is the Riemannian volume on M . The *Fisher information* at inverse temperature $\beta > 0$ is the functional (see Definition 3.1 and (3.6) for further details)

$$I_\beta: \mathcal{P}(M) \rightarrow [0, +\infty],$$

$$I_\beta(\mu) := \begin{cases} \frac{1}{2\beta^2} \int dm_\beta \frac{|\nabla \varrho|^2}{\varrho} & \text{if } \frac{d\mu}{dm_\beta} = \varrho; \\ +\infty & \text{otherwise.} \end{cases} \quad (2.10)$$

We are interested in the variational convergence of I_β in the low temperature regime, namely when $\beta \rightarrow \infty$. In order to describe our main result we need to define further notation.

For $z \in \wp$, we denote by $(\xi_i(z))_{i=1, \dots, d}$ the eigenvalues of $\text{Hess } V(z)$, labelled by ordering $\xi_1(z) \leq \xi_2(z) \leq \dots \leq \xi_d(z)$. Then define

$$\zeta: M \rightarrow [0, +\infty]$$

$$\zeta(z) := \begin{cases} \sum_{i=1}^d |\xi_i(z)| - \xi_i(z) = 2 \sum_{i: \xi_i(z) < 0} |\xi_i(z)| & \text{if } z \in \wp; \\ +\infty & \text{otherwise.} \end{cases} \quad (2.11)$$

For $k \geq 1$ and $x_k \in \wp_0$, the saddle point \hat{x}_k defined in A.4 is easily seen to satisfy $\xi_1(\hat{x}_k) < 0$ and $\xi_i(\hat{x}_k) > 0$ for $i \geq 2$. Recalling the labelling (2.8) we define for $k = 1, \dots, n$

$$\eta_k: M \rightarrow [0, +\infty]$$

$$\eta_k(x) := \begin{cases} 0 & \text{if } x \in \{x_0, \dots, x_{k-1}\}; \\ \frac{|\xi_1(\hat{x}_k)|}{\pi} \sqrt{\frac{\det(\text{Hess } V)(x_k)}{|\det(\text{Hess } V)(\hat{x}_k)|}} = \sqrt{\frac{|\xi_1(\hat{x}_k)| \prod_{i=1}^d \xi_i(x_k)}{\pi^2 \prod_{i=2}^d \xi_i(\hat{x}_k)}} & \text{if } x = x_k; \\ +\infty & \text{otherwise.} \end{cases} \quad (2.12)$$

The functions ζ and η_k are lower semicontinuous and coercive. Their expression naturally appears when studying the asymptotic behaviour of eigenvalues of L_β (see Theorem 4.1 and 4.5 for this interpretation). Our main result is the following.

Theorem 2.3. *Assume A.1-A.5. Then (I_β) is an equicoercive sequence of lower semicontinuous functionals. Moreover*

$$\Gamma\text{-}\lim_{\beta} I_\beta = I, \quad (2.13)$$

$$\Gamma\text{-}\lim_{\beta} \beta I_\beta = J, \quad (2.14)$$

$$\Gamma\text{-}\lim_{\beta} (\beta e^{\beta W_k} I_\beta) = J_k \quad \text{for } k = 1, \dots, n, \quad (2.15)$$

where the lower semicontinuous, coercive functionals $I, J, J_k: \mathcal{P}(M) \rightarrow [0, +\infty]$ are defined as

$$I(\mu) := \int d\mu(x) |\nabla V|^2(x). \quad (2.16)$$

$$J(\mu) = \int d\mu(x) \zeta(x) = \begin{cases} \sum_{y \in \wp} \alpha_y \zeta(y) & \text{if } \mu = \sum_{y \in \wp} \alpha_y \delta_y; \\ +\infty & \text{otherwise.} \end{cases} \quad (2.17)$$

$$J_k(\mu) = \int d\mu(x) \eta_k(x) = \begin{cases} \alpha_k \eta_k(x_k) & \text{if } \mu = \sum_{j=0}^k \alpha_j \delta_{x_j}; \\ +\infty & \text{otherwise.} \end{cases} \quad (2.18)$$

Remark 2.4. It holds $\inf_{\mu} I(\mu) = \inf_{\mu} J(\mu) = \inf_{\mu} J_k(\mu) = 0$. The number of minimizers of the functionals in the sequence I, J, J_n, \dots, J_1 decreases from $|\wp|$ to 1. More precisely we have

- $I(\mu) = 0$ iff $J(\mu) < +\infty$, namely iff μ is concentrated on \wp .
- $J(\mu) = 0$ iff $J_n(\mu) < +\infty$, namely iff μ is concentrated on \wp_0 .
- for $k = 1, \dots, n-1$, $J_{k+1}(\mu) = 0$ iff $J_k(\mu) < +\infty$, and finally $J_1(\mu) = 0$ iff $\mu = \delta_{x_0}$ (that is the unique limit point of m_{β} , the minimizer of I_{β}).

In other words, I_{β} admits the following full development by Γ -convergence, see [4, Chap. 1.10], as $\beta \rightarrow \infty$:

$$I_{\beta}(\mu) \sim I(\mu) + \frac{1}{\beta} J(\mu) + \sum_{k=1}^n \frac{1}{\beta} e^{-\beta W_k} J_k(\mu). \quad (2.19)$$

In particular the asymptotic behavior of infima of I_{β} on closed and open subsets is characterized by a finite and non-zero leading order, see [4, Theorem 1.18].

Corollary 2.5. Consider the diffusion process X^{β} defined through

$$\begin{aligned} \dot{X}_t^{\beta} &= -\nabla V(X_t^{\beta}) + \sqrt{2\beta^{-1}} \dot{W}_t \\ X^{\beta}(0) &= x_0. \end{aligned} \quad (2.20)$$

Equivalently, let X^{β} be the Markov process with generator $\beta^{-1}\Delta - \nabla V \cdot \nabla$, and starting at $x_0 \in M$. For $\beta, T > 0$, consider the empirical measure

$$\theta_{\beta, T} := \frac{1}{T} \int_0^T \delta_{X_t^{\beta}} dt \in \mathcal{P}(M). \quad (2.21)$$

In other terms, $\theta_{\beta, T}$ is the random probability measure on M such that for all test functions φ it holds $\int d\theta_{\beta, T}(\varphi) = \frac{1}{T} \int_0^T \varphi(X_t^{\beta}) dt$. Then, in the sense of large deviations [6], and in the limit $T \gg \beta \rightarrow +\infty$, $\theta_{\beta, T}$ satisfies (independently of x_0)

$$\mathbb{P}(\theta_{\beta, T} \sim \mu) \sim e^{-\beta T (I(\mu) + \frac{1}{\beta} J(\mu) + \sum_{k=1}^n \frac{e^{-\beta W_k}}{\beta} J_k(\mu))}. \quad (2.22)$$

More precisely, for all I -regular (respectively J -regular and J_k -regular) sets $\mathcal{A} \subset \mathcal{P}(M)$ it holds

$$\lim_{\beta \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{1}{\beta T} \log \mathbb{P}(\theta_{\beta, T} \in \mathcal{A}) = - \inf_{\mu \in \mathcal{A}} I(\mu), \quad (2.23)$$

$$\lim_{\beta \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{1}{T} \log \mathbb{P}(\theta_{\beta, T} \in \mathcal{A}) = - \inf_{\mu \in \mathcal{A}} J(\mu), \quad (2.24)$$

$$\lim_{\beta \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{e^{\beta W_k}}{T} \log \mathbb{P}(\theta_{\beta, T} \in \mathcal{A}) = - \inf_{\mu \in \mathcal{A}} J_k(\mu). \quad (2.25)$$

Proof. It is not hard to check that, under **A.1-A.3**, the hypotheses in [5] are satisfied, and thus for each fixed $\beta > 0$ the empirical measure $\theta_{\beta, T}$ satisfies a large deviations principle with rate βI_{β} as $T \rightarrow +\infty$. As well known and easy to prove, the rate function of the large deviations with speed $a_{\beta} T$, for the directed family $\theta_{\beta, T}$ as $T \rightarrow \infty$ and $\beta \rightarrow \infty$ is then given by the Γ -limit of $\frac{1}{a_{\beta}} \beta I_{\beta}$, see [17]. Thus the statement follows from Theorem 2.3 when using respectively $a_{\beta} = \beta$, $a_{\beta} = 1$ and $a_{\beta} = e^{-\beta W_k}$. \square

3. THE FISHER INFORMATION

In this section we shortly collect some basic facts concerning the Fisher information. We only sketch the proofs here since we just restate some facts in what is a well understood framework. In this section we omit the dependence on β for the sake of readability.

Definition 3.1. Let $V \in C^0(M)$. The Fisher information $I: \mathcal{P}(M) \rightarrow [0, +\infty]$ induced by V is defined as

$$I(\mu) = \sup_{\psi \in \Omega} \int d\mu \left(e^V \nabla \cdot \psi - \frac{1}{2} e^{2V} \psi^2 \right). \quad (3.1)$$

Define the measure $m \in \mathcal{P}(M)$ as $dm(x) = e^{-V(x)} dx$.

Remark 3.2. As a supremum of linear and continuous functionals, I is convex and lower semicontinuous. Moreover if $V \in C^1(M)$, the change of variable $\psi \rightarrow -e^{-V} \psi$ shows

$$\begin{aligned} I(\mu) &= \sup_{\psi \in \Omega} \int d\mu \left(\nabla V \cdot \psi - \nabla \cdot \psi - \frac{1}{2} |\psi|^2 \right) \\ &= \begin{cases} \frac{1}{2} \int dm \frac{|\nabla \varrho|^2}{\varrho} & \text{if } d\mu = \varrho dm \text{ and } \nabla \log \varrho \in L^2(\mu) \\ +\infty & \text{otherwise} \end{cases} \\ &= \begin{cases} \int dx \, 2|\nabla h|^2 + h^2 \left(\frac{|\nabla V|^2}{2} - \Delta V \right) & \text{if } d\mu = h^2 dx \text{ and } h \in H^1(M) \\ +\infty & \text{otherwise.} \end{cases} \end{aligned} \quad (3.2)$$

Let now

$$\tilde{\mathcal{P}}(M) := \left\{ \mu \in \mathcal{P}(M) : \frac{d\mu}{dm} \in C^2(M), \exists \varepsilon > 0 : \frac{d\mu}{dm} \geq \varepsilon \right\}. \quad (3.3)$$

Proposition 3.3. Assume that $Z := \int dx e^{-V(x)} < +\infty$ and $V \in C^1(M)$. Then I is the lower semicontinuous envelope of $\tilde{I}: \mathcal{P}(M) \rightarrow [0, +\infty]$ defined as

$$\tilde{I}(\mu) = \begin{cases} \frac{1}{2} \int dm \frac{|\nabla \varrho|^2}{\varrho} & \text{if } \mu \in \tilde{\mathcal{P}}(M) \\ +\infty & \text{otherwise.} \end{cases} \quad (3.4)$$

Proof. Since changing V to $V + \log Z$ does not change I , here we assume $Z = 1$. We need to prove that for each μ there exists $\mu^n \in \tilde{\mathcal{P}}(M)$ such that $\mu^n \rightarrow \mu$ and $\liminf_n \tilde{I}(\mu^n) \leq I(\mu)$. Otherwise said, that $\tilde{\mathcal{P}}(M)$ is I -dense in $\mathcal{P}(M)$. Setting

$$\mu^n = \left(1 - \frac{1}{n}\right)\mu + \frac{1}{n}m \quad (3.5)$$

one easily gathers $\mu^n \rightarrow \mu$ and $I(\mu^n) \leq \tilde{I}(\mu^n)$. Therefore it's enough to prove that $\tilde{\mathcal{P}}(M)$ is I -dense in the set of $\mu \in \mathcal{P}(M)$ with density bounded away from 0. This is immediate from the density of smooth functions in weighted Sobolev spaces. \square

In view of Remark 3.2, the functional I_β , already introduced in (2.10) and appearing in our main theorem, can be equivalently defined as

$$I_\beta(\mu) := \beta^{-2} I^{\beta V}, \quad (3.6)$$

where $I^{\beta V}$ is the Fisher information induced by βV as defined in Definition 3.1.

4. SPECTRAL ANALYSIS OF THE GENERATOR

In this section we denote by $\langle \cdot, \cdot \rangle$ the inner product in $L^2(m_\beta)$. Consider the operator

$$L_\beta f := \Delta f - \beta \nabla V \cdot \nabla f \quad (4.1)$$

defined for $f \in C_c^\infty(M)$. By [A.2](#) and standard results, it uniquely extends to a self-adjoint operator in $L^2(m_\beta)$ with compact resolvent. We still denote by L_β such an extension.

4.1. Quasimodes of the bounded spectrum. For $z \in \wp$ and $\underline{n} = (n_1, \dots, n_d) \in \mathbb{N}^d$ let

$$\lambda_{z, \underline{n}} := \frac{\zeta(z)}{2} + \sum_{k=1}^d n_k |\xi_k(z)|, \quad (4.2)$$

where ζ and the ξ_k 's are defined in Subsection [2.4](#). The set $(\lambda_{z, \underline{n}})_{\underline{n} \in \mathbb{N}^d}$ is nothing but the spectrum of a suitably rescaled quadratic approximation (i.e. of a harmonic oscillator) around the point $z \in \wp$ of the Schrödinger operator [\(1.8\)](#), see also the proof of Lemma [4.3](#) for this interpretation. Define also

$$S_\lambda := \{(z, \underline{n}) \in \wp \times \mathbb{N}^d : \lambda_{z, \underline{n}} = \lambda\}. \quad (4.3)$$

The following theorem conveniently resumes in our setting some of the main results obtained in the paper [\[21\]](#) in a more general framework of semiclassical Schrödinger operators. Throughout this Subsection [4.1](#) it is sufficient to assume just [A.1](#) and [A.2](#).

Theorem 4.1 (Bounded eigenvalues). *Fix $\Lambda > 0$. There exists $\varepsilon_\Lambda > 0$ such that for each $\varepsilon \in (0, \varepsilon_\Lambda)$ the following holds: there exists $\beta_\varepsilon > 0$ so that for $\beta \geq \beta_\varepsilon$*

$$\text{Spec}(-\frac{1}{\beta}L_\beta) \cap [0, \Lambda] \subset \bigcup_{\lambda: S_\lambda \neq \emptyset} (\lambda - \varepsilon, \lambda + \varepsilon) \cap [0, \Lambda]. \quad (4.4)$$

Moreover, for each $\lambda \in [0, \Lambda]$ such that $S_\lambda \neq \emptyset$, the cardinality of $\text{Spec}(-\frac{1}{\beta}L_\beta) \cap (\lambda - \varepsilon, \lambda + \varepsilon)$ equals, when each eigenvalue is counted with its multiplicity, the cardinality of S_λ .

This theorem states that in the limit $\beta \rightarrow \infty$, counting multiplicity, the spectrum of $-\frac{1}{\beta}L_\beta$ is well-approximated by the spectrum of the direct union of suitable Harmonic oscillators. It is necessary to fix a threshold Λ , since this harmonic approximation is not uniform for $\Lambda \rightarrow \infty$.

For $\lambda \geq 0$ and $\varepsilon > 0$ denote by

$$P_{\beta, \varepsilon, \lambda} := \mathbf{1}_{(\lambda - \varepsilon, \lambda + \varepsilon)}(-\frac{1}{\beta}L_\beta) \quad (4.5)$$

the spectral projection of $-\frac{1}{\beta}L_\beta$ associated to the interval $(\lambda - \varepsilon, \lambda + \varepsilon)$.

Proposition 4.2. *There exists an orthonormal base $(\Psi_{\beta, z, \underline{n}})_{z \in \wp, \underline{n} \in \mathbb{N}^d}$ of $L^2(m_\beta)$ such that for every $\varepsilon > 0, z \in \wp$ and $\underline{n} \in \mathbb{N}^d$ the following holds: there exists a $\beta_{\varepsilon, z, \underline{n}} > 0$ such that for $\beta > \beta_{\varepsilon, z, \underline{n}}$ and for every $\varphi \in C_b(M)$,*

$$\Psi_{\beta, z, \underline{n}} \in \text{Range}(P_{\beta, \varepsilon, \lambda_{z, \underline{n}}}), \quad (4.6)$$

$$\lim_{\beta} \int \Psi_{\beta, z, \underline{n}} \Psi_{\beta, z', \underline{n}'} \varphi dm_\beta = \begin{cases} \varphi(z) & \text{if } z = z' \text{ and } \underline{n} = \underline{n}' \\ 0 & \text{otherwise} \end{cases}. \quad (4.7)$$

We stress that eigenbases of L_β in general fail to satisfy (4.6)-(4.7), due to possible resonances (that is $\lambda_{z,\underline{n}} = \lambda_{z',\underline{n}'}$ for some $z \neq z'$ and $\underline{n}, \underline{n}'$). We prove the proposition after the preliminary Lemma 4.3.

Lemma 4.3. *For each $z \in \wp$, $\underline{n} \in \mathbb{N}^d$ there exists $\tilde{\Psi}_{\beta,z,\underline{n}} \in C_c^2(M)$ such that for every $\varphi \in C_b(M)$*

$$\lim_{\beta} \int |(-\frac{1}{\beta}L_\beta - \lambda_{z,\underline{n}})\tilde{\Psi}_{\beta,z,\underline{n}}(x)|^2 dm_\beta = 0, \quad (4.8)$$

$$\lim_{\beta} \int \tilde{\Psi}_{\beta,z,\underline{n}} \tilde{\Psi}_{\beta,z',\underline{n}'} \varphi dm_\beta = \begin{cases} \varphi(z) & \text{if } z = z' \text{ and } \underline{n} = \underline{n}' \\ 0 & \text{otherwise} \end{cases}. \quad (4.9)$$

Proof. First consider first the case $M = \mathbb{R}^d$. Define for $\beta > 0$ the differential operator (see also (1.8))

$$A_\beta := -\Delta + \frac{1}{4}\beta^2|\nabla V|^2 - \frac{1}{2}\beta\Delta V \quad (4.10)$$

and let for $z \in \wp$

$$H_{\beta,z} := -\Delta + \beta^2 Q_z - \beta C_z, \quad (4.11)$$

where

$$Q_z(x) = \frac{1}{4} \text{Hess}^2 V(z)(x-z) \cdot (x-z), \quad C_z = \frac{1}{2} \text{Trace}(\text{Hess} V(z)). \quad (4.12)$$

The operator $H_{\beta,z}$ extends to a self-adjoint operator in $L^2(dx)$, which is nothing but a harmonic oscillator shifted by the constant βC_z . In particular its spectrum is given by $(\beta \lambda_{z,\underline{n}})_{\underline{n} \in \mathbb{N}^d}$. Let now $(\Theta_{z,\underline{n}})_{\underline{n} \in \mathbb{N}^d}$ be a corresponding orthonormal basis of eigenfunctions of $H_{z,\beta=1}$; the $\Theta_{z,\underline{n}}$ are Hermite functions centered at z . It is easy to check that $(\Theta_{\beta,z,\underline{n}})_{\underline{n}}$ defined by

$$\Theta_{\beta,z,\underline{n}}(x) = \beta^{1/4} \Theta_{z,\underline{n}}(z + \sqrt{\beta}(x-z)) \quad (4.13)$$

is an orthonormal base of eigenfunctions of $H_{z,\beta}$ and

$$\lim_{\beta \rightarrow +\infty} \Theta_{\beta,z,\underline{n}}^2 dx = \delta_z(dx) \quad \text{in } \mathcal{P}(M). \quad (4.14)$$

Then define $\tilde{\Theta}_{\beta,z,\underline{n}}(x) := \frac{\chi_z(x)\Theta_{\beta,z,\underline{n}}(x)}{\sqrt{Z_{\beta,z,\underline{n}}}}$, where $\chi_z \in C_c^\infty(M; [0,1])$ is a smooth cut-off function such that $\chi \equiv 1$ on a ball $B_r(z)$ centered at z of radius r , and $\chi \equiv 0$ on $B_{2r}^c(z)$, where $r > 0$ is chosen sufficiently small (in particular such that the χ_z 's have pairwise disjoint supports).

It follows from Taylor expansion of the Schrödinger potential $\frac{1}{4}\beta^2|\nabla V|^2 - \frac{1}{2}\beta\Delta V$ that, as $x \rightarrow z$,

$$A_\beta = H_{\beta,z} + O(\beta^2|x-z|^3) + O(\beta|x-z|). \quad (4.15)$$

Thus one obtains

$$\begin{aligned} \int \left[(A_\beta - \beta \lambda_{z,\underline{n}}) \tilde{\Theta}_{\beta,z,\underline{n}}(x) \right]^2 dx = \\ \frac{1}{Z_{\beta,z,\underline{n}}} \int \left[\Theta_{\beta,z,\underline{n}} \Delta \chi_z + 2 \nabla \chi_z \cdot \nabla \Theta_{\beta,z,\underline{n}} \right. \\ \left. + (O(\beta^2|x-z|^3) + O(\beta|x-z|)) \chi_z \Theta_{\beta,z,\underline{n}} \right]^2 dx. \end{aligned} \quad (4.16)$$

Hence, using the explicit form of the $\Theta_{\beta,z,\underline{n}}$'s as Hermite functions centered at z , it follows by Laplace asymptotics that

$$\frac{1}{\beta^2} \int \left[(A_\beta - \beta \lambda_{z,\underline{n}}) \tilde{\Theta}_{\beta,z,\underline{n}}(x) \right]^2 dx = O(\beta^{-1}). \quad (4.17)$$

Moreover, from (4.14) and $L^2(dx)$ orthogonality of the Hermite functions $(\Theta_{z,\underline{n}})_n$ it easily follows for $\varphi \in C_b(M)$

$$\lim_{\beta} \int \tilde{\Theta}_{\beta,z,\underline{n}} \tilde{\Theta}_{\beta,z',\underline{n}'} \varphi dx = \begin{cases} \varphi(z) & \text{if } z = z' \text{ and } \underline{n} = \underline{n}' \\ 0 & \text{otherwise} \end{cases}. \quad (4.18)$$

Finally define $\tilde{\Psi}_{\beta,z,\underline{n}} = \tilde{\Theta}_{\beta,z,\underline{n}} e^{\frac{\beta V}{2}}$ and notice that

$$\int |(-\frac{1}{\beta} L_\beta - \lambda_{z,\underline{n}}) \tilde{\Psi}_{\beta,z,\underline{n}}(x)|^2 dm_\beta = \frac{1}{\beta^2} \int |(A_\beta - \beta \lambda_{z,\underline{n}}) \tilde{\Theta}_{\beta,z,\underline{n}}(x)|^2 dx$$

and

$$\int \tilde{\Psi}_{\beta,z,\underline{n}} \tilde{\Psi}_{\beta,z',\underline{n}'} \varphi dm_\beta = \int \tilde{\Theta}_{\beta,z,\underline{n}} \tilde{\Theta}_{\beta,z',\underline{n}'} \varphi dx.$$

Therefore (4.8) and (4.9) follow from (4.17) and (4.18).

The proof in the case of M a compact manifold follows from a straightforward adaptation of the previous arguments: since the Laplace-Beltrami operator in coordinates takes the form

$$\sum_{i,j} g^{ij} \partial_i \partial_j + \left(\partial_j g^{ij} + g^{ij} \partial_j \log \sqrt{\det g} \right) \partial_j, \quad (4.19)$$

using in particular local coordinates $\{y = y^{(z)}\}$ around each $z \in \wp$ such that the metric tensor is the identity in 0, leads (instead of (4.15)) to the local estimate

$$A_\beta = H_{\beta,z} + \sum_i [O(|y|) \partial_i \partial_i + O(1) \partial_i] + O(\beta^2 |y|^3) + O(\beta |y|). \quad (4.20)$$

Choosing r sufficiently small such that the support of χ_z is contained in the corresponding local chart $\{y^{(z)}\}$, one can argue as before through Laplace asymptotics and show that the additional terms appearing in (4.20) give again an $O(\beta)$ contribution. \square

Remark 4.4. Let T be a bounded operator on a Hilbert space H and let $u, v \in H$ be normalized. Then

$$|\langle v, Tv \rangle - \langle u, Tu \rangle| \leq 2 \|T\| \left(\sqrt{1 - \langle u, v \rangle^2} + \sqrt{1 - \langle u', v' \rangle^2} \right). \quad (4.21)$$

Proof. Write $v = \langle u, v \rangle u + (v - \langle u, v \rangle u)$ and notice $\|v - \langle u, v \rangle u\|_H = \sqrt{1 - \langle u, v \rangle^2}$. Using the inequality $\sqrt{1 - a^2} \sqrt{1 - a'^2} + \sqrt{1 - aa'} \leq \sqrt{1 - a^2} + \sqrt{1 - a'^2}$ for $a = \langle u, v \rangle$ and $a' = \langle u', v' \rangle$ one gets the result by straightforward linear algebra. \square

Proof of Proposition 4.2. We use the same notation as in Theorem 4.1. Fix $\Lambda > 0$ large enough. For $\lambda < \Lambda$ such that $S_\lambda \neq \emptyset$, for $(z, \underline{n}) \in S_\lambda$ take $\tilde{\Psi}_{\beta,z,\underline{n}}$ as in Lemma 4.3. Define $\bar{\Psi}_{\beta,z,\underline{n}} := P_{\beta,\varepsilon_\Lambda,\lambda} \tilde{\Psi}_{\beta,z,\underline{n}}$ as the spectral projection of $\tilde{\Psi}_{\beta,z,\underline{n}}$ corresponding to the interval $(\lambda - \varepsilon_\Lambda, \lambda + \varepsilon_\Lambda)$, see (4.5).

Now for $(z, \underline{n}), (z', \underline{n}') \in S_\lambda$, since $P_{\beta,\varepsilon_\Lambda,\lambda}$ is a projector,

$$\begin{aligned} & \langle \bar{\Psi}_{\beta,z,\underline{n}}, \bar{\Psi}_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)} = \\ & \langle \tilde{\Psi}_{\beta,z,\underline{n}}, \tilde{\Psi}_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)} - \langle \tilde{\Psi}_{\beta,z,\underline{n}} - \bar{\Psi}_{\beta,z,\underline{n}}, \tilde{\Psi}_{\beta,z',\underline{n}'} - \bar{\Psi}_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)}. \end{aligned} \quad (4.22)$$

The definition of $\bar{\Psi}_{\beta,z,\underline{n}}$ readily implies

$$\begin{aligned} \|\tilde{\Psi}_{\beta,z,\underline{n}} - \bar{\Psi}_{\beta,z,\underline{n}}\|_{L^2(m_\beta)} &= \|(I - P_{\beta,\varepsilon_\Lambda,\lambda})\tilde{\Psi}_{\beta,z,\underline{n}}\|_{L^2(m_\beta)} \\ &\leq \frac{1}{\varepsilon_\Lambda} \|(-\frac{1}{\beta}L_\beta - \lambda_{z,\underline{n}})\tilde{\Psi}_{\beta,z,\underline{n}}\|_{L^2(m_\beta)}. \end{aligned} \quad (4.23)$$

In view of (4.8) this vanishes as $\beta \rightarrow \infty$. Therefore the last term in (4.22) vanishes as $\beta \rightarrow \infty$ and (4.9) now gives

$$\lim_{\beta} \langle \bar{\Psi}_{\beta,z,\underline{n}}, \bar{\Psi}_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)} = \begin{cases} 1 & \text{if } z = z' \text{ and } \underline{n} = \underline{n}' \\ 0 & \text{otherwise.} \end{cases} \quad (4.24)$$

In particular for β large enough the $(\bar{\Psi}_{\beta,z,\underline{n}})_{(z,\underline{n}) \in S_\lambda}$ are linearly independent, and span $\text{Range}(P_{\beta,\varepsilon_\Lambda,\lambda})$ by Theorem 4.1. Now construct $(\Psi_{\beta,z,\underline{n}})_{(z,\underline{n}) \in S_\lambda}$ by applying the Gram-Schmidt procedure on $(\bar{\Psi}_{\beta,z,\underline{n}})_{(z,\underline{n}) \in S_\lambda}$. From (4.24) and Lemma 4.3-(ii) (with $\varphi \equiv 1$) it follows that

$$\lim_{\beta} \langle \tilde{\Psi}_{\beta,z,\underline{n}}, \Psi_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)} = \begin{cases} 1 & \text{if } z = z' \text{ and } \underline{n} = \underline{n}' \\ 0 & \text{otherwise} \end{cases}. \quad (4.25)$$

Now apply Remark 4.4 with $H = L^2(m_\beta)$, $v = \Psi_{\beta,z,\underline{n}}$, $v' = \Psi_{\beta,z',\underline{n}'}$, $u = \tilde{\Psi}_{\beta,z,\underline{n}}$, $u' = \tilde{\Psi}_{\beta,z',\underline{n}'}$ and $T \equiv T_\varphi$ the pointwise multiplication by φ to get

$$\begin{aligned} &\left| \langle \Psi_{\beta,z,\underline{n}}, \varphi \Psi_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)} - \langle \tilde{\Psi}_{\beta,z,\underline{n}}, \varphi \tilde{\Psi}_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)} \right| \leq \\ &2 \|\varphi\|_\infty \left(\sqrt{1 - \langle \tilde{\Psi}_{\beta,z,\underline{n}}, \Psi_{\beta,z,\underline{n}} \rangle_{L^2(m_\beta)}} + \sqrt{1 - \langle \tilde{\Psi}_{\beta,z',\underline{n}'}, \Psi_{\beta,z',\underline{n}'} \rangle_{L^2(m_\beta)}} \right). \end{aligned} \quad (4.26)$$

Thus we obtain (4.7) from Lemma 4.3-(ii) and (4.25).

Thus the $(\Psi_{\beta,z,\underline{n}})_{(z,\underline{n}) \in S_\lambda}$ are an orthonormal base of $\text{Range}(P_{\beta,\varepsilon_\Lambda,\lambda})$ satisfying (4.7). Since this holds for any λ such that S_λ is not empty and $L^2(m_\beta)$ is a direct sum of eigenspaces of L_β , the $(\Psi_{\beta,z,\underline{n}})_{(z,\underline{n}) \in S_\lambda}$ are an orthonormal base of $L^2(m_\beta)$ as λ runs over the positive real numbers such that S_λ is nonempty. \square

4.2. Eigenfunctions of the split spectrum. We denote by $\ell_{\beta,0}, \dots, \ell_{\beta,n}$ the first $n+1$ eigenvalues of $-\frac{1}{\beta}L_\beta$ counted with multiplicity. It follows from the smoothness of V , A.2, A.3 and general principles that $\ell_{\beta,0}$ equals zero for every β and is simple with constant eigenfunction $\Phi_{\beta,0} \equiv 1/\sqrt{Z_\beta}$. Moreover, with the notation of the previous Subsection 4.1, $\lambda_{x,\underline{0}} = 0$ whenever $x \in \wp_0$ is a local minimum, and $\lambda_{z,\underline{n}} > 0$ otherwise. It follows then from Theorem 4.1 that there exist $\varepsilon > 0$ and $\beta_0 > 0$ such that for each $\beta \geq \beta_0$

$$\text{Spec}(-\frac{1}{\beta}L_\beta) \cap [0, \varepsilon] = \{\ell_{\beta,0} = 0, \ell_{\beta,1}, \dots, \ell_{\beta,n}\}. \quad (4.27)$$

It is not difficult to see that the eigenvalues $\ell_{\beta,1}, \dots, \ell_{\beta,n}$ are indeed exponentially small in β . A much stronger statement, giving the precise leading behaviour of the $\ell_{\beta,k}$'s in a general setting encompassing hypotheses A.1-A.5, was given in [11], (see also [3] and [8]). The following theorem conveniently resumes in our framework a weak version of the main result in [11].

Theorem 4.5 (Low-lying eigenvalues). *For $k = 1, \dots, n$ the eigenvalue $\ell_{\beta,k}$ is simple, admits a normalized eigenfunction $\Phi_{\beta,k} \in C^\infty(M)$ and satisfies, for η_k as*

in (2.12),

$$\lim_{\beta} e^{\beta W_k} \ell_{\beta,k} = \frac{1}{2} \eta_k(x_k). \quad (4.28)$$

Lemma 4.6. *For $k = 1, \dots, n$ there exists $\tilde{\Phi}_{\beta,k} \in C_c^\infty(M)$ with $\|\tilde{\Phi}_{\beta,k}\|_{L^2(m_\beta)} = 1$, such that*

- (i) *the probability measure $\tilde{\Phi}_{\beta,k}^2 dm_\beta$ converges to δ_{x_k} in $\mathcal{P}(M)$.*
- (ii) $\lim_{\beta \rightarrow \infty} \langle \tilde{\Phi}_{\beta,k}, \Phi_{\beta,k} \rangle^2 = 1$.

Proof. In this proof the W_k 's are defined as in A.4-A.5, and we set for convenience $W_{n+1} = 0$ and $\ell_{\beta,n+1} = \varepsilon$, with ε as in (4.27) (notice that this is *not* an eigenvalue of $-\frac{1}{\beta}L_\beta$).

Fix $\delta > 0$ such that

$$\delta < \min_{k=1, \dots, n} (W_k - W_{k+1}). \quad (4.29)$$

Let $B_k \subset M$, respectively $B_{k,\delta}$, be the connected component of $V^{-1}((-\infty, V(\hat{x}_k)))$, respectively $V^{-1}((-\infty, V(\hat{x}_k) - \delta))$, containing x_k . The B_k 's are precompact by Remark 2.1, and the closure of $B_{k,\delta}$ is contained in B_k . In particular there exists $\chi_k \in C_c^\infty(M; [0, 1])$ such that $\chi_k \equiv 1$ on $B_{k,\delta}$ and $\chi_k \equiv 0$ on $M \setminus B_k$.

For $k = 1, \dots, n$ define $\tilde{\Phi}_{\beta,k} = \chi_k / \sqrt{Z_{\beta,k}}$ where

$$Z_{\beta,k} = \int e^{-\beta V(x)} \chi_k^2(x) dx. \quad (4.30)$$

$V(x_k)$ is the unique minimum of $V(x)$ on B_k , and $\chi(x_k) = 1$. Therefore (i) holds. By Laplace principle

$$\lim_{\beta} \frac{1}{\beta} \log Z_{\beta,k} = -V(x_k), \quad (4.31)$$

$$\lim_{\beta} \langle \tilde{\Phi}_{\beta,j}, \tilde{\Phi}_{\beta,k} \rangle = 0 \quad j, k = 1, \dots, n, \quad j \neq k, \quad (4.32)$$

$$\lim_{\beta} \langle \tilde{\Phi}_{\beta,0}, \tilde{\Phi}_{\beta,k} \rangle = 0 \quad k = 1, \dots, n. \quad (4.33)$$

Notice moreover

$$\inf_{x: |\nabla \chi_k(x)| > 0} V(x) \geq V(\hat{x}_k) - \delta = V(x_k) + W_k - \delta. \quad (4.34)$$

Denote now by $P_{\beta,k} := \mathbf{1}_{[\ell_{\beta,k+1}, +\infty)}(-\frac{1}{\beta}L_\beta)$ the spectral projection of $-\frac{1}{\beta}L_\beta$ associated to the interval $[\ell_{\beta,k+1}, +\infty)$. By spectral decomposition

$$P_{\beta,k} \Phi = \Phi - \sum_{j=0}^k \langle \Phi, \Phi_{\beta,j} \rangle \Phi_{\beta,j}, \quad \forall \Phi \in L^2(m_\beta). \quad (4.35)$$

The Markov inequality for spectral projections, an integration by parts and (4.34) yield

$$\begin{aligned} \left\| P_{\beta,k} \tilde{\Phi}_{\beta,k} \right\|_{L^2(m_\beta)}^2 &\leq \frac{1}{\ell_{\beta,k+1}} \langle \tilde{\Phi}_{\beta,k}, -L_\beta \tilde{\Phi}_{\beta,k} \rangle = \frac{1}{\ell_{\beta,k+1} Z_{\beta,k}} \int |\nabla \chi_k|^2(x) e^{-\beta V(x)} dx \\ &\leq C_k \frac{\exp(-\beta(V(x_k) + W_k - \delta))}{\ell_{\beta,k+1} Z_{\beta,k}}, \end{aligned} \quad (4.36)$$

where $C_k = \int |\nabla \chi_k|^2(x) dx < \infty$. The estimates of $\ell_{\beta, k+1}$ and $Z_{\beta, k}$ provided respectively in (4.28) and (4.31), and the choice (4.29) of δ thus imply

$$\lim_{\beta} \left\| P_{\beta, k} \tilde{\Phi}_{\beta, k} \right\|_{L^2(m_{\beta})} = 0. \quad (4.37)$$

Taking the scalar product with $\tilde{\Phi}_{\beta, k}$ in both sides of (4.35) calculated for $\Phi = \tilde{\Phi}_{\beta, k}$, gives

$$\begin{aligned} 1 - \langle \tilde{\Phi}_{\beta, k}, \Phi_{\beta, k} \rangle^2 &= \langle \tilde{\Phi}_{\beta, k}, P_{\beta, k} \tilde{\Phi}_{\beta, k} \rangle + \sum_{j=0}^{k-1} \langle \tilde{\Phi}_{\beta, k}, \Phi_{\beta, j} \rangle^2 \\ &= \|P_{\beta, k} \tilde{\Phi}_{\beta, k}\|_{L^2(m_{\beta})}^2 + \langle \tilde{\Phi}_{\beta, k}, \Phi_{\beta, 0} \rangle^2 \\ &\quad + \sum_{j=1}^{k-1} \left(\langle \tilde{\Phi}_{\beta, j}, \Phi_{\beta, j} \rangle \langle \tilde{\Phi}_{\beta, k}, \tilde{\Phi}_{\beta, j} \rangle \right. \\ &\quad \left. + \langle \tilde{\Phi}_{\beta, k}, \Phi_{\beta, j} - \langle \tilde{\Phi}_{\beta, j}, \Phi_{\beta, j} \rangle \tilde{\Phi}_{\beta, j} \rangle \right)^2 \\ &\leq \|P_{\beta, k} \tilde{\Phi}_{\beta, k}\|_{L^2(m_{\beta})}^2 + \langle \tilde{\Phi}_{\beta, k}, \Phi_{\beta, 0} \rangle^2 \\ &\quad + 2 \sum_{j=1}^{k-1} \langle \tilde{\Phi}_{\beta, k}, \tilde{\Phi}_{\beta, j} \rangle^2 + 1 - \langle \tilde{\Phi}_{\beta, j}, \Phi_{\beta, j} \rangle^2 \\ &= o_{\beta}(1) + 2 \sum_{j=1}^{k-1} \left(1 - \langle \tilde{\Phi}_{\beta, j}, \Phi_{\beta, j} \rangle^2 \right), \end{aligned} \quad (4.38)$$

where in the last line we used (4.32), (4.33) and (4.37).

In order to prove (ii), we now proceed by finite induction over k . The statement (ii) holds for $k = 1$ as the sum in the last line of (4.38) is actually empty. But then from (4.38) one immediately yields the inductive step. \square

Proposition 4.7. *For $k = 0, \dots, n$ let $\Phi_{\beta, k}$ be a normalized eigenfunction corresponding to $\ell_{\beta, k}$ and define the probability measure $m_{\beta, k}$ by*

$$dm_{\beta, k} = \Phi_{\beta, k}^2 dm_{\beta}. \quad (4.39)$$

Then $m_{\beta, k}$ converges to δ_{x_k} in $\mathcal{P}(M)$ as $\beta \rightarrow \infty$. In particular for $h \neq k$ it holds

$$\lim_{\beta} \int |\Phi_{\beta, h} \Phi_{\beta, k}| dm_{\beta} = 0. \quad (4.40)$$

Proof. The statement (4.39) is immediate for $k = 0$, since we assumed x_0 to be the unique global minimizer of V . Let $k \geq 1$, take $\tilde{\Phi}_{\beta, k}$ as in Lemma 4.6 and fix a test function $\varphi \in C_b(M)$. Now apply Remark 4.4 with $H = L^2(m_{\beta})$, $v = v' = \Phi_{\beta, k}$, $u = u' = \tilde{\Phi}_{\beta, k}$, and $T \equiv T_{\varphi}$ the pointwise multiplication by φ . We get from (4.21)

$$\begin{aligned} \left| \int \varphi dm_{\beta, k} - \int \varphi \tilde{\Phi}_{\beta, k}^2 dm_{\beta} \right| &= \left| \langle \Phi_{\beta, k}, T_{\varphi} \Phi_{\beta, k} \rangle - \langle \tilde{\Phi}_{\beta, k}, T_{\varphi} \tilde{\Phi}_{\beta, k} \rangle \right| \\ &\leq 4 \|\varphi\|_{C(M)} \sqrt{1 - \langle \tilde{\Phi}_{\beta, k}, \Phi_{\beta, k} \rangle^2}. \end{aligned} \quad (4.41)$$

This vanishes by Lemma 4.6-(ii). Therefore by Lemma 4.6-(i)

$$\lim_{\beta} \int \varphi dm_{\beta,k} = \lim_{\beta} \int \varphi \tilde{\Phi}_{\beta,k}^2 dm_{\beta}(x) = \varphi(x_k), \quad (4.42)$$

namely $m_{\beta,k} \rightarrow \delta_{x_k}$ as $\beta \rightarrow \infty$. Now (4.40) is an immediate consequence of this fact, since for $E \subset M$ a neighborhood of x_h not containing x_k

$$\int |\Phi_{\beta,h} \Phi_{\beta,k}| dm_{\beta} \leq \left(\int_E |\Phi_{\beta,k}|^2 dm_{\beta} \right)^{1/2} + \left(\int_{E^c} |\Phi_{\beta,h}|^2 dm_{\beta} \right)^{1/2}, \quad (4.43)$$

and both terms vanish as $\beta \rightarrow \infty$. \square

5. Γ -CONVERGENCE OF I_{β}

Proposition 5.1. *Assume $V \in C^2(M)$ and A.2. Then (I_{β}) is equicoercive.*

Proof. Let $R(x) := \inf_{\beta \geq \beta_0} |\nabla V|^2(x) - \frac{2}{\beta} \Delta V(x)$. Taking $\psi = \beta \nabla V$ in the first line of (3.2) and recalling (3.6), one obtains for $\beta \geq \beta_0$ and each $\mu \in \mathcal{P}(M)$,

$$\begin{aligned} I_{\beta}(\mu) &\geq \beta^{-2} \int d\mu \left(\beta^2 |\nabla V|^2 - \beta \Delta V - \frac{\beta^2}{2} |\nabla V|^2 \right) \\ &= \frac{1}{2} \int d\mu \left(|\nabla V|^2 - \frac{2}{\beta} \Delta V \right) \geq \frac{1}{2} \int d\mu R. \end{aligned} \quad (5.1)$$

In particular, for any $t > 0$ and $\mu \in \mathcal{P}(M)$, it holds $\mu(\{R \leq t\}) \geq 1 - 2t^{-1} I_{\beta}(\mu)$. By A.2, R has compact sublevel sets, therefore any family $(\mu_{\beta}) \subset \mathcal{P}(M)$ such that $(I_{\beta}(\mu_{\beta}))$ is uniformly bounded, is tight. And, by Prohorov's Theorem, precompact. \square

Proof of (2.13), Γ -liminf. Assume that $\mu_{\beta} \rightarrow \mu$. Then, replacing ψ by $\beta \psi$ in (3.2), one obtains for each $\psi \in \Omega$

$$I_{\beta}(\mu_{\beta}) \geq \int d\mu_{\beta} \left(\nabla V \cdot \psi - \frac{1}{\beta} \nabla \cdot \psi - \frac{1}{2} \psi^2 \right), \quad (5.2)$$

which implies

$$\liminf_{\beta} I_{\beta}(\mu_{\beta}) \geq \int d\mu \left(\nabla V \cdot \psi - \frac{1}{2} \psi^2 \right). \quad (5.3)$$

Optimizing over ψ we get the result. \square

Proof of (2.13), Γ -limsup. We proceed in three steps.

Step 1. First assume $\mu = \delta_{\bar{x}}$ for some $\bar{x} \in M$. Take $U \equiv U_{\bar{x}} \in C^2(M; [0, +\infty))$ a smooth function such that

- (i) $U(x) = \text{distance}(x, \bar{x})^2$ in a neighborhood of \bar{x} , and U is strictly positive elsewhere.
- (ii) If $M = \mathbb{R}^d$, then $U(x) \geq |x|^2 + |\nabla V|^2(x) + |\Delta V|(x)$ for x large enough and $\nabla \exp(-U) \in L^2(dx)$ (it's immediate to check that such a U exists).

Let then

$$\mu_{\beta, \bar{x}}(dx) = \frac{1}{C_{\beta}} \exp(-2\beta U(x)) dx. \quad (5.4)$$

By Laplace principle $\mu_{\beta, \bar{x}} \rightarrow \delta_{\bar{x}}$. On the other hand an explicit calculation shows

$$I_{\beta}(\mu_{\beta, \bar{x}}) = \int d\mu_{\beta, \bar{x}} \left(\frac{|\nabla V|^2}{2} + 2|\nabla U|^2 - \frac{1}{\beta} \Delta V \right). \quad (5.5)$$

If M is compact, then

$$\lim_{\beta} \int d\mu_{\beta, \bar{x}} |\nabla U|^2 = |\nabla U|^2(\bar{x}) = 0, \quad (5.6)$$

$$\lim_{\beta} \int d\mu_{\beta, \bar{x}} \Delta V = \Delta V(\bar{x}), \quad (5.7)$$

so that the second and third term in the l.h.s. of (5.5) vanish to get

$$\overline{\lim}_{\beta} I_{\beta}(\mu_{\beta, \bar{x}}) = \overline{\lim}_{\beta} \int d\mu_{\beta, \bar{x}} \frac{|\nabla V|^2}{2} = \frac{|\nabla V|^2(\bar{x})}{2} = I(\delta_{\bar{x}}). \quad (5.8)$$

If $M = \mathbb{R}^d$, (5.6), (5.7) and (5.8) still hold if we restrict the integral to a (large) ball B containing \bar{x} . Since $e^{-2\beta U}/C_{\beta}$ vanishes pointwise out of B , it's enough to show that the integrands in (5.6), (5.7) and (5.8) are uniformly integrable. This is easily established by condition (ii) above.

Step2. If $\mu = \sum_{k=1}^N \alpha_k \delta_{\bar{x}_k}$, then define $\mu_{\beta} = \sum_{k=1}^N \alpha_k \mu_{\beta, \bar{x}_k}$, where $\mu_{\beta, \bar{x}}$ is defined as in (5.4). Clearly $\mu_{\beta} \rightarrow \mu$. On the other hand, since I_{β} is convex and I is linear, again $\overline{\lim}_{\beta} I_{\beta}(\mu_{\beta}) \leq I(\mu)$.

Step3. By a standard diagonal argument, it's now enough to show that finite convex combinations of Dirac masses are I -dense in $\mathcal{P}(M)$. This is trivial, since I is linear. \square

6. FIRST ORDER DEVELOPMENT BY Γ -CONVERGENCE

In this section we prove (2.14). The following remark is a restatement of (3.2).

Remark 6.1. *If $\mu = \varrho m_{\beta}$ and $h \in C^2(M)$ is such that $h^2 = \varrho$, then*

$$I_{\beta}(\mu) = -\frac{2}{\beta^2} \int dm_{\beta}(x) h(x) (L_{\beta} h)(x). \quad (6.1)$$

In particular if $d\mu = h^2 dm_{\beta}$ and h is an $L^2(m_{\beta})$ -normalized eigenfunction of $-\frac{1}{\beta} L_{\beta}$ with eigenvalue λ , then

$$I_{\beta}(\mu) = \frac{2}{\beta} \lambda. \quad (6.2)$$

More generally, for $P_{\beta, \varepsilon, \lambda}$ defined as in (4.5) and for $h \in \text{Range}(P_{\beta, \varepsilon, \lambda})$

$$\frac{2}{\beta}(\lambda - \varepsilon) \leq I_{\beta}(\mu) \leq \frac{2}{\beta}(\lambda + \varepsilon). \quad (6.3)$$

Proof of (2.14): Γ -liminf inequality. Let μ_{β} be a sequence converging to μ in $\mathcal{P}(M)$, we need to show that

$$\underline{\lim}_{\beta} \beta I_{\beta}(\mu_{\beta}) \geq J(\mu). \quad (6.4)$$

From the Γ -liminf (2.13) proved in Section 5, the liminf in (6.4) equals $+\infty$ unless $I(\mu) = 0$, namely μ has the form

$$\mu = \sum_{z \in \mathcal{P}} \alpha_z \delta_z. \quad (6.5)$$

Up to passing to a suitable subsequence (still labeled β hereafter), we can assume that the liminf is actually a limit, so that with no loss of generality $I_{\beta}(\mu_{\beta}) < +\infty$ for all β large enough. Then by Proposition 3.3 we can assume that $\varrho_{\beta} = d\mu_{\beta}/dm_{\beta}$

is in $C^2(M)$ and bounded away from 0. In particular $h_\beta := \sqrt{\varrho_\beta} \in C^2(M)$. Fix $\varepsilon > 0$, Λ large enough and such that

$$\Lambda > \max_{z \in \wp} \lambda_{z, \underline{0}}, \quad (6.6)$$

and let $\beta \geq \max_{(z, \underline{n}) : \lambda_{z, \underline{n}} \leq \Lambda} \beta_{\varepsilon, z, \underline{n}}$. By Proposition 4.2 and using the notation therein introduced, recalling also (4.3)-(4.5), we can write

$$h_\beta = \sum_{\lambda \leq \Lambda} P_{\beta, \varepsilon, \lambda} h_\beta + P_{\beta, \Lambda} h_\beta, \quad (6.7)$$

where

$$P_{\beta, \Lambda} := \mathbf{1}_{(\Lambda, +\infty)}(-\frac{1}{\beta} L_\beta) \quad , \quad P_{\beta, \varepsilon, \lambda} h_\beta = \sum_{(z, \underline{n}) \in S_\lambda} \gamma_{\beta, z, \underline{n}} \Psi_{\beta, z, \underline{n}} \quad ,$$

$$\gamma_{\beta, z, \underline{n}} := \langle h_\beta, \Psi_{\beta, z, \underline{n}} \rangle \in [-1, 1].$$

By (6.1), Proposition 4.2 and the Markov spectral inequality

$$\begin{aligned} \beta I_\beta(\mu_\beta) &= 2 \sum_{\lambda \leq \Lambda} \langle -\frac{1}{\beta} L_\beta P_{\beta, \varepsilon, \lambda} h_\beta, P_{\beta, \varepsilon, \lambda} h_\beta \rangle_{m_\beta} \\ &\quad + 2 \langle -\frac{1}{\beta} L_\beta P_{\beta, \Lambda} h_\beta, P_{\beta, \Lambda} h_\beta \rangle_{m_\beta} \\ &\geq 2 \sum_{\lambda \leq \Lambda} (\lambda - \varepsilon) \|P_{\beta, \varepsilon, \lambda} h_\beta\|_{L^2(m_\beta)}^2 + 2\Lambda \|P_{\beta, \Lambda} h_\beta\|_{L^2(m_\beta)}^2 \\ &= 2 \sum_{\lambda \leq \Lambda} \sum_{(z, \underline{n}) \in S_\lambda} \gamma_{\beta, z, \underline{n}}^2 (\lambda_{z, \underline{n}} - \varepsilon) + 2\Lambda \|P_{\beta, \Lambda} h_\beta\|_{L^2(m_\beta)}^2 \\ &\geq 2 \sum_{z \in \wp} \alpha_{\beta, z, \Lambda} (\lambda_{z, \underline{0}} - \varepsilon) + 2\Lambda \|P_{\beta, \Lambda} h_\beta\|_{L^2(m_\beta)}^2, \end{aligned} \quad (6.8)$$

where we used in the last line $\lambda_{z, \underline{n}} \geq \lambda_{z, \underline{0}}$ and introduced

$$\alpha_{\beta, z, \Lambda} = \sum_{\underline{n} : \lambda_{z, \underline{n}} \leq \Lambda} \gamma_{\beta, z, \underline{n}}^2. \quad (6.9)$$

As we take $\beta \rightarrow \infty$, (6.8) holds for any $\varepsilon > 0$, in particular we gather

$$\varliminf_{\beta} \|P_{\beta, \Lambda} h_\beta\|_{L^2(m_\beta)}^2 \leq \varliminf_{\beta} \frac{1}{2\Lambda} \beta I_\beta(\mu_\beta) \quad (6.10)$$

and, since

$$\sum_{z \in \wp} \alpha_z = 1 = \|h_\beta\|_{L^2(m_\beta)}^2 = \|P_{\beta, \Lambda} h_\beta\|_{L^2(m_\beta)}^2 + \sum_{z \in \wp} \alpha_{\beta, z, \Lambda}, \quad (6.11)$$

still by (6.8) and the fact that ε is arbitrary (once we take $\beta \rightarrow \infty$)

$$\begin{aligned} \varliminf_{\beta} \beta I_\beta(\mu_\beta) &\geq \varliminf_{\beta} 2 \sum_{z \in \wp} \alpha_{\beta, z, \Lambda} \lambda_{z, \underline{0}} + 2\Lambda \left(\sum_{z \in \wp} \alpha_z - \alpha_{\beta, z, \Lambda} \right) \\ &= 2 \sum_{z \in \wp} \alpha_z \lambda_{z, \underline{0}} + 2 \varliminf_{\beta} \sum_{z \in \wp} (\alpha_z - \alpha_{\beta, z, \Lambda}) (\Lambda - \lambda_{z, \underline{0}}) \\ &= J(\mu) + 2 \varliminf_{\beta} \sum_{z \in \wp} (\alpha_z - \alpha_{\beta, z, \Lambda}) (\Lambda - \lambda_{z, \underline{0}}), \end{aligned} \quad (6.12)$$

where in the last line we used (4.2). Since the sum above is finite, in view of (6.6), we conclude once we show that

$$\overline{\lim}_{\beta} \alpha_{\beta, z, \Lambda} \leq \alpha_z, \quad \forall z \in \wp. \quad (6.13)$$

To this aim, fix $z \in \wp$ and $\chi \in C_b(M)$, $0 \leq \chi \leq 1$, such that $\chi(z) = 1$ and $\chi(z') = 0$ for $z' \in \wp$, $z' \neq z$. Then

$$\begin{aligned} \alpha_z &= \mu(\chi) = \lim_{\beta} \mu_{\beta}(\chi) = \lim_{\beta} m_{\beta}(h_{\beta}^2 \chi) \\ &= \lim_{\beta} \sum_{\lambda, \lambda' \leq \Lambda} \sum_{(z, \underline{n}) \in S_{\lambda}} \sum_{(z', \underline{n}') \in S_{\lambda'}} \gamma_{\beta, z, \underline{n}} \gamma_{\beta, z', \underline{n}'} \langle \chi \Psi_{\beta, z, \underline{n}}, \Psi_{\beta, z', \underline{n}'} \rangle_{L^2(m_{\beta})} \\ &\quad + \lim_{\beta} \langle \chi P_{\beta, \Lambda} h_{\beta}, 2h_{\beta} - P_{\beta, \Lambda} h_{\beta} \rangle_{L^2(m_{\beta})}. \end{aligned} \quad (6.14)$$

Using (4.7) both for the on- and off-diagonal terms in the above sum and recalling (6.9) we obtain

$$\alpha_z \geq \overline{\lim}_{\beta} \alpha_{\beta, z, \Lambda} - 2\|\chi\|_{C_b} \|P_{\Lambda, \beta} h_{\beta}\|_{L^2(m_{\beta})} \geq \overline{\lim}_{\beta} \alpha_{\beta, z, \Lambda} - \lim_{\beta} \sqrt{\frac{2\beta I_{\beta}(\mu_{\beta})}{\Lambda}}, \quad (6.15)$$

where in the last inequality we used (6.10). Since we can assume $\lim_{\beta} \beta I_{\beta}(\mu_{\beta}) = C < +\infty$ with no loss of generality, and since $\alpha_{\beta, z, \Lambda}$ is increasing in Λ , from (6.15) we gather

$$\overline{\lim}_{\beta} \alpha_{\beta, z, \Lambda} \leq \inf_{\Lambda' \geq \Lambda} \overline{\lim}_{\beta} \alpha_{\beta, z, \Lambda'} \leq \alpha_z + \inf_{\Lambda' \geq \Lambda} \sqrt{\frac{2C}{\Lambda}} = \alpha_z, \quad (6.16)$$

namely (6.13). \square

Proof of (2.14): Γ -limsup inequality. If $J(\mu) = +\infty$ there is nothing to prove. So we can assume $\mu = \sum_{z \in \wp} \alpha_z \delta_z$. Recall the functions $(\Psi_{\beta, z, \underline{n}})_{z \in \wp, \underline{n} \in \mathbb{N}^d}$ introduced in Proposition 4.2 and define $\mu_{\beta, z} \in \mathcal{P}(M)$ and the recovery sequence $\mu_{\beta} \in \mathcal{P}(M)$ by

$$d\mu_{\beta, z} := \Psi_{\beta, z, \underline{0}}^2 dm_{\beta}, \quad (6.17)$$

$$\mu_{\beta} := \sum_{z \in \wp} \alpha_z m_{\beta, z}. \quad (6.18)$$

By (4.7), $\mu_{\beta, z} \rightarrow \delta_z$ in $\mathcal{P}(M)$, so that $\mu_{\beta} \rightarrow \mu$.

Using the notation of Proposition 4.2, for each $\varepsilon > 0$ and for each $\beta \geq \max_{z \in \wp} \beta_{\varepsilon, z, \underline{0}}$, by (6.3) and (4.2)

$$I_{\beta}(m_{\beta, z}) \leq \frac{2}{\beta}(\lambda_{z, \underline{0}} + \varepsilon) = \frac{1}{\beta}(\zeta(z) + 2\varepsilon). \quad (6.19)$$

Now, since I_{β} is convex by Remark 3.2

$$\beta I_{\beta}(\mu_{\beta}) \leq \beta \sum_{z \in \wp} \alpha_z I_{\beta}(m_{\beta, z}) \leq \sum_{z \in \wp} \alpha_z (\zeta(z) + 2\varepsilon) = J(\mu) + 2\varepsilon. \quad (6.20)$$

As we take the limsup $\beta \rightarrow +\infty$, (6.20) holds for any $\varepsilon > 0$, and thus $\overline{\lim}_{\beta} I_{\beta}(\mu_{\beta}) \geq I(\mu)$. \square

7. EXPONENTIAL DEVELOPMENT BY Γ -CONVERGENCE

In this section we prove (2.15).

Proof of (2.15): Γ -liminf inequality. Fix some $k = 1, \dots, n$ and let μ_β be a sequence converging to μ . We need to show that

$$\liminf_{\beta} \beta e^{\beta W_k} I_{\beta}(\mu_{\beta}) \geq J_k(\mu). \quad (7.1)$$

Up to passing to a suitable subsequence (still labeled β hereafter), we can assume that the liminf is actually a limit, so that with no loss of generality $I_{\beta}(\mu_{\beta}) < +\infty$ for all β large enough. Then by Proposition 3.3 we can assume that $\varrho_{\beta} = d\mu_{\beta}/dm_{\beta}$ is in $C^2(M)$ and bounded away from 0. In particular $h_{\beta} := \sqrt{\varrho_{\beta}} \in C^2(M)$. As in the proof of Lemma 4.6 we denote by $P_{\beta,k} := \mathbf{1}_{[\ell_{\beta,k+1}, +\infty)}(-\frac{1}{\beta}L_{\beta})$ the spectral projection of $-\frac{1}{\beta}L_{\beta}$ associated to the interval $[\ell_{\beta,k+1}, +\infty)$. Then, since $h_{\beta} \in L^2(m_{\beta})$, we can write

$$\begin{aligned} h_{\beta} &= \sum_{j=0}^k \gamma_{\beta,j} \Phi_{\beta,j} + P_{\beta,k} h_{\beta}, \\ \gamma_{\beta,j} &= \langle h_{\beta}, \Phi_{\beta,j} \rangle \in [-1, 1]. \end{aligned} \quad (7.2)$$

By (6.1) and the spectral Markov inequality

$$\begin{aligned} I_{\beta}(\mu_{\beta}) &= \frac{2}{\beta} \sum_{j=0}^k \gamma_{\beta,j}^2 \ell_{\beta,j} - \frac{2}{\beta^2} \int dm_{\beta}(x) P_{\beta,k} h_{\beta}(x) (L_{\beta} P_{\beta,k} h_{\beta})(x) \\ &\geq \frac{2}{\beta} \sum_{j=0}^k \gamma_{\beta,j}^2 \ell_{\beta,j} + \frac{2\ell_{\beta,k+1}}{\beta} \|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})}^2, \end{aligned} \quad (7.3)$$

i.e.

$$\begin{aligned} \beta e^{\beta W_k} I_{\beta}(\mu_{\beta}) &\geq 2\gamma_{\beta,k}^2 e^{\beta W_k} \ell_{\beta,k} \\ &\quad + 2 \sum_{j=0}^{k-1} \gamma_{\beta,j}^2 e^{\beta W_k} \ell_{\beta,j} + 2e^{\beta W_k} \ell_{\beta,k+1} \|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})}^2. \end{aligned} \quad (7.4)$$

From (4.28) and assumption A.5, the terms $\gamma_{\beta,j}^2 e^{\beta W_k} \ell_{\beta,j}$ with an index $j \leq k-1$ vanish as $\beta \rightarrow \infty$, since $\gamma_{\beta,j}^2 \leq 1$. On the other hand, still by (4.28) and A.5, the term $e^{\beta W_k} \ell_{\beta,k+1} \|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})}^2$ diverges to $+\infty$ unless $\|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})}$ vanishes. Thus setting $\underline{\alpha} := \liminf_{\beta} \gamma_{\beta,k}^2$ we gather again by (4.28)

$$\liminf_{\beta} \beta e^{\beta W_k} I_{\beta}(\mu_{\beta}) \geq \begin{cases} +\infty & \text{if } \liminf_{\beta} \|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})} > 0, \\ \underline{\alpha} \eta_k(x_k) & \text{otherwise.} \end{cases} \quad (7.5)$$

In particular, if $\liminf_{\beta} \|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})} > 0$, we proved the inequality (7.1) no matter what the limit μ of the μ_{β} is.

Now we claim that if $\liminf_{\beta} \|P_{\beta,k} h_{\beta}\|_{L^2(m_{\beta})} = 0$, then necessarily $\lim_{\beta} \mu_{\beta} = \mu = \sum_{j=0}^k \alpha_j \delta_{x_j}$ for some α_j , with $\alpha_k = \underline{\alpha}$, so that $\liminf_{\beta} \beta e^{\beta W_k} I_{\beta}(\mu_{\beta}) \geq \alpha_k \eta_k(x_k)$,

namely (7.1). To prove this claim notice that

$$\begin{aligned} d\mu_\beta &= (h_\beta)^2 dm_\beta \\ &= \left(\sum_{j=0}^k \gamma_{\beta,j}^2 \Phi_{\beta,j}^2 \right) dm_\beta + \left(\sum_{i \neq j, i,j=0}^k \gamma_{\beta,i} \gamma_{\beta,j} \Phi_{\beta,i} \Phi_{\beta,j} \right) dm_\beta \\ &\quad + (P_{\beta,k} h_\beta) \left(2 \sum_{j=0}^k \gamma_{\beta,j} \Phi_{\beta,j} + P_{\beta,k} h_\beta \right) dm_\beta. \end{aligned} \quad (7.6)$$

Since $\|(P_{\beta,k} h_\beta)\|_{L^2(m_\beta)}$ vanishes as $\beta \rightarrow \infty$ and (4.40) holds, the last two term above also vanish (weakly) as measures as $\beta \rightarrow \infty$. On the other hand, since $\mu_\beta \rightarrow \mu$, it follows from Proposition 4.7 that $\alpha_j = \lim_\beta \gamma_{\beta,j}^2$ exists and $\mu = \sum_{j=0}^k \alpha_j \delta_{x_j}$. \square

Proof of (2.15): Γ -limsup inequality. If $J_k(\mu) = +\infty$ there is nothing to prove. So we can assume $\mu = \sum_{j=0}^k \alpha_j \delta_{x_j}$. For $m_{\beta,j}$ as in (4.39), define the recovery sequence μ_β by

$$\mu_\beta := \sum_{j=0}^k \alpha_j m_{\beta,j}. \quad (7.7)$$

By Proposition 4.7, $\mu_\beta \rightarrow \mu$ in $\mathcal{P}(M)$. I_β is convex, and by (6.2)

$$I_\beta(\mu_\beta) \leq \sum_{j=0}^k \alpha_j I(m_{\beta,j}) = \frac{2}{\beta} \sum_{j=0}^k \alpha_j \ell_{\beta,j} \quad (7.8)$$

By (4.28) and hypotheses A.5 one finally gets

$$\overline{\lim}_\beta \beta e^{\beta W_k} I_\beta(\mu_\beta) \leq 2 \alpha_k \lim_\beta e^{\beta W_k} \ell_{\beta,k} = \alpha_k \eta_k(x_k) = J_k(\mu). \quad (7.9)$$

\square

Acknowledgements: GDG gratefully acknowledges the financial support of the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) / ERC Grant Agreement number 614492, helpful discussions with Tony Lelièvre and Tom Hudson, and the warm hospitality at the University of Rome La Sapienza during his frequent visits.

This work has been carried out thanks to the support of the A*MIDEX project (n. ANR11IDEX000102) funded by the *Investissements d'Avenir* French Government program, managed by the French National Research Agency (ANR).

We are grateful to Lorenzo Bertini for introducing us to the problem.

REFERENCES

- [1] Bakry D., Gentil I., Ledoux M. *Analysis and geometry of Markov diffusion operators*. Grundle Math. Wiss. 348, Springer (2014).
- [2] Berglund N., *Kramers' law: Validity, derivations and generalisations*. Markov Processes Relat. Fields 19:459-490 (2013).
- [3] Bovier A., Gayraud V., Klein M., *Metastability in reversible diffusion processes II. Precise asymptotics for small eigenvalues*, J. Eur. Math. Soc. 7, 69–99 (2005).
- [4] Braides A., *Γ -convergence for beginners*, Oxford University Press, (2002).
- [5] Donsker M.D., Varadhan S.R.S., *Asymptotic evaluation of certain Markov process expectations for large time (III)*, Comm. Pure Appl. Math. 29, 389–461 (1976).

- [6] Dembo A., Zeitouni O., *Large Deviations Techniques and Applications, 2nd ed. Corr. pr.* Springer (2009).
- [7] Di Gesù, Tony Lelièvre, Dorian Le Peutrec, Boris Nectoux *Jump Markov models and transition state theory: the Quasi-Stationary Distribution approach.* arxiv 1605.02643 (2016).
- [8] Eckhoff M., *Precise asymptotics of small eigenvalues of reversible diffusions in the metastable regime.* Ann. Prob. 33 (1), 244-299 (2005).
- [9] Freidlin M. I., Wentzell A. D., *Random perturbations of dynamical systems, 2nd ed.* Springer (1998).
- [10] Hänggi P., Talkner P., Borkovec M., *Reaction-rate theory. Fifty Years after Kramers.* Rev. of Mod. Phys., Vol.62 no.2 252-342 (1990).
- [11] Helffer B., Klein M., Nier F., *Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach,* Matemática Contemp. 26 (Brazilian Math. Soc.), 41-85 (2004).
- [12] Jordan R., Kinderlehrer D., Otto F. *The variational formulation of the Fokker–Planck equation,* SIAM J. Math. Anal. 29–1 (1998).
- [13] Kifer Y., *Large deviations in dynamical systems and stochastic processes,* Trans. American Math. Society, 321-2 (1990).
- [14] Kramers H.A., *Brownian motion in a field of force and the diffusion model of chemical reactions,* Physica VII, no. 4 (1940)
- [15] Le Peutrec D., *Small eigenvalues of the Neumann realization of the semiclassical Witten Laplacian,* Ann. Fac. Sci. Toulouse Math. (6) 19, no. 3–4, 735–809 (2010).
- [16] Lelièvre T., *Two mathematical tools to analyze metastable stochastic processes.* in Numerical Mathematics and Advanced Applications 2011, A. Cangiani et al. eds., Springer, p. 791-810, (2013).
- [17] Mariani M., *A Γ -convergence approach to large deviations,* arxiv:1204.0640 (2012).
- [18] Menz G., Schlichting A., *Poincaré and logarithmic Sobolev inequalities by decomposition of the energy landscape.* , Ann. Probab. 42, no. 5, pp. 1809–1884 (2014).
- [19] Peletier M., Savaré G., Veneroni M., *From diffusion to reaction via Γ -convergence,* SIAM J. Math. Anal. 42-4, 1805–1825, (2010).
- [20] Sandier E., Serfaty S., *Gamma-convergence of gradient flows with applications to Ginzburg-Landau,* Comm. Pure Appl. Math. 57-12, 1627-1672 (2004).
- [21] Simon B., *Semi-classical analysis of low lying eigenvalues. Non-degenerate minima: asymptotic expansion,* Annales de l’I.H.P. Sect. A, 38–3, 295-308 (1983).
- [22] Stroock D.W., *Probability Theory. An analytic view,* Cambridge University Press (1994).
- [23] Witten E., *Supersymmetry and Morse Theory.* J. Diff. Geom. 17, 661-692 (1982).

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