

A general two-scale criteria for logarithmic Sobolev inequalities

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A general two-scale criteria for logarithmic Sobolev inequalities

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Abstract

We present a general criteria to prove that a probability measure satisfies a logarithmic Sobolev inequality, knowing that some of its marginals and associated conditional laws satisfy a logarithmic Sobolev inequality. This is a generalization of a result by N. Grunewald et al. [5].

1 Motivation and notation

The motivation behind this work is molecular dynamics (in the canonical statistical ensemble), and more precisely, (i) the analysis of numerical methods for the computation of *free energy differences* [7] and (ii) the derivation of *effective dynamics on coarse-grained variables* [6]. In both cases, it appears that estimates based on entropies for measures related to the Boltzmann-Gibbs measure is a useful tool. One important question is the following: what is the link between the logarithmic Sobolev inequality (LSI) constant of the Boltzmann-Gibbs measure for the original variables (microscopic level) and the LSI constant of the Boltzmann-Gibbs measure for some coarse-grained variables (macroscopic level). The aim of this work is to give an answer, which is a generalization to non-linear coarse-graining operators of results in [8,5].

Let \mathcal{D} be a domain of \mathbb{R}^n representing the configuration space of the system under consideration, and $V : \mathcal{D} \rightarrow \mathbb{R}$ a potential, associating to each configuration an energy. Let us consider a function (representing the coarse-grained

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variables, also called the *reaction coordinates*)

$$\xi : \mathcal{D} \rightarrow \mathcal{M},$$

with $\mathcal{M} \subset \mathbb{R}^p$ (and $1 \leq p < n$). Let us introduce the Gram matrix $G : \mathcal{D} \rightarrow \mathbb{R}^{p \times p}$ of the derivative $\nabla \xi : \mathcal{D} \rightarrow \mathbb{R}^{p \times n}$: $G = \nabla \xi \nabla \xi^T$, *i.e.*, componentwise, $\forall \alpha, \beta \in \{1, \dots, p\}$,

$$G_{\alpha, \beta} = \nabla \xi_\alpha \cdot \nabla \xi_\beta. \quad (1)$$

We suppose that ξ is such that

$$[\mathbf{H1}] \quad \xi \text{ is a smooth function such that } \det G \neq 0 \text{ on } \mathcal{D}.$$

The submanifolds

$$\Sigma_z = \{x \in \mathcal{D}, \xi(x) = z\}$$

are then smooth submanifolds of \mathcal{D} of codimension p . We denote by σ_{Σ_z} the surface measure on Σ_z , *i.e.* the Lebesgue measure on Σ_z induced by the Lebesgue measure in the ambient Euclidean space \mathcal{D} . The submanifold Σ_z naturally has a (complete and locally compact) Riemannian structure induced by the Euclidean structure of the ambient space \mathcal{D} .

Let us define the density ψ_0 (with respect to the Lebesgue measure on \mathcal{D}) of the Boltzmann-Gibbs probability measure $d\mu_0(x) = \psi_0(x) dx$ associated to the potential V :

$$\psi_0 = Z^{-1} \exp(-V),$$

where $Z = \int_{\mathcal{D}} \exp(-V)$. We denote by ψ_0^ξ the density (with respect to the Lebesgue measure on \mathcal{M}) of the image $d\mu_0^\xi(z) = \psi_0^\xi(z) dz$ of the measure μ_0 by ξ :

$$\psi_0^\xi(z) = Z^{-1} \int_{\Sigma_z} \exp(-V) (\det G)^{-1/2} d\sigma_{\Sigma_z}.$$

Let us introduce then the conditional measure $\mu_{0,z}$ of μ_0 at a fixed value of ξ :

$$d\mu_{0,z} = \frac{Z^{-1} \exp(-V) (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi_0^\xi(z)}.$$

Let us introduce the effective potential A_0 associated to ξ (also called *free energy*), defined by

$$A_0(z) = -\ln \psi_0^\xi(z). \quad (2)$$

The following expression for the derivative of A_0 (also called *the mean force*) is obtained:

$$\nabla A_0(z) = \int_{\Sigma_z} F d\mu_{0,z}, \quad (3)$$

where F is defined by: $\forall \alpha \in \{1, \dots, p\}$,

$$F_\alpha = \sum_{\beta=1}^p G_{\alpha, \beta}^{-1} \nabla \xi_\beta \cdot \nabla V - \operatorname{div} \left(\sum_{\beta=1}^p G_{\alpha, \beta}^{-1} \nabla \xi_\beta \right), \quad (4)$$

where $G_{\alpha,\beta}^{-1}$ denotes the (α, β) -component of the inverse of the matrix G . All these results can be derived using the co-area formula (see Lemma 2.2 below), using similar computations as in Lemma 2.3 below.

Let us also introduce the following projection operators: For any $x \in \mathcal{D}$, we denote by

$$P(x) = \text{Id} - \sum_{\alpha,\beta=1}^p G_{\alpha,\beta}^{-1} \nabla \xi_\alpha \otimes \nabla \xi_\beta(x) \quad (5)$$

the orthogonal projection operator onto the tangent space $T_x \Sigma_{\xi(x)}$ to $\Sigma_{\xi(x)}$ at point x , and by

$$Q(x) = \text{Id} - P(x) = \sum_{\alpha,\beta=1}^p G_{\alpha,\beta}^{-1} \nabla \xi_\alpha \otimes \nabla \xi_\beta(x) \quad (6)$$

the orthogonal projection operator onto the normal space $N_x \Sigma_{\xi(x)}$ to $\Sigma_{\xi(x)}$ at point x . We denote by \otimes the tensor product: for two vectors $u, v \in \mathbb{R}^n$, $u \otimes v$ is a $n \times n$ matrix with components $(u \otimes v)_{i,j} = u_i v_j$.

For any two probability measures μ and ν such that μ is absolutely continuous with respect to ν (this property being denoted $\mu \ll \nu$ in the following), we introduce the relative entropy

$$H(\mu|\nu) = \int \ln \left(\frac{d\mu}{d\nu} \right) d\mu.$$

Let us also introduce the Fisher information: For any two probability measures μ and ν such that $\mu \ll \nu$,

$$I(\mu|\nu) = \int \left| \nabla \ln \left(\frac{d\mu}{d\nu} \right) \right|^2 d\mu. \quad (7)$$

In (7) and in the following, $|\cdot|$ denotes the Euclidean norm (in \mathbb{R}^n or in \mathbb{R}^p). In the case ν is a probability measure on the (Riemannian) submanifold Σ_z , ∇ actually denotes the gradient on Σ_z in (7), namely

$$\nabla_{\Sigma_z} = P \nabla. \quad (8)$$

We recall the definition of the Logarithmic Sobolev Inequality (LSI):

Definition 1.1 *The probability measure ν satisfies a logarithmic Sobolev inequality with constant $\rho > 0$ (in short: LSI(ρ)) if for all probability measures μ such that $\mu \ll \nu$,*

$$H(\mu|\nu) \leq \frac{1}{2\rho} I(\mu|\nu).$$

The main result of this paper states under which condition a LSI holds for μ_0 ,

assuming that a LSI holds for the conditional probability measure $\mu_{0,z}$ (this is [H2]) and for the marginal μ_0^ξ (this is [H3]).

Theorem 1.2 *In addition to [H1], let us assume (recall that the local mean force F is defined by (4)):*

$$[\mathbf{H2}] \quad \begin{cases} V \text{ and } \xi \text{ are such that } \exists \rho > 0, \text{ for all } z \in \mathcal{M}, \\ \text{the conditional measure } \mu_{0,z} \text{ satisfies } LSI(\rho). \end{cases}$$

[H3] V and ξ are such that $\exists r > 0$, the measure $d\mu_0^\xi = \psi_0^\xi(z) dz$ satisfies $LSI(r)$.

$$[\mathbf{H4}] \quad \begin{cases} V \text{ and } \xi \text{ are sufficiently differentiable functions such that: } \exists m > 0, G \geq m \text{ Id and} \\ (a) \|\nabla_{\Sigma_z} F\|_{L^\infty} \leq M < \infty \text{ or } (b) \|F\|_{L^\infty} \leq \frac{M}{\sqrt{\rho}} < \infty. \end{cases}$$

Then μ_0 satisfies $LSI(R)$ for some constant R which satisfies:

$$R \geq \frac{1}{2} \left(rm + \frac{M^2 m}{\rho} + \rho - \sqrt{\left(rm + \frac{M^2 m}{\rho} + \rho \right)^2 - 4rm\rho} \right). \quad (9)$$

In [H4], $G \geq m \text{ Id}$ should be understood in the following sense: for any vector $u \in \mathbb{R}^p$, $u^T G u \geq m|u|^2$. In [H4-a] or [H4-b], the L^∞ norm is with respect to $x \in \mathcal{D}$: $\|F\|_{L^\infty} = \sup_{x \in \mathcal{D}} |F|$ and $\|\nabla_{\Sigma_z} F\|_{L^\infty} = \sup_{x \in \mathcal{D}} |\nabla_{\Sigma_z} F|$, where $|\cdot|$ here denotes the operator norm on the matrix $\nabla_{\Sigma_z} F$ associated to the Euclidean norm on the vectors: $|\nabla_{\Sigma_z} F(x)| = \sup_{u \in T_x \Sigma_z} \frac{|\nabla F(x)u|}{|u|}$.

Assumption [H4-a] is an assumption on the coupling in the following sense. Assume that $V(x) = \frac{1}{2}x^T H x$ for some symmetric positive matrix $H \in \mathbb{R}^{n \times n}$ (so that μ_0 is a Gaussian law), and that $\xi(x_1, \dots, x_n) = (x_1, \dots, x_p)$. In this case, $G = \text{Id}$, and $\nabla_{\Sigma_z} F = 0$ is equivalent to the fact that the covariance $\text{Cov}((X_1, \dots, X_p), (X_{p+1}, \dots, X_n)) = 0$, where (X_1, \dots, X_n) is a random variable with law μ_0 . In this case of Gaussian laws and a linear function ξ , it can be checked that (9) is optimal (see [8]).

2 Proof

To prove the result, we need to introduce a few other notation. Let ψ be a probability density functional on \mathcal{D} . We denote the *total entropy* by

$$E = H(\psi|\psi_0),$$

and the *macroscopic entropy* by

$$E_M = H(\psi^\xi|\psi_0^\xi),$$

where

$$\psi^\xi(z) = \int_{\Sigma_z} \psi(\det G)^{-1/2} d\sigma_{\Sigma_z}.$$

We denote the conditioned probability measures of ψ at a fixed value z of the reaction coordinate by

$$d\mu_z = \frac{\psi(\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi(z)},$$

the “local entropy” by

$$e_m(z) = H(\mu_z | \mu_{0,z}) = \int_{\Sigma_z} \ln \left(\frac{\psi}{\psi^\xi(z)} / \frac{\psi_0}{\psi_0^\xi(z)} \right) d\mu_z,$$

and finally the *microscopic entropy* by

$$E_m = \int_{\mathcal{M}} e_m(z) \psi^\xi(z) dz.$$

It is straightforward to obtain the following result which can be seen as a property of extensivity of the entropy:

Lemma 2.1 *It holds*

$$E = E_M + E_m.$$

We will need the co-area formula (see [1,4]):

Lemma 2.2 *For any smooth function $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$,*

$$\int_{\mathbb{R}^n} \phi(x) (\det G(x))^{1/2} dx = \int_{\mathbb{R}^p} \int_{\Sigma_z} \phi d\sigma_{\Sigma_z} dz, \quad (10)$$

where G is defined by (1).

Remark 1 The co-area formula shows that if the random variable X has law $\psi(x) dx$ in \mathbb{R}^n , then $\xi(X)$ has law

$$\int_{\Sigma_z} \psi (\det G)^{-1/2} d\sigma_{\Sigma_z} dz,$$

and the law of X conditioned to a fixed value z of $\xi(X)$ is

$$d\mu_z = \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\int_{\Sigma_z} \psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}.$$

Indeed, for any bounded functions f and g ,

$$\begin{aligned}\mathbb{E}(f(\xi(X))g(X)) &= \int_{\mathbb{R}^n} f(\xi(x))g(x)\psi(x) dx, \\ &= \int_{\mathbb{R}^p} \int_{\Sigma_z} f \circ \xi g \psi (\det G)^{-1/2} d\sigma_{\Sigma_z} dz, \\ &= \int_{\mathbb{R}^p} f(z) \frac{\int_{\Sigma_z} g \psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\int_{\Sigma_z} \psi (\det G)^{-1/2} d\sigma_{\Sigma_z}} \int_{\Sigma_z} \psi (\det G)^{-1/2} d\sigma_{\Sigma_z} dz.\end{aligned}$$

The measure $(\det G)^{-1/2} d\sigma_{\Sigma_z}$ is sometimes denoted by $\delta_{\xi(x)-z}$ in the literature.

From the co-area formula, we get:

Lemma 2.3 *The derivative of ψ^ξ reads: $\forall \alpha \in \{1, \dots, p\}$,*

$$\partial_{z_\alpha} \psi^\xi(z) = \int_{\Sigma_z} \sum_{\beta=1}^p \left(G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \psi + \operatorname{div} \left(G_{\alpha,\beta}^{-1} \nabla \xi_\beta \right) \psi \right) (\det G)^{-1/2} d\sigma_{\Sigma_z}.$$

Proof : For any smooth test function $g : \mathcal{M} \rightarrow \mathbb{R}^p$, we obtain (using the co-area formula (10) and an integration by parts)¹:

$$\begin{aligned}\int_{\mathcal{M}} \psi^\xi \operatorname{div} g &= \int_{\mathcal{D}} \psi (\operatorname{div} g) \circ \xi, \\ &= \int_{\mathcal{D}} \psi G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla (g_\alpha \circ \xi), \\ &= - \int_{\mathcal{D}} \operatorname{div} \left(\psi G_{\alpha,\beta}^{-1} \nabla \xi_\beta \right) g_\alpha \circ \xi, \\ &= - \int_{\mathcal{M}} g_\alpha(z) \int_{\Sigma_z} \left(G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \psi + \operatorname{div} \left(G_{\alpha,\beta}^{-1} \nabla \xi_\beta \right) \psi \right) (\det G)^{-1/2} d\sigma_{\Sigma_z} dz,\end{aligned}$$

which yields the result. ◇

A corollary of Lemma 2.3 applied with $\psi = \psi_0$ is Equation (3). Let us now introduce the mean force associated with ψ (compare with (3)):

$$D(z) = \int_{\Sigma_z} F d\mu_z.$$

Notice that, in general, $D \neq -\nabla \ln \psi^\xi$, and $\operatorname{curl} D \neq 0$. We need a measure of the difference between D and ∇A_0 , in terms of the difference between ψ and ψ_0 :

Lemma 2.4 *The difference between D and ∇A_0 can be expressed in terms*

¹ In all the following proofs, we use the summation convention on repeated Greek indices going from 1 to p .

of ψ and ψ_0 as: for $\alpha \in \{1, \dots, p\}$, for all $z \in \mathcal{M}$,

$$(D_\alpha - \partial_{z_\alpha} A_0)(z) = \int_{\Sigma_z} \sum_{\beta=1}^p G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \ln \left(\frac{\psi}{\psi_0} \right) \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} - \partial_{z_\alpha} \ln \left(\frac{\psi^\xi}{\psi_0^\xi} \right).$$

Proof : Using Lemma 2.3 and the definition of D , it holds:

$$\begin{aligned} & \int_{\Sigma_z} G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \ln \left(\frac{\psi}{\psi_0} \right) \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} - \partial_{z_\alpha} \ln \left(\frac{\psi^\xi}{\psi_0^\xi} \right) \\ &= \frac{1}{\psi^\xi} \int_{\Sigma_z} G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \psi (\det G)^{-1/2} d\sigma_{\Sigma_z} + \int_{\Sigma_z} G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla V \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} \\ & \quad - \partial_{z_\alpha} \ln \psi^\xi + \partial_{z_\alpha} \ln \psi_0^\xi \\ &= - \int_{\Sigma_z} \operatorname{div} (G_{\alpha,\beta}^{-1} \nabla \xi_\beta) \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} + \int_{\Sigma_z} G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla V \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} \\ & \quad - \partial_{z_\alpha} A_0 \\ &= D_\alpha - \partial_{z_\alpha} A_0. \end{aligned}$$

◇

From Lemma 2.4, the following estimates are obtained:

Lemma 2.5 *Let us assume [H2] and [H4]. Then for all $z \in \mathcal{M}$,*

$$|D(z) - \nabla A_0(z)| \leq M \sqrt{\frac{2}{\rho} e_m(z)}.$$

Proof : If we suppose [H4-b], then we have:

$$\begin{aligned} |D(z) - \nabla A_0(z)| &= \left| \int F d\mu_z - \int F d\mu_{0,z} \right| \\ &\leq \|F\|_{L^\infty} \|\mu_z - \mu_{0,z}\|_{VT}, \\ &\leq \frac{M}{\sqrt{\rho}} \|\mu_z - \mu_{0,z}\|_{VT}, \end{aligned}$$

where $\|\mu_z - \mu_{0,z}\|_{VT}$ denotes the total variation norm of the signed measure $(\mu_z - \mu_{0,z})$. The result then follows from the Csiszar-Kullback inequality (see for example [2]):

$$\|\mu_z - \mu_{0,z}\|_{VT} \leq \sqrt{2H(\mu_z | \mu_{0,z})}.$$

Let us now assume [H4-a]. For any coupling measure $\pi \in \Pi(\mu_z, \mu_{0,z})$ defined on $\Sigma_z \times \Sigma_z$ (namely any probability measure on $\Sigma \times \Sigma$ such that its marginals

are μ_z and $\mu_{0,z}$, it holds:

$$\begin{aligned} |D(z) - \nabla A_0(z)| &= \left| \int_{\Sigma_z \times \Sigma_z} (F(x) - F(x')) \pi(dx, dx') \right|, \\ &\leq \|\nabla_{\Sigma_z} F\|_{L^\infty} \int_{\Sigma_z \times \Sigma_z} d_{\Sigma_z}(x, x') \pi(dx, dx'), \\ &\leq M \int_{\Sigma_z \times \Sigma_z} d_{\Sigma_z}(x, x') \pi(dx, dx'), \end{aligned}$$

where d_{Σ_z} denotes the geodesic distance on Σ_z : $\forall x, y \in \Sigma_z$,

$$d_{\Sigma_z}(x, y) = \inf \left\{ \sqrt{\int_0^1 |\dot{w}(t)|^2 dt} \mid w \in \mathcal{C}^1([0, 1], \Sigma_z), w(0) = x, w(1) = y \right\}.$$

Taking now the infimum over all $\pi \in \Pi(\mu_z, \mu_{0,z})$, we obtain

$$|D(z) - \nabla A_0(z)| \leq MW(\mu_z, \mu_{0,z})$$

where $W(\mu_z, \mu_{0,z})$ denotes the Wasserstein distance with linear cost (see for example [2]). It is known that if $\mu_{0,z}$ satisfies a LSI (which is [H2]), then we have the following Talagrand inequality (see [3,9]):

$$W(\mu_z, \mu_{0,z}) \leq \sqrt{\frac{2}{\rho} H(\mu_z | \mu_{0,z})}.$$

This implies the result. ◇

Lemma 2.6 *Let us assume [H2]. Then it holds*

$$E_m \leq \frac{1}{2\rho} \int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi.$$

Proof: Notice that the Fisher information of μ_z with respect to $\mu_{0,z}$ writes

$$I(\mu_z | \mu_{0,z}) = \int_{\Sigma_z} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi(z)}.$$

Therefore, using [H2], it follows:

$$\begin{aligned} E_m &= \int_{\mathcal{M}} e_m \psi^\xi dz, \\ &\leq \int_{\mathcal{M}} \frac{1}{2\rho} \int_{\Sigma_z} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi(z)} \psi^\xi dz, \end{aligned}$$

which yields the result, using the co-area formula (10). ◇

We are now in position to prove Theorem 1.2. We have (using [H2], [H3], Lemma 2.1, Lemma 2.4, and the inequality $(a + b)^2 \leq (1 + \varepsilon)a^2 + (1 + \varepsilon^{-1})b^2$, for a positive ε to be fixed later on):

$$\begin{aligned} E = E_m + E_M &\leq \frac{1}{2\rho} \int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi + \frac{1}{2r} \int_{\mathcal{M}} \left| \nabla \ln \left(\frac{\psi^\xi}{\psi_0^\xi} \right) \right|^2 \psi^\xi, \\ &\leq \frac{1}{2\rho} \int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi + \frac{1 + \varepsilon}{2r} \int_{\mathcal{M}} |D - \nabla A_0|^2 \psi^\xi \\ &\quad + \frac{1 + \varepsilon^{-1}}{2r} \int_{\mathcal{M}} \sum_{\alpha=1}^p \left| \int_{\Sigma_z} G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \ln \left(\frac{\psi}{\psi_0} \right) \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} \right|^2 \psi^\xi. \end{aligned}$$

Using the Cauchy-Schwarz inequality:

$$\begin{aligned} &\left| \int_{\Sigma_z} G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \ln \left(\frac{\psi}{\psi_0} \right) \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} \right|^2 \\ &\leq \int_{\Sigma_z} \left| G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \frac{\psi (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\psi^\xi} \end{aligned}$$

and Lemma 2.5, we thus obtain

$$\begin{aligned} E &\leq \frac{1}{2\rho} \int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi + \frac{(1 + \varepsilon)M^2}{r\rho} \int_{\mathcal{M}} e_m \psi^\xi \\ &\quad + \frac{1 + \varepsilon^{-1}}{2r} \int_{\mathcal{M}} \int_{\Sigma_z} \sum_{\alpha=1}^p \left| G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot \nabla \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi (\det G)^{-1/2} d\sigma_{\Sigma_z}. \end{aligned}$$

For any vector $u \in \mathbb{R}^n$, notice that $|Qu|^2 = G_{\alpha,\beta}^{-1} \nabla \xi_\alpha \cdot u \nabla \xi_\beta \cdot u$, and that $|u|^2 = |Pu|^2 + |Qu|^2$ (where P and Q are the projection operators defined by (5) and (6)). Using [H4], we thus have:

$$\begin{aligned} \sum_{\alpha=1}^p |G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot u|^2 &= G_{\alpha,\beta}^{-1} \nabla \xi_\beta \cdot u G_{\alpha,\gamma}^{-1} \nabla \xi_\gamma \cdot u, \\ &\leq \frac{1}{m} G_{\beta,\gamma}^{-1} \nabla \xi_\beta \cdot u \nabla \xi_\gamma \cdot u, \\ &= \frac{1}{m} |Qu|^2. \end{aligned}$$

Applying this inequality with $u = \nabla \ln \left(\frac{\psi}{\psi_0} \right)$ and using Lemma 2.6, we get:

$$\begin{aligned}
E &\leq \frac{1}{2\rho} \int_{\mathcal{D}} \left| P \nabla \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi + \frac{(1+\varepsilon)M^2}{r\rho} E_m \\
&\quad + \frac{1+\varepsilon^{-1}}{2rm} \int_{\mathcal{M}} \int_{\Sigma_z} \left| Q \nabla \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi (\det G)^{-1/2} d\sigma_{\Sigma_z}, \\
&\leq \left(\frac{1}{2\rho} + \frac{(1+\varepsilon)M^2}{2r\rho^2} \right) \int_{\mathcal{D}} \left| P \nabla \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi \\
&\quad + \frac{1+\varepsilon^{-1}}{2rm} \int_{\mathcal{D}} \left| Q \nabla \ln \left(\frac{\psi}{\psi_0} \right) \right|^2 \psi.
\end{aligned}$$

This shows that ψ satisfies a LSI with constant R satisfying

$$\begin{aligned}
R &\geq \frac{1}{2} \left(\max \left(\frac{1}{2\rho} + \frac{(1+\varepsilon)M^2}{2r\rho^2}, \frac{1+\varepsilon^{-1}}{2rm} \right) \right)^{-1}, \\
&= \min \left(\frac{\rho^2}{\rho + (1+\varepsilon)M^2/r}, \frac{rm}{1+\varepsilon^{-1}} \right).
\end{aligned}$$

Optimizing in ε , namely solving $\frac{\rho^2}{\rho + (1+\varepsilon)M^2/r} = \frac{rm}{1+\varepsilon^{-1}}$ concludes the proof.

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