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Spectral Analysis of Discrete Metastable Diffusions

Giacomo Di Gesù

Dipartimento di Matematica, Università di Roma 'La Sapienza', P.le Aldo Moro 5, 00185 Rome, Italy.
E-mail: giacomo.digesu@uniroma1.it

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Abstract: We consider a discrete Schrödinger operator $H_\varepsilon = -\varepsilon^2 \Delta_\varepsilon + V_\varepsilon$ on $\ell^2(\varepsilon\mathbb{Z}^d)$, where $\varepsilon > 0$ is a small parameter and the potential V_ε is defined in terms of a multi-well energy landscape f on $\mathbb{R}^d$. This operator can be seen as a discrete analog of the semiclassical Witten Laplacian of $\mathbb{R}^d$. It is unitarily equivalent to the generator of a diffusion on $\varepsilon\mathbb{Z}^d$, satisfying the detailed balance condition with respect to the Boltzmann weight $\exp(-f/\varepsilon)$. These type of diffusions exhibit metastable behavior and arise in the context of disordered mean field models in Statistical Mechanics. We analyze the bottom of the spectrum of H_ε in the semiclassical regime $\varepsilon \ll 1$ and show that there is a one-to-one correspondence between exponentially small eigenvalues and local minima of f. Then we analyze in more detail the bistable case and compute the precise asymptotic splitting between the two exponentially small eigenvalues. Through this purely spectral-theoretical analysis of the discrete Witten Laplacian we recover in a self-contained way the Eyring–Kramers formula for the metastable tunneling time of the underlying stochastic process.

1. Introduction

This paper derives sharp semiclassical spectral asymptotics for Schrödinger operators acting on $\ell^2(\varepsilon\mathbb{Z}^d)$ of the form

$$H_\varepsilon = -\varepsilon^2 \Delta_\varepsilon + V_\varepsilon, \quad 0 < \varepsilon \ll 1, \tag{1}$$

where Δ_ε is the discrete nearest-neighbor Laplacian of $\varepsilon\mathbb{Z}^d$ and V_ε is a possibly unbounded multiplication operator, defined in terms of a multiwell energy landscape f. More precisely, given $f \in C^2(\mathbb{R}^d)$, we identify V_ε with the function

$$V_\varepsilon(x) = e^{\frac{f(x)}{2\varepsilon}} (\varepsilon^2 \Delta_\varepsilon e^{-\frac{f}{2\varepsilon}})(x). \tag{2}$$

We shall dub H_ε the discrete semiclassical Witten Laplacian associated with f. This is motivated by the following observation: the continuous space version of H_ε, i.e. the Schrödinger operator $\mathcal{H}_\varepsilon$ on $L^2(\mathbb{R}^d)$ obtained from (1),(2) by substituting Δ_ε with the Laplacian Δ of $\mathbb{R}^d$, reads

$$\mathcal{H}_\varepsilon = -\varepsilon^2\Delta + \tfrac{1}{4}|\nabla f|^2 - \tfrac{\varepsilon}{2}\Delta f, \tag{3}$$

and thus coincides with the restriction on functions of the Witten Laplacian of $\mathbb{R}^d$ [27,30,40,46]. It is well known that the latter has deep connections to problems in Statistical Mechanics [24]. In some situations, e.g. when considering lattice models of Statistical Mechanics as discussed below, one is led in a natural way to its discrete version (1),(2). The continuous space operator (3) is then rather a simplifying idealization of (1),(2): it is indeed easier to analyze $\mathcal{H}_\varepsilon$ by exploiting the standard machinery of differential and semiclassical calculus, but the results might be a priori less accurate in making predictions. This paper shows a general strategy which permits to obtain sharp semiclassical estimates directly in the discrete setting.

We are mainly inspired by the analysis [26] on the continuous space Witten Laplacian and by the series of papers [33–36] by M. Klein and E. Rosenberger, who develop an approach to the semiclassical spectral analysis of discrete Schrödinger operators of the form (1) via microlocalization techniques. We refer also to the earlier work [31] and to [13,14,39] for semiclassical investigations in discrete settings.

Brief description of the main results. Following in particular the approach of [34] we show that under mild regularity assumptions on f there is a low-lying spectrum of exponentially small eigenvalues which is well separated from the rest of the spectrum. Moreover the number of exponentially small eigenvalues equals the number of local minima of f, see Theorem 2.2 below.

Then we analyze in more detail the case of two local minima of f and compute the precise asymptotic splitting between the two small eigenvalues. From a general point of view, this corresponds to a subtle tunneling calculation through other, non-resonant wells [29] of the Schrödinger potential V_ε, corresponding to saddle points of f.

As opposed to [26] we work again under mild regularity assumptions on f and proceed with a streamlined, direct strategy that avoids WKB expansions, a priori Agmon estimates and also the underlying complex structure of the Witten Laplacian. Much of the simplification is obtained via a suitable choice of global quasimodes. We show that the leading asymptotic of the exponentially small eigenvalue gap is given by an Eyring-Kramers formula:

$$\lambda(\varepsilon) = \varepsilon A e^{-\frac{E}{\varepsilon}}(1 + o(1)),$$

where $A, E > 0$ are explicit constants depending on f (see Theorem 2.3 for a precise statement) that turn out to coincide with the one obtained in the continuous case for $\mathcal{H}_\varepsilon$ in [26] (see also [10,21]). In other terms, the geometric constraint imposed by the lattice turns out to be negligible in first order approximation. The vanishing rate of the remainder term depends on the regularity of f around its critical points. We show that $f \in C^3(\mathbb{R}^d)$ leads to an error of order $O(\sqrt{\varepsilon})$, while for $f \in C^4(\mathbb{R}^d)$ this error improves to $O(\varepsilon)$.

The spectral Eyring-Kramers formula in the discrete setting considered here is not new. Indeed, up to some minor variants, this type of result has been derived in the framework of discrete metastable diffusions, by analyzing mean transition times of Markov processes via potential theory [8]. We shall discuss below more in detail the probabilistic interpretation of our results. The present paper shows that, as in the continuous setting, also in the discrete setting the Eyring-Kramers formula can be obtained by a direct and self-contained spectral approach, without relying at all on probabilistic potential theory.

We remark that the method we use to analyze the exponentially small eigenvalues can be extended also to the general case with more than two local minima. The extension is based on an iterative finite-dimensional matrix procedure, very similar to the one considered in [26] (see also [16] and references therein). This procedure is independent of the rest and not related to the peculiar analytical difficulties arising from the discrete character of the setting. To not obscure the exposition of the main ideas of this paper, the general case will be discussed somewhere else.

Connection to discrete metastable diffusions. Our main motivation for investigating the spectral properties of H_ε stems from its close connection to certain metastable diffusions with state space $\varepsilon\mathbb{Z}^d$. These have been extensively studied in the probabilistic literature, mainly due to their paradigmatic properties and their applications to problems in Statistical Mechanics [2,5,8,12,20,38,42]. The general, continuous time version might be described in terms of a Markovian generator L_ε of the form

$$L_\varepsilon \psi(x) = \sum_{v\in\mathbb{Z}^d} r_\varepsilon(x, x+\varepsilon v)\,[\psi(x+\varepsilon v) - \psi(x)]\,, \tag{4}$$

with $r_\varepsilon(x, x+\varepsilon v)$ being the rate of a jump from x to $x+\varepsilon v$. The jump rates are assumed to satisfy the detailed balance condition with respect to the Boltzmann weight $\rho_\varepsilon = e^{-f/\varepsilon}$ on $\varepsilon\mathbb{Z}^d$, so that L_ε may be realized as a selfadjoint operator acting on the weighted space $\ell^2(\varepsilon\mathbb{Z}^d;\,\rho_\varepsilon)$. Moreover the scaling is chosen so that L_ε formally converges for $\varepsilon \to 0$ to a first order differential operator on $\mathbb{R}^d$, corresponding to a deterministic transport along a vector field. One might thus think of the dynamics as a small stochastic perturbation of a deterministic motion. A standard choice of jump rates satisfying the above requirements is given by

$$r_\varepsilon(x, x+\varepsilon v) = \begin{cases} \frac{1}{\varepsilon} e^{-\frac{1}{2\varepsilon}[(f(x+\varepsilon v) - f(x)]} & \text{if } v \in \{-e_k, e_k\}_{k=1,\dots,d}, \\ 0 & \text{otherwise,} \end{cases} \tag{5}$$

where $(e_1, \dots, e_d)$ is the standard basis of $\mathbb{R}^d$.

There is a direct link between the discrete Witten Laplacian and discrete diffusions as described above: up to a change of sign and multiplicative factor ε, the Markovian generator L_ε given by (4),(5) and the discrete Witten Laplacian given by (1),(2) are formally unitarily equivalent. This can be seen by the well-known ground state transformation, which turns a Schrödinger operator into a diffusion operator [32], see Proposition 2.5 below for the precise statement. As a consequence, our spectral analysis of H_ε can be immediately translated into analogous results on L_ε, see Corollary 2.6. The advantage of working with H_ε is that in the flat space $\ell^2(\varepsilon\mathbb{Z}^d)$ one can exploit Fourier analysis and related microlocalization techniques.

We remark that discrete diffusions as described above naturally arise in the context of disordered mean field models in Statistical Mechanics. A prominent example is the dynamical random field Curie-Weiss model [5,8,22,42], which is well described by a discrete diffusion on $\varepsilon\mathbb{Z}^d$ after a suitable reduction in terms of order parameters. The limit $\varepsilon \to 0$ then corresponds to the thermodynamic limit of infinite volume.

A characteristic feature of the dynamics $\partial_t \psi = L_\varepsilon \psi$ for small ε is metastability: if f admits several local minima the system remains trapped for exponentially large times in neighborhoods of local minima of f before exploring the whole state space. This is due to the fact that the local minima of f turn out to be exactly the stable equilibrium points of the limiting deterministic motion. We refer to [7,23,41] for comprehensive introductions to metastability of Markov processes and e.g. to [3,17,37] for shorter surveys.

A key issue in the understanding of metastability is to quantify the time scales at which metastable transitions between local minima occur. For discrete diffusions of type (4) sharp asymptotic estimates have been obtained in [8,9] in terms of average hitting times. The formula for the leading asymptotics is called Eyring-Kramers formula. In [8] it is also shown that there is a very clean relationshp between the metastable transition times and the low-lying spectrum of $-L_\varepsilon$. Indeed, there is a cluster of exponentially small eigenvalues, each one being asymptotically equivalent to the inverse of a metastable transition time.

The problem of determining the asymptotic behavior of metastable transition times can therefore be equivalently phrased as a problem of spectral asymptotics of the generator L_ε and thus of H_ε. Due to these facts, one can view the method presented in this paper as a spectral approach to the computation of metastable transition times in discrete setting.

Plan of the paper In Sect. 2 we introduce the setting, provide precise definitions and basic properties for the discrete Witten Laplacian H_ε, the diffusion generator L_ε and state our main results: Theorem 2.2, saying that there are as many exponentially small eigenvalues of H_ε as minima of f and that there is a large gap of order ε between them and the rest of the spectrum; Theorem 2.3, giving the precise splitting between exponentially small eigenvalues due to the tunnel effect (Eyring-Kramers formula). In Sect. 3 we collect some preliminary tools which can be seen as general means for a semiclassical analysis on the lattice: the IMS formula for the discrete Laplacian which permits to localize quadratic forms on the lattice; estimates on the discrete semiclassical Harmonic oscillator based on microlocalization techniques; and results on sharp Laplace asymptotics on the lattice $\varepsilon\mathbb{Z}^d$ based on the Poisson summation formula. In Sects. 4 and 5 we provide the proofs of Theorems 2.2 and 2.3 respectively.

2. Precise Setting and Main Results

Throughout the paper we shall use the following notation. We consider the symmetric set

$$\mathcal{N} = \{e_k, -e_k : k = 1, \dots, d\} \subset \mathbb{Z}^d,$$

where $(e_1, \dots, e_d)$ is the standard basis of $\mathbb{R}^d$. For $\varepsilon > 0$ the symbols ∇_ε and Δ_ε denote respectively the rescaled discrete gradient and the rescaled discrete Laplacian of the lattice $\varepsilon\mathbb{Z}^d$, with graph structure induced by $\varepsilon\mathcal{N}$. More precisely, for every $\psi : \varepsilon\mathbb{Z}^d \to \mathbb{R}$ we define

$$\begin{aligned}\nabla_\varepsilon \psi(x, v) &= \varepsilon^{-1}[\psi(x + \varepsilon v) - \psi(x)], \quad \forall x \in \varepsilon\mathbb{Z}^d \quad \text{and} \quad v \in \mathcal{N}, \\ \Delta_\varepsilon \psi(x) &= \varepsilon^{-2} \sum_{v \in \mathcal{N}} [\psi(x + \varepsilon v) - \psi(x)], \quad \forall x \in \varepsilon\mathbb{Z}^d.\end{aligned}$$

We shall work on the Hilbert space $\ell^2(\varepsilon\mathbb{Z}^d) = \{\psi \in \mathbb{R}^{\varepsilon\mathbb{Z}^d} : \|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)} < \infty\}$, where $\|\cdot\|_{\ell^2(\varepsilon\mathbb{Z}^d)}$ is the norm corresponding to the scalar product

$$\langle\psi,\psi'\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \varepsilon^d \sum_{x\in\varepsilon\mathbb{Z}^d} \psi(x)\,\psi'(x).$$

The discrete Laplacian Δ_ε is a bounded linear operator on $\ell^2(\varepsilon\mathbb{Z}^d)$. It is also selfadjoint and $-\Delta_\varepsilon$ is nonnegative. More precisely, for $\psi,\psi' \in \ell^2(\varepsilon\mathbb{Z}^d)$, once can check that

$$\langle -\Delta_\varepsilon\psi,\psi'\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \langle\psi,-\Delta_\varepsilon\psi'\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \langle\nabla_\varepsilon\psi,\nabla_\varepsilon\psi'\rangle_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})},$$

and in particular

$$\langle -\Delta_\varepsilon\psi,\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \|\nabla_\varepsilon\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})} \geqslant 0.$$

Here $\|\cdot\|_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})}$ is the norm induced by the scalar product

$$\langle\alpha,\alpha'\rangle_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})} = \frac{\varepsilon^d}{2}\sum_{x\in\varepsilon\mathbb{Z}^d}\sum_{v\in\mathcal{N}} \alpha(x,v)\,\alpha'(x,v),$$

defined for $\alpha,\alpha' \in \ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}}) := \{\alpha \in \mathbb{R}^{\varepsilon\mathbb{Z}^d\times\mathcal{N}} : \|\alpha(\cdot,v)\|_{\ell^2(\varepsilon\mathbb{Z}^d)} < \infty \text{ forall } v \in \mathcal{N}\}$ (the space of square integrable 1-forms on the graph $\varepsilon\mathbb{Z}^d$).

2.1. Definition and basic properties of H_ε. Given a function $f : \mathbb{R}^d \to \mathbb{R}$ and a parameter $\varepsilon > 0$, we define a new function $V_\varepsilon : \mathbb{R}^d \to \mathbb{R}$ by setting

$$V_\varepsilon(x) = \sum_{v\in\mathcal{N}} \left[e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)} - 1\right], \quad \forall x \in \mathbb{R}^d. \tag{6}$$

Note that the expression (6) for V_ε and the one given in the introduction in (2) are equal by definition of Δ_ε and ∇_ε. We shall identify in the sequel V_ε with the corresponding multiplication operator in $\ell^2(\varepsilon\mathbb{Z}^d)$ having dense domain $\mathrm{Dom}(V_\varepsilon) = \{\psi \in \ell^2(\varepsilon\mathbb{Z}^d) : V_\varepsilon\psi \in \ell^2(\varepsilon\mathbb{Z}^d)\}$. The restriction of V_ε to $C_c(\varepsilon\mathbb{Z}^d)$ (i.e. the set of $\psi \in \mathbb{R}^{\varepsilon\mathbb{Z}^d}$ such that $\psi(x) = 0$ for all but finitely many x) is essentially selfadjoint.
We are interested in the Schrödinger-type operator $H_\varepsilon : \mathrm{Dom}(V_\varepsilon) \to \ell^2(\varepsilon\mathbb{Z}^d)$ given by

$$H_\varepsilon = -\varepsilon^2\Delta_\varepsilon + V_\varepsilon.$$

Note that H_ε is a selfadjoint operator in $\ell^2(\varepsilon\mathbb{Z}^d)$ and its restriction to $C_c(\varepsilon\mathbb{Z}^d)$ is essentially selfadjoint. This follows e.g. from the Kato-Rellich Theorem [45, Theorem 6.4], using the analogous properties of V_ε and the fact that Δ_ε is bounded and selfadjoint.

Moreover, from the pointwise bound $V_\varepsilon \geqslant -2d$ and the nonnegativity of $-\Delta_\varepsilon$ it follows immediately that H_ε is bounded from below. An important observation is that the quadratic form associated with H_ε is not only bounded from below, but even nonnegative. This is due to the special form of the potential V_ε. Indeed, a straightforward computation yields

$$\langle H_\varepsilon\psi,\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \|\nabla_{f,\varepsilon}\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})} \geqslant 0, \quad \forall\psi \in \mathrm{Dom}(V_\varepsilon), \tag{7}$$

where $\nabla_{f,\varepsilon}$ denotes a suitably weighted discrete gradient:

$$\nabla_{f,\varepsilon}\psi\,(x,v) = \varepsilon e^{-\frac{f(x)+f(x+\varepsilon v)}{4\varepsilon}}\nabla_\varepsilon(e^{\frac{f}{2\varepsilon}}\psi)\,(x,v), \quad \forall x \in \varepsilon\mathbb{Z}^d \quad \text{and} \quad v \in \mathcal{N}.$$

It follows in particular that the spectrum of H_ε is contained in $[0,\infty)$.

Remark 2.1. The property (7) states that H_ε is the Laplacian associated to the distorted gradient $\nabla_{f,\varepsilon}$. As it is done for the continuous space Witten Laplacian [30,46], it is possible to give an extension of H_ε in the sense of Hodge theory. The extended operator is then defined on a suitable algebra of discrete differential forms and satisfies the usual intertwining relations. We shall not use this fact and refer to [16] for details.

2.2. Assumptions and main results. We shall consider the following two sets of hypotheses on the function f. Here and in the following $|\cdot|$ denotes the standard euclidean norm on $\mathbb{R}^d$. The gradient and Hessian of a function on $\mathbb{R}^d$ are denoted by ∇ and Hess.

H1. $f \in C^3(\mathbb{R}^d)$ and all its critical points are nondegenerate. Moreover

(i) $\liminf_{|x|\to\infty} |\nabla f(x)| > 0$.
(ii) Hess f is bounded on $\mathbb{R}^d$.

Note that **H**1 implies that the set of critical points of f is finite. Indeed, nondegenerate critical points are necessarily isolated and by (i) the critical points of f must be contained in a compact subset of $\mathbb{R}^d$.
To analyze the exponential splitting between small eigenvalues we will assume for simplicity the following more restrictive hypothesis.

H2. Hyptohesis **H**1 holds true. Moreover

(i) $\liminf_{|x|\to\infty} \frac{f(x)}{|x|} > 0$.
(ii) The function f has exactly two local minimum points $m_0, m_1 \in \mathbb{R}^d$.

The first result we present shows that under Assumption **H**1 the essential spectrum of H_ε, denoted by $\mathrm{Spec}_{\mathrm{ess}}(H_\varepsilon)$, is uniformly bounded away from zero and that its discrete spectrum, denoted by $\mathrm{Spec}_{\mathrm{disc}}(H_\varepsilon)$, is well separated into two parts: one consists of exponentially small eigenvalues, the other of eigenvalues which are at least at distance of order ε from zero. Moreover, counting multiplicity, the number of exponentially small eigenvalues equals exactly the number of local minima of f:

Theorem 2.2. *Assume **H1** and denote by $N_0 \in \mathbb{N}_0$ the number of local minima of f. There exist constants $\varepsilon_0 \in (0,1)$ and $C > 0$ such that for each $\varepsilon \in (0, \varepsilon_0]$ the following properties hold true.*

(i) $\mathrm{Spec}_{ess}(H_\varepsilon) \subset [C, \infty)$.
(ii) $|\,\mathrm{Spec}_{disc}(H_\varepsilon) \cap [0, C\varepsilon]| \leqslant N_0$.
(iii) *H_ε admits at least N_0 eigenvalues counting multiplicity. In the nontrivial case that $N_0 \neq 0$, the N_0-th eigenvalue $\lambda_{N_0}(\varepsilon)$ (according to increasing order and counting multiplicity) satisfies the bounds*

$$0 \leqslant \lambda_{N_0}(\varepsilon) \leqslant e^{-C/\varepsilon}.$$

The properties stated in Theorem 2.2 are well-known in the continous space setting [28,43] and have also been recently extended to certain infinite-dimensional situations [11]. In the finite-dimensional continuous space setting the standard proof consists in approximating the Schrödinger operator with harmonic oscillators around the critical points of f. The error is then estimated using the IMS localization formula, which permits to connect the local estimates around the critical points to global estimates. The discrete case is analytically more difficult, due to the nonlocal character of the discrete

Laplacian. The main idea to overcome these difficulties is taken from [34] and consists in localizing not only the potential V_ε but the full operator H_ε. This amounts in localizing the symbol in phase space and is also referred to as micolocalization. The setting in [34] is very general and requires the machinery of pseudodifferential operators, which makes the proof rather involved and requires strong regularity assumptions on the potential V_ε which are not assumed here. Here we give a more elementary proof which is adapted to our special case and works well under Hypthesis **H**1.

We now assume the stronger Hypothesis **H**2. Then, thanks to the superlinear growth condition **H**2 (i), it holds

$$\|e^{-\frac{f}{2\varepsilon}}\|_{\ell^2(\varepsilon\mathbb{Z}^d)} < \infty, \quad \forall\varepsilon > 0.$$

This implies that $e^{-\frac{f}{2\varepsilon}}$ is in the domain of H_ε and therefore, since $H_\varepsilon e^{-\frac{f}{2\varepsilon}} = 0$ by direct computation, that 0 is an eigenvalue of H_ε. Moreover, due to the fact that $\mathcal{N}$ generates the group $\mathbb{Z}^d$, it follows for example from (7) that only multiples of Ψ_ε can be eigenfunctions corresponding to the eigenvalue 0. Thus we conclude that 0 is an eigenvalue with multiplicity 1 for every $\varepsilon > 0$.

Since, by assumption, there are $N_0 = 2$ local minima of f, it follows from Theorem 2.2 that, for $\varepsilon > 0$ sufficiently small, there is exactly one eigenvalue λ_ε of H_ε, which is different from 0 and is exponentially small in ε. Moreover, by the same theorem, λ_ε must have multiplicity 1. Our second main result provides the precise leading asymptotic behavior of $\lambda(\varepsilon)$. This behavior is expressed in terms of two constants $A, E > 0$, giving respectively the prefactor and the exponential rate. More precisely one defines

$$E := h^* - h_*, \tag{8}$$

where $h_* := \max\{f(m_0), f(m_1)\} \in \mathbb{R}$ and where $h^* \in \mathbb{R}$ is given by the height of the barrier which separates the two minima. More precisely, h^* can be defined as follows [26]. For $h \in \mathbb{R}$ we denote by $\mathcal{S}_f(h) := f^{-1}((-\infty, h))$ the (open) sublevel set of f corresponding to the height h and by $N_f(h)$ the number of connected components of $\mathcal{S}_f(h)$. Then $h^*(f) \in \mathbb{R}$ is defined as the maximal height which disconnects $\mathcal{S}_f(h)$ into two components (Fig. 1):

$$h^* := \max\left\{h \in \mathbb{R} : N_f(h) = 2\right\}. \tag{9}$$

By simple topological arguments, on the level set $f^{-1}(h^*)$ there must be at least one critical point of f of index 1 and at most a finite number n of them, which we label in an arbitrary order as $s_1, \ldots, s_n$. We denote by $\mu(s_k)$ the only negative eigenvalue of Hess $f(s_k)$. The constant A is then defined in terms of the quadratic curvature of f around the two minima and the relevant saddle points. More precisely, one defines

$$A := \begin{cases} \sum_{k=1}^n \frac{|\mu(s_k)|}{2\pi} \frac{(\det \text{Hess } f(m_1))^{\frac{1}{2}}}{|\det \text{Hess } f(s_k)|^{\frac{1}{2}}}, & \text{if} \quad f(m_0) < f(m_1), \\ \sum_{k=1}^n \frac{|\mu(s_k)|}{2\pi} \frac{(\det \text{Hess } f(m_0))^{\frac{1}{2}} + (\det \text{Hess } f(m_1))^{\frac{1}{2}}}{|\det \text{Hess } f(s_k)|^{\frac{1}{2}}}, & \text{if} \quad f(m_0) = f(m_1). \end{cases} \tag{10}$$

Our second main theorem is the following.

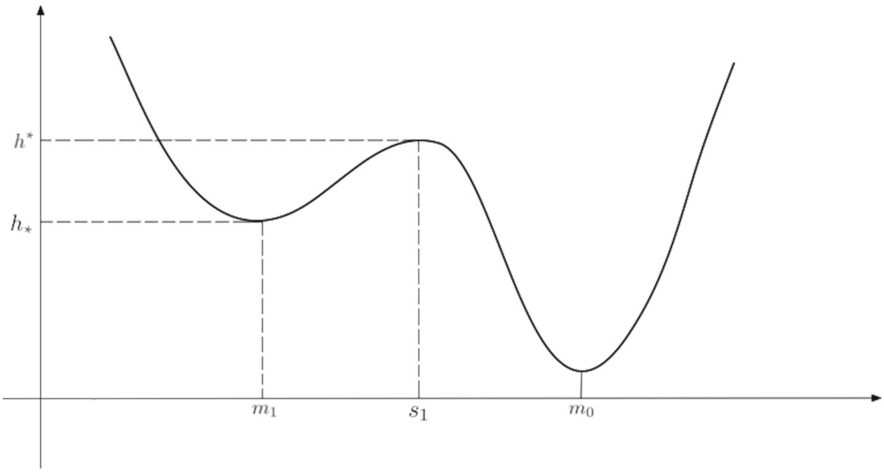

Fig. 1. A double-well potential f on $\mathbb{R}$

Theorem 2.3. *Assume **H2** and take $\varepsilon_0 > 0$ as in Theorem 2.2. Let A, E be given respectively by (8), (10) and let, for $\varepsilon \in (0, \varepsilon_0)$, $\lambda(\varepsilon)$ be the smallest non-zero eigenvalue of H_ε. Then the error term $\mathcal{R}(\varepsilon)$, defined for $\varepsilon \in (0, \varepsilon_0)$ by*

$$\lambda(\varepsilon) = \varepsilon A e^{-\frac{E}{\varepsilon}} \left(1 + \mathcal{R}(\varepsilon)\right),$$

satisfies the following: there exists a constant $C > 0$ such that $|\mathcal{R}(\varepsilon)| \leqslant C\varepsilon^\gamma$ for every $\varepsilon \in (0, \varepsilon_0)$, with $\gamma = \frac{1}{2}$. The same holds true with $\gamma = 1$ under the additional asumption $f \in C^4(\mathbb{R}^d)$.

Remark 2.4. As shown in the author's PhD thesis [16], using the underlying Witten complex structure, the additional assumption $f \in C^\infty(\mathbb{R}^d)$ implies that $\mathcal{R}_\varepsilon$ admits full asymptotic expansions in powers of ε. The latter result is analogous to the result of [26] in continuous space setting. However the proof of complete expansions given in [16] is substantially more involved, since it requires a construction and detailed analysis of discrete WKB expansions on the level of 1-forms. We remark also that the geometric constraint imposed by the lattice becomes appreciable at the level of higher order corrections since the asymptotic expansion of $\mathcal{R}_\varepsilon$ differs in general from the one given in the continous setting.

As anticipated in the introduction, our main results can be easily translated into results on spectral properties of the class of metastable discrete diffusions with generator (4), (5). Since this might be a particularly interesting application of our results, we shall spell out precisely their consequences from the stochastic point of view.

2.3. Results on the diffusion operator L_ε. Given a function $f : \mathbb{R}^d \to \mathbb{R}$ and a parameter $\varepsilon > 0$, we consider the weight functions

$$\rho_\varepsilon(x) = e^{-\frac{f(x)}{\varepsilon}} \quad \text{and} \quad r_\varepsilon(x, x') = \frac{1}{\varepsilon} e^{-\frac{f(x')-f(x)}{2\varepsilon}}, \quad \forall x, x' \in \mathbb{R}^d.$$

Note that ρ_ε and r_ε are related by the identity

$$\rho_\varepsilon(x) r_\varepsilon(x, x') = \rho_\varepsilon(x') r_\varepsilon(x', x), \quad \forall \varepsilon > 0 \quad \text{and} \quad x, x' \in \mathbb{R}^d. \tag{11}$$

We work now in the weighted Hilbert space $\ell^2(\rho_\varepsilon)$ obtained as subspace of $\mathbb{R}^{\varepsilon\mathbb{Z}^d}$ by introducing the weighted scalar product

$$\langle \psi, \psi' \rangle_{\ell^2(\rho_\varepsilon)} = \varepsilon^d \sum_{x \in \varepsilon\mathbb{Z}^d} \psi(x)\, \psi'(x)\, \rho_\varepsilon(x),$$

and the corresponding induced norm $\|\cdot\|_{\ell^2(\rho_\varepsilon)}$. We shall denote by L_ε the Laplacian of the weighted graph $\varepsilon\mathbb{Z}^d$, whose vertices are weighted by ρ_ε and whose edges (determined by $\mathcal{N}$) are weighted by $\rho_\varepsilon r_\varepsilon$. More precisely we define $L_\varepsilon : \mathrm{Dom}(L_\varepsilon) \to \ell^2(\rho_\varepsilon)$ by setting

$$\mathrm{Dom}(L_\varepsilon) = \left\{ \psi \in \ell^2(\rho_\varepsilon) : L_\varepsilon \psi \in \ell^2(\rho_\varepsilon) \right\},$$

and, for each $x \in \varepsilon\mathbb{Z}^d$,

$$L_\varepsilon \psi(x) = \sum_{v \in \mathcal{N}} r_\varepsilon\,(x, x + \varepsilon v)\,[\psi(x + \varepsilon v) - \psi(x)], \quad \forall \psi \in \mathrm{Dom}(L_\varepsilon).$$

This provides a Hilbert space realization of the formal operator (4), (5).

Proposition 2.5. *For each $\varepsilon > 0$ the operators $-\varepsilon L_\varepsilon$ and H_ε are unitarily equivalent.*

Proof. Let $\varepsilon > 0$. We consider the unitary operator

$$\Phi_\varepsilon : \ell^2(\rho_\varepsilon) \to \ell^2(\varepsilon\mathbb{Z}^d), \quad \Phi_\varepsilon[\psi](x) = \sqrt{\rho_\varepsilon}(x)\psi(x).$$

Then a direct computation shows that

$$H_\varepsilon \psi = -\varepsilon \Phi_\varepsilon \left[L_\varepsilon \Phi_\varepsilon^{-1}[\psi] \right], \quad \forall \psi \in \mathrm{Dom}(\mathrm{V}_\varepsilon), \tag{12}$$

and that $\Phi_\varepsilon[\mathrm{Dom}(L_\varepsilon)] = \mathrm{Dom}(\mathrm{V}_\varepsilon)$. □

From the unitarily equivalence it follows that L_ε is not only symmetric and nonnegative (this can be checked by summation by parts and using the detailed balance condition (11)), but also selfadjoint. We remark also that $C_c(\varepsilon\mathbb{Z}^d)$, which is a core for H_ε and is invariant under Φ_ε, is also a core of L_ε.
Combining Proposition 2.5 with Theorems 2.2 and 2.3 yields then the following result.

Corollary 2.6. *Assume **H1** and denote by $N_0 \in \mathbb{N}_0$ the number of local minima of f. There exist constants $\varepsilon_0 \in (0, 1)$, $C > 0$ such that for each $\varepsilon \in (0, \varepsilon_0]$ the following properties hold true.*

(i) $\mathrm{Spec}_{ess}(-L_\varepsilon) \subset [\varepsilon^{-1}C, \infty)$ *and* $|\,\mathrm{Spec}_{disc}(-L_\varepsilon) \cap [0, C]| \leqslant N_0$.
(ii) $-L_\varepsilon$ *admits at least N_0 eigenvalues $\lambda_1, \ldots, \lambda_{N_0}(\varepsilon)$ counting multiplicity. In the nontrivial case that $N_0 \neq 0$, the N_0-th eigenvalue $\lambda_{N_0}(\varepsilon)$ (according to increasing order and counting multiplicity) satisfies the bounds*

$$0 \leqslant \lambda_{N_0}(\varepsilon) \leqslant e^{-\frac{C}{\varepsilon}}.$$

Moreover, assuming in addition ***H****2, it holds* $\lambda_1(\varepsilon) = 0$ *and, taking* A, E *as in* (8), (10), *the error term* $\mathcal{R}(\varepsilon)$, *defined for* $\varepsilon \in (0, \varepsilon_0)$ *by*

$$\lambda_2(\varepsilon) = Ae^{-\frac{E}{\varepsilon}} (1 + \mathcal{R}(\varepsilon)) , \tag{13}$$

satisfies the following: there exists a constant $C > 0$ *such that* $|\mathcal{R}(\varepsilon)| \leqslant C\varepsilon^\gamma$ *for every* $\varepsilon \in (0, \varepsilon_0)$, *with* $\gamma = \frac{1}{2}$. *The same holds true with* $\gamma = 1$ *under the additional asumption* $f \in C^4(\mathbb{R}^d)$.

We stress that (i) implies a quantitative scale separation between the N_0 slow modes, corresponding to the metastable tunneling times, and all the other modes, corresponding to fast relaxations to local equilibria. In principle it is also possible to refine the analysis of the fast modes revealing the full hierarchy of scales governing the dynamics in the small ε regime, see [19] for a Γ-convergence formulation in continuous space setting and the recent [4].

As already mentioned, the rigorous derivation of an Eyring-Kramers formula of type (13) in the setting of discrete metastable diffusions had already been derived by a different approach based on capacity estimates [7,9]. Compared to these previous results the formula given in (13) differs in two aspects:

(1) The estimate on the error term $\mathcal{R}(\varepsilon)$ is improved by our approach, since in [7, Theorems 10.9 and 10.10], under the same regularity assumptions as considered here ($f \in C^3(\mathbb{R}^d)$) a logarithmic correction appears. More precisely our result improves the error estimate from $\mathcal{R}(\varepsilon) = \mathcal{O}(\sqrt{\varepsilon[\log 1/\varepsilon]^3})$ to $\mathcal{R}(\varepsilon) = \mathcal{O}(\sqrt{\varepsilon})$. Further, we show that $\mathcal{R}(\varepsilon) = \mathcal{O}(\varepsilon)$ under the stronger assumption $f \in C^4(\mathbb{R}^d)$.
(2) The prefactor A given in (13) differs from the one given in [7,9]. This is due to our slightly different choice of jump rates, compare (5) with [7, (10.1.2.), p. 248]. Indeed it is clear that the prefactor is sensible to the particular choice of jump rates among the infinitely many possible jump rates satisfying the detailed balance condition with respect to the Boltzmann weight $e^{-f/\varepsilon}$. This sensitivity of the prefactor is opposed to the robustness of the exponential rate E, which is universal as can be seen e.g. via a Large Deviations analysis. We remark that, while the rates chosen in [7] correspond to a Metropolis algorithm, our choice (5) corresponds, in the context of the Statistical Mechanics models mentioned above, to a heat bath algorithm. This is a very natural choice and is considered for example in [38]. As observed in the introduction, it is the choice which in first order approximation gives the same prefactor as the continuous space model (3). Furthermore, [7,9] concerns discrete time processes, which means that the rates are normalized and thus bounded over $\mathbb{R}^d$. Our setting includes also the case of possibly unbounded rates which requires some additional technical work for the analysis outside compact sets.

3. General Tools for a Semiclassical Analysis on the Lattice

This section is devoted to some preliminary tools for a semiclassical analysis on the lattice.

Section 3.1 concerns a discrete IMS localization formula, see [45, Lemma 11.3] or [15, Theorem 3.2], where also an explanation of the name can be found, for the standard continuous space setting and [34]. The IMS formula is a simple observation based on a computation of commutators. It will be used repeteadly for decomposing the quadratic form induced by a Schrödinger operator into localized parts.

Section 3.2 provides estimates on the first two eigenvalues of the discrete semiclassical Harmonic oscillator. These estimates follow from more general results proven in [34]. Nevertheless we shall include a relatively short and completely selfcontained proof, which focuses on the estimates needed to prove the separation between exponentially small eigenvalues of H_ε and the rest of its spectrum, as provided by Theorem 2.2. The proof is based on a microlocalization which permits to separate high and low frequency actions of the operator.

Section 3.3 provides sharp asymptotic results for Laplace-type sums. These are instrumental in almost all the computations necessary for deriving the Eyring-Kramers formula for the eigenvalue splitting and for tunneling calculations in general. Our proofs are again based on Fourier analysis. In particular, following [16], we shall use the Poisson summation formula: shifting a function by an integer vector and summing over all shifts produces the same periodization as taking the Fourier series of the Fourier transform. Compared to [16], where it is shown how to get complete asymptotic expansions in the smooth setting, here we shall relax the regularity assumptions on the phase function to cover the applications we have in mind.

3.1. The discrete IMS formula. We say that the set $\{\chi_j\}_{j\in J}$ is a smooth quadratic partition of unity of $\mathbb{R}^d$ if J is a finite set, $\chi_j \in C^\infty(\mathbb{R}^d)$ for every $j \in J$ and $\sum_{j\in J}\chi_j^2 \equiv 1$.

Proposition 3.1. *There exists a constant $C > 0$ such that for every $\varepsilon > 0$, every $\psi \in \ell^2(\varepsilon\mathbb{Z}^d)$ and every smooth quadratic partition of unity $\{\chi_j\}_{j\in J}$ it holds*

$$\Big\|\Delta_\varepsilon\psi - \sum_{j\in J}\chi_j\,\Delta_\varepsilon\left(\chi_j\,\psi\right)\Big\|_{\ell^2(\varepsilon\mathbb{Z}^d)} \leqslant C\sup_{x,j}|\operatorname{Hess}\chi_j(x)|\|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)}.$$

Proof. We have

$$\Delta_\varepsilon\psi(x) - \sum_j\chi_j(x)\,\Delta_\varepsilon\left(\chi_j\,\psi\right)(x) = \tfrac{1}{\varepsilon^2}\sum_{v\in\mathcal{N}}\Big[1-\sum_j\chi_j(x)\chi_j(x+\varepsilon v)\Big]\psi(x+\varepsilon v),$$

thus

$$\begin{aligned}&\Big\|\Delta_\varepsilon\psi - \sum_j\chi_j\,\Delta_\varepsilon\left(\chi_j\,\psi\right)\Big\|_{\ell^2(\varepsilon\mathbb{Z}^d)}\\ &\quad\leqslant \tfrac{1}{\varepsilon^2}\sum_{v\in\mathcal{N}}\sup_{x\in\mathbb{R}^d}\Big|1-\sum_j\chi_j(x)\chi_j(x+\varepsilon v)\Big|\,\|\psi(\cdot+\varepsilon v)\|_{\ell^2(\varepsilon\mathbb{Z}^d)}.\end{aligned}\tag{14}$$

Differentiating the relation $\sum_j\chi_j^2 \equiv 1$ yields $\sum_j\chi_j\nabla\chi_j\cdot v \equiv 0$ for every v and therefore, by Taylor expansion, for every $x\in\mathbb{R}^d$, $v\in\mathcal{N}$ and $\varepsilon>0$,

$$\Big|1-\sum_j\chi_j(x)\chi_j(x+\varepsilon v)\Big| \leqslant \tfrac{\varepsilon^2}{2}\sup_{y\in\mathbb{R}^d}\sum_j|\chi_j(y)|\,|\operatorname{Hess}\chi_j(y)v\cdot v|.\tag{15}$$

The claim follows now from (14) and (15) by noting that the assumption $\sum_j\chi_j^2\equiv 1$ also implies $\sup_{j,x}|\chi_j(x)|\leqslant 1$, that $\|\psi(\cdot+\varepsilon v)\|_{\ell^2(\varepsilon\mathbb{Z}^d)} = \|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)}$ for every v and recalling that $\mathcal{N}$ is bounded. □

3.2. Estimates on the discrete semiclassical Harmonic oscillator. We provide lower bounds for the first and the second eigenvalue of the semiclassical discrete Harmonic oscillator.

Proposition 3.2. *For every $x \in \mathbb{R}^d$ let $U(x) = \langle x - \bar{x}, M(x - \bar{x})\rangle$, where $\bar{x} \in \mathbb{R}^d$ and M is a symmetric $d \times d$ real matrix with strictly positive eigenvalues denoted by $\kappa_1, \dots, \kappa_d$. Moreover let $\lambda_0 = \sum_j \sqrt{\kappa_j}$ and $\lambda_1 = \sum_j \sqrt{\kappa_j} + 2\min_j \sqrt{\kappa_j}$. Then there exist for every $\varepsilon > 0$ a function $\Psi_\varepsilon \in \ell^2(\varepsilon\mathbb{Z}^d)$ and constants $\varepsilon_0, C > 0$ such that for every $\varepsilon \in (0, \varepsilon_0]$ and $\psi \in C_c(\varepsilon\mathbb{Z}^d)$ the following hold:*

(i) $\langle\left(-\varepsilon^2\Delta_\varepsilon + U\right)\psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant \varepsilon\left(\lambda_0 - C\varepsilon^{\frac{1}{5}}\right)\|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}$.

(ii) $\langle\left(-\varepsilon^2\Delta_\varepsilon + U\right)\psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant \varepsilon\left(\lambda_1 - C\varepsilon^{\frac{1}{5}}\right)\|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} - \langle\psi, \Psi_\varepsilon\rangle^2_{\ell^2(\varepsilon\mathbb{Z}^d)}$.

The proof is by localization around low frequencies in Fourier space and comparison with the corresponding continuous Harmonic oscillator on $\mathbb{R}^d$, whose first and second eigenvalue are given respectively by $\varepsilon\lambda_0$ and $\varepsilon\lambda_1$. At low frequencies, discrete and continuous Harmonic oscillators are close, while the high frequencies do not contribute to the bottom of the spectrum.

In the proof we shall use the following notation: for $\varepsilon > 0$ and $\psi \in \ell^1(\varepsilon\mathbb{Z}^d)$ we define

$$\hat{\psi}(\xi) := \mathcal{F}[\psi](\xi) := (2\pi)^{-\frac{d}{2}} \sum_{x\in\varepsilon\mathbb{Z}^d} \psi(x)\, e^{-\frac{\mathrm{i}x\cdot\xi}{\varepsilon}} \quad \text{for} \quad \xi \in \mathbb{R}^d,$$

and for $\varepsilon > 0$ and $\phi \in L^1(\mathbb{R}^d)$ we define

$$\check{\phi}(\xi) := \mathcal{G}[\psi](\xi) := (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \phi(x)\, e^{\frac{\mathrm{i}x\cdot\xi}{\varepsilon}}\, dx \quad \text{for} \quad \xi \in \mathbb{R}^d.$$

Then by Parseval's theorem

$$\|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)} = \|\hat{\psi}\|_{L^2([-\pi,\pi]^d)} \quad \forall\psi \in \ell^2(\varepsilon\mathbb{Z}^d), \tag{16}$$

and by Plancherel's theorem

$$\|\phi\|_{L^2(\mathbb{R}^d)} = \|\check{\phi}\|_{L^2(\mathbb{R}^d)} \quad \forall\phi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d). \tag{17}$$

We recall also the inversion theorem for the Fourier transform and Fourier series, which in our notation reads as follows. Let $\phi \in S(\mathbb{R}^d)$, the Schwartz space on $\mathbb{R}^d$, and let $\tilde{\phi}(x) = \check{\phi}(-x)$ for every $x \in \mathbb{R}^d$. Then

$$\phi(\xi) = \check{\tilde{\phi}}(\xi) \quad \forall\xi \in \mathbb{R}^d. \tag{18}$$

Moreover, for every $\phi \in C^\infty(\mathbb{R}^d)$ with $\operatorname{supp}(\phi) \subset (-\pi, \pi)^d$ it holds $\check{\phi} \in \ell^1(\varepsilon\mathbb{Z}^d)$ and

$$\phi(\xi) = \hat{\check{\phi}}(\xi) = \mathcal{F}[\mathcal{G}[\phi]](\xi) \quad \forall\xi \in [-\pi, \pi]^d. \tag{19}$$

Proof of Proposition 3.2. Let $\varepsilon \in (0, 1]$, $\psi \in C_c(\varepsilon\mathbb{Z}^d)$ and let $\varphi := \left(-\varepsilon^2\Delta_\varepsilon + U\right)\psi$. Then $\phi \in C_c(\varepsilon\mathbb{Z}^d)$ and $\hat{\varphi} = (W - A_\varepsilon)\hat{\psi}$, where $W : \mathbb{R}^d \to \mathbb{R}$ is a multiplication operator given by

$$W(\xi) := 4\sum_{j=1}^{d}\sin^2\left(\frac{\xi_j}{2}\right),$$

and A_ε is a second order differential operator given by

$$A_\varepsilon := \sum_{j,k=1}^{d} M_{j,k}\left(\varepsilon^2\partial_j\partial_k + \varepsilon\, 2\bar{x}_k \mathrm{i}\partial_j - \bar{x}_k\bar{x}_j\right).$$

It follows then by Parseval's theorem (16) that

$$\langle\left(-\varepsilon^2\Delta_\varepsilon \; + U\right)\psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \langle(W - A_\varepsilon)\hat{\psi}, \hat{\psi}\rangle_{L^2([-\pi,\pi]^d)}. \tag{20}$$

We now consider a cut-off function $\theta \in C^\infty(\mathbb{R}^d; [0, 1])$ which equals 1 on $\{\xi : |\xi| \leqslant 1\}$ and vanishes on $\{\xi : |\xi| \geqslant 2\}$. For $j = 1, \ldots, N$ we define with $s = \frac{2}{5}$ the ε-dependent smooth quadratic partition of unity $\{\theta_{0,\varepsilon}, \theta_{1,\varepsilon}\}$ by setting

$$\theta_{0,\varepsilon}(\xi) := \theta\left(\varepsilon^{-s}(\xi)\right) \quad \theta_{1,\varepsilon}(\xi) := \sqrt{1 - \theta_{0,\varepsilon}^2(\xi)}.$$

Moreover we denote by W_0 the leading term in the ξ-expansion of the function W around the origin, i.e.

$$W_0(\xi) := \tfrac{1}{2}\,\mathrm{Hess}\,W(0)\,\xi\cdot\xi = |\xi|^2 \quad \forall\xi \in \mathbb{R}^d.$$

A simple rearrangement of terms gives

$$\begin{aligned}\langle(W - A_\varepsilon)\hat{\psi}, \hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} &= \langle(W_0 - A_\varepsilon)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)}\\ &\quad+\langle(W - A_\varepsilon)\;\theta_{1,\varepsilon}\hat{\psi}, \theta_{1,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)}\\ &\quad+\mathcal{E}_1(\varepsilon) + \mathcal{E}_2(\varepsilon),\end{aligned} \tag{21}$$

where the localization errors $\mathcal{E}_1(\varepsilon)$, $\mathcal{E}_2(\varepsilon)$ are given by

$$\begin{aligned}\mathcal{E}_1(\varepsilon) &:= \langle(W - W_0)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)},\\ \mathcal{E}_2(\varepsilon) &:= -\sum_{j=0}^{1}\langle\left(\theta_{j,\varepsilon}A_\varepsilon - A_\varepsilon\theta_{j,\varepsilon}\right)\hat{\psi}, \theta_{j,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)}.\end{aligned}$$

The four terms in the right hand side of (21) are analyzed separately in the following.

(1) *Analysis of the first term in the right hand side of* (21).

Using that $\operatorname{supp}\theta_{0,\varepsilon} \subset (-\pi, \pi)^d$ for $\varepsilon \in (0, 1]$, Plancherel's theorem (17) and that the smallest eigenvalue of the Harmonic Oscillator $-\varepsilon^2\Delta + U$ on $\mathbb{R}^d$ is λ_0, gives

$$\begin{aligned}&\langle(W_0 - A_\varepsilon)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} = \langle(W_0 - A_\varepsilon)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2(\mathbb{R}^d)}\\ &= \langle\left(-\varepsilon^2\Delta + U\right)\mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}]\rangle_{L^2(\mathbb{R}^d)} \geqslant \varepsilon\lambda_0\left\|\mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}]\right\|^2_{L^2(\mathbb{R}^d)}\end{aligned}$$

$$= \varepsilon\lambda_0 \|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2(\mathbb{R}^d)} = \varepsilon\lambda_0 \|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} \quad \forall\varepsilon \in (0,1]. \tag{22}$$

Moreover, considering for $\varepsilon > 0$ the ground state

$$g_\varepsilon(x) := \frac{e^{-\frac{\langle x,\sqrt{M}x\rangle}{2\varepsilon}}}{\left\|e^{-\frac{\langle x,\sqrt{M}x\rangle}{2\varepsilon}}\right\|_{L^2(\mathbb{R}^d)}},$$

an analogous computation gives for $\varepsilon \in (0, 1]$ the estimate

$$\begin{aligned}
&\langle (W_0 - A_\varepsilon)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} = \langle \left(-\varepsilon^2\Delta + U\right)\mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}]\rangle_{L^2(\mathbb{R}^d)} \\
&\geqslant \varepsilon\lambda_0 \langle \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], g_\varepsilon\rangle^2_{L^2(\mathbb{R}^d)} + \varepsilon\lambda_1\left(\|\mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}]\|^2_{L^2(\mathbb{R}^d)} - \langle \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], g_\varepsilon\rangle^2_{L^2(\mathbb{R}^d)}\right) \\
&= \varepsilon\lambda_1 \|\mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}]\|^2_{L^2(\mathbb{R}^d)} - 2\varepsilon \min_j \sqrt{\kappa_j}\langle \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], g_\varepsilon\rangle^2_{L^2(\mathbb{R}^d)} \\
&= \varepsilon\lambda_1 \|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} - 2\varepsilon \min_j \sqrt{\kappa_j}\langle \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], \mathcal{G}[\tilde{g}_\varepsilon]\rangle^2_{L^2(\mathbb{R}^d)},
\end{aligned}$$

where for the last equality the Fourier inversion theorem (18) is used for g_ε. Moreover using (17), (19) and (16) we get

$$\begin{aligned}
&\langle \mathcal{G}[\theta_{0,\varepsilon}\hat{\psi}], \mathcal{G}[\tilde{g}_\varepsilon]\rangle_{L^2(\mathbb{R}^d)} = \langle \theta_{0,\varepsilon}\hat{\psi}, \tilde{g}_\varepsilon\rangle_{L^2(\mathbb{R}^d)} = \langle \hat{\psi}, \theta_{0,\varepsilon}\tilde{g}_\varepsilon\rangle_{L^2([-\pi,\pi]^d)} \\
&\quad = \langle \mathcal{F}[\psi], \mathcal{F}[\mathcal{G}[\theta_{0,\varepsilon}\tilde{g}]]_\varepsilon\rangle_{L^2([-\pi,\pi]^d)} = \langle \psi, \mathcal{G}[\theta_{0,\varepsilon}\tilde{g}_\varepsilon]\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}.
\end{aligned}$$

Thus, setting for shortness

$$\Phi_\varepsilon(\xi) := \sqrt{2\varepsilon}\min_j \kappa_j^{\frac{1}{4}}\tilde{g}_\varepsilon(\xi) \quad \text{for } \xi \in \mathbb{R}^d,$$

we can conclude that

$$\begin{aligned}
&\langle (W_0 - A_\varepsilon)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} \\
&\quad \geqslant \varepsilon\lambda_1 \|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} - \langle \psi, \mathcal{G}[\theta_{0,\varepsilon}\Phi_\varepsilon]\rangle^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall\varepsilon \in (0,1].
\end{aligned} \tag{23}$$

(2) *Analysis of the second term in the right hand side of* (21).
Using the inequality $\sin\frac{t}{2} \geqslant \frac{t}{4}$ for $t \in [0, \pi]$ gives

$$W(\xi) = 4\sum_{j=1}^{d}\sin^2\left(\frac{\xi_j}{2}\right) \geqslant \frac{1}{4}|\xi|^2 \quad \forall\xi \in [-\pi,\pi]^d. \tag{24}$$

Since $\operatorname{supp}\theta_{1,\varepsilon} \subset \{\xi \in \mathbb{R}^d : |\xi| \geqslant 2\varepsilon^{\frac{2}{5}}\}$ for $\varepsilon \in (0, 1]$, the bound (24) implies

$$\langle W\theta_{1,\varepsilon}\hat{\psi}, \theta_{1,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} \geqslant \varepsilon^{\frac{4}{5}}\|\theta_{1,\varepsilon}\hat{\psi}|^2_{L^2([-\pi,\pi]^d)} \quad \forall\varepsilon \in (0,1]. \tag{25}$$

Moreover, since $\hat{\psi}$ is periodic and $\theta_{1,\varepsilon}$ equals 1 around the boundary of $[-\pi,\pi]^d$ for $\varepsilon \in (0, 1]$, integration by parts gives

$$\langle -A_\varepsilon\,\theta_{1,\varepsilon}\hat{\psi}, \theta_{1,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} \geqslant 0 \quad \forall\xi \in (0,1]. \tag{26}$$

In particular, it follows from (25) and (26) that there exists an $\varepsilon_0' \in (0, 1]$ such that for all $\varepsilon \in (0, \varepsilon_0']$

$$\langle (W - A_\varepsilon)\ \theta_{1,\varepsilon}\hat{\psi}, \theta_{1,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)} \geqslant \varepsilon\lambda_1 \|\theta_{1,\varepsilon}\hat{\psi}|^2_{L^2([-\pi,\pi]^d)}. \tag{27}$$

(3) *Analysis of the localization error $\mathcal{E}_1$.*
Since by Taylor expansion there exists a $C' > 0$ such that $|W(\xi) - W_0(\xi)| \leqslant C'|\xi|^3$ for $|\xi| \leqslant 2$, one gets

$$\begin{aligned}|\mathcal{E}_1(\varepsilon)| &= \left|\langle (W - W_0)\,\theta_{0,\varepsilon}\hat{\psi}, \theta_{0,\varepsilon}\hat{\psi}\rangle_{L^2([-\pi,\pi]^d)}\right| \\ &\leqslant \sup_{|\xi|<2\varepsilon^{\frac{2}{5}}} |W(\xi) - W_0(\xi)|\ \|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} \\ &\leqslant 8C'\,\varepsilon^{\frac{6}{5}}\ \|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} \quad \forall\varepsilon \in (0, 1].\end{aligned}$$

In particular, since $\|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} \leqslant \|\hat{\psi}\|^2_{L^2([-\pi,\pi]^d)} = \|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}$, it follows that

$$\mathcal{E}_1(\varepsilon) \geqslant -8C'\,\varepsilon^{\frac{6}{5}}\ \|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall\varepsilon \in (0, 1]. \tag{28}$$

(4) *Analysis of the localization error $\mathcal{E}_2$.*
A straightforward computation (see also [45, Lemma 11.3]) gives the IMS localization formula

$$A_\varepsilon\hat{\psi} - \sum_{j=0}^{1}\theta_{j,\varepsilon}A_\varepsilon(\theta_{j,\varepsilon}\hat{\psi}) = \varepsilon^2\sum_{j=0}^{1}\langle\nabla\theta_{j,\varepsilon}, M\nabla\theta_{j,\varepsilon}\rangle\hat{\psi}(\xi) \ \text{ on } \mathbb{R}^d.$$

Thus there exists a constant $C'' > 0$ such that

$$\begin{aligned}|\mathcal{E}_2(\varepsilon)| &\leqslant \varepsilon^2\sum_{j=0}^{1}\sup_{\xi\in\mathbb{R}^d}|\langle\nabla\theta_{j,\varepsilon}(\xi), M\nabla\theta_{j,\varepsilon}(\xi)\rangle|\ \|\hat{\psi}\|_{L^2([-\pi,\pi]^d)} \\ &\leqslant C''\,\varepsilon^{2-2s}\ \|\hat{\psi}\|_{L^2([-\pi,\pi]^d)} \quad \forall\varepsilon \in (0, 1].\end{aligned}$$

Recalling that $s = \frac{2}{5}$ and the Parseval theorem (16) we conclude that

$$\mathcal{E}_2(\varepsilon) \geqslant -C''\varepsilon^{\frac{6}{5}}\ \|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall\varepsilon \in (0, 1]. \tag{29}$$

Final step.
Statement (i) in the theorem follows by putting together (20), (21), (22), (27), (28) and (29), chosing $C = 8C' + C''$ and $\varepsilon_0 = \varepsilon_0'$ and observing that

$$\|\theta_{0,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d} + \|\theta_{1,\varepsilon}\hat{\psi}\|^2_{L^2([-\pi,\pi]^d} = \|\hat{\psi}\|^2_{L^2([-\pi,\pi]^d} = \|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}.$$

Statement (ii) follows similarly, but using (23) instead of (22) and chosing $\Psi_\varepsilon = \widetilde{\theta_{0,\varepsilon}\Phi_\varepsilon}\Big|_{\varepsilon\mathbb{Z}^d}$. □

3.3. Laplace asymptotics on $\varepsilon\mathbb{Z}^d$. Given $x_0 \in \mathbb{R}^d$ and $\delta > 0$ we denote by $B_\delta(x_0) = \{x \in \mathbb{R}^d : |x - x_0| < \delta\}$ the open ball of radius δ around x_0 and, for each $\varepsilon > 0$, by $B_\delta^\varepsilon(x_0) = B_\delta(x_0) \cap \varepsilon\mathbb{Z}^d$ its intersection with $\varepsilon\mathbb{Z}^d$ and by $[B_\delta^\varepsilon(x_0)]^c = \varepsilon\mathbb{Z}^d \backslash B_\delta^\varepsilon(x_0)$ the complementary of $B_\delta^\varepsilon(x_0)$.

Proposition 3.3. *Let $q(x) = \frac{1}{2}x \cdot Qx$, where Q is a symmetric, positive definite $d \times d$ matrix and let $x_0 \in \mathbb{R}^d$ and $m \in \mathbb{N}_0$. Then there exists a $\gamma > 0$ such that for every $\varepsilon \in (0, 1]$*

$$\varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} |x - x_0|^{2m} e^{-\frac{q(x-x_0)}{\varepsilon}} = \varepsilon^m \int_{\mathbb{R}^d} |x - x_0|^{2m} e^{-q(x-x_0)}\, dx + \mathcal{O}(e^{-\frac{\gamma}{\varepsilon}}). \quad (30)$$

Moreover for every $\delta > 0$ there exists $\gamma(\delta) > 0$ such that for every $\varepsilon \in (0, 1]$

$$\sum_{x \in B_\delta^\varepsilon(x_0)} |x - x_0|^{2m} e^{-\frac{q(x-x_0)}{\varepsilon}} = \sum_{x \in \varepsilon\mathbb{Z}^d} |x - x_0|^{2m} e^{-\frac{q(x-x_0)}{\varepsilon}} \left(1 + \mathcal{O}(e^{-\frac{\gamma(\delta)}{\varepsilon}})\right). \quad (31)$$

Remark 3.4. The Gaussian integrals appearing on the right hand side of (30) can be computed explicitly. We shall use in the sequel the explicit value only for $m = 0$, in which case (30) becomes

$$\varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} e^{-\frac{q(x-x_0)}{\varepsilon}} = \sqrt{\frac{(2\pi)^d}{\det Q}} + \mathcal{O}(e^{-\frac{\gamma}{\varepsilon}}).$$

We shall also use the following estimate for odd moments:

$$\varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} |x - x_0|^m e^{-\frac{q(x-x_0)}{\varepsilon}} = \mathcal{O}(\varepsilon^{\frac{m}{2}}) \quad \text{for} \quad m = 1, 3, \ldots, \quad (32)$$

The latter follows from Proposition 3.3 and the Cauchy–Schwarz inequality

$$\left| \varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} |x - x_0|^m e^{-\frac{q(x-x_0)}{\varepsilon}} \right| \leqslant \left(\varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} |x - x_0|^{2m} e^{-\frac{q(x-x_0)}{\varepsilon}} \right)^{\frac{1}{2}} \left(\varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} e^{-\frac{q(x-x_0)}{\varepsilon}} \right)^{\frac{1}{2}}.$$

Proof of Proposition 3.3. The function $x \mapsto u(x) := |x|^{2m} e^{-q(x-x_0)}$ is in the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ and its Fourier transform $\hat{u}(x) := \int_{\mathbb{R}^d} u(y)\, e^{-2\pi \mathrm{i} x \cdot y}\, dy$ satisfies the Poisson summation formula (see e.g. [44, Corollary 2.6, p. 252])

$$\sum_{x \in \mathbb{Z}^d} u(x) = \sum_{x \in \mathbb{Z}^d} \hat{u}(x).$$

It follows that

$$\varepsilon^{\frac{d}{2}} \sum_{x \in \varepsilon\mathbb{Z}^d} |x - x_0|^{2m} e^{-\frac{q(x-x_0)}{\varepsilon}} = \varepsilon^{\frac{d}{2}+m} \sum_{x \in \mathbb{Z}^d} |\sqrt{\varepsilon}(x - \tfrac{x_0}{\varepsilon})|^{2m}\, e^{q(\sqrt{\varepsilon}(x - \frac{x_0}{\varepsilon}))} =$$

$$= \varepsilon^{\frac{d}{2}+m} \sum_{x\in\mathbb{Z}^d} u(\sqrt{\varepsilon}(x - \tfrac{x_0}{\varepsilon})) = \varepsilon^m \sum_{x\in\mathbb{Z}^d} e^{-\frac{2\pi i x\cdot x_0}{\varepsilon}} \hat{u}(\tfrac{x}{\sqrt{\varepsilon}})$$
$$= \varepsilon^m \int_{\mathbb{R}^d} u(x)\, dx + R_\varepsilon,$$

with

$$R_\varepsilon := \varepsilon^m \sum_{x\in\mathbb{Z}^d\setminus\{0\}} e^{-\frac{2\pi i x\cdot x_0}{\varepsilon}} \hat{u}(\tfrac{x}{\sqrt{\varepsilon}}).$$

Since $\hat{u}$ is a linear combination of derivatives of Gaussian functions, there exist constants $C, \gamma > 0$ such that

$$|\hat{u}(x)| \leqslant Ce^{-2\gamma|x|^2} \quad \forall x \in \mathbb{R}^d.$$

It follows that for every $\varepsilon \in (0, 1]$

$$|R_\varepsilon| \leqslant C\varepsilon^m \sum_{x\in\mathbb{Z}^d\setminus\{0\}} e^{-\frac{2\gamma|x|^2}{\varepsilon}} = C\varepsilon^m e^{-\frac{\gamma}{\varepsilon}} \sum_{x\in\mathbb{Z}^d\setminus\{0\}} e^{-\frac{\gamma}{\varepsilon}(2|x|^2-1)} \leqslant C' e^{-\frac{\gamma}{\varepsilon}},$$

with $C' := C \sum_{x\in\mathbb{Z}^d\setminus\{0\}} e^{-\gamma(2|x|^2-1)}$ which concludes the proof of (30).

In order to prove (31), fix $\delta > 0$ and note that, due to the positive definiteness of Q, there exists a constant $C > 0$ such that $q(x) > C\delta^2$ for every $x \in [B_\delta^\varepsilon(x_0)]^c$. Thus, for $\varepsilon \in (0, 1]$,

$$\sum_{x\in[B_\delta^\varepsilon(x_0)]^c} e^{-\frac{q(x-x_0)}{\varepsilon}} = e^{-\frac{C\delta^2}{\varepsilon}} \sum_{x\in[B_\delta^\varepsilon(x_0)]^c} e^{-\frac{q(x-x_0)-C\delta^2}{\varepsilon}} \leqslant$$
$$\leqslant \varepsilon^{-d} e^{-\frac{C\delta^2}{\varepsilon}} e^{C\delta^2} \varepsilon^d \sum_{x\in[B_\delta^\varepsilon(x_0)]^c} e^{-q(x-x_0)} \leqslant \varepsilon^{-d} e^{-\frac{C\delta^2}{\varepsilon}} K, \tag{33}$$

with $K = e^{C\delta^2}\left(\int_{\mathbb{R}^d} e^{-q(x-x_0)} dx + 1\right)$. To see the last inequality one can use e.g. the Poisson summation formula for $\varepsilon^d \sum_{x\in\varepsilon\mathbb{Z}^d} e^{-q(x-x_0)}$. From (33), chosing $\gamma > 0$ sufficiently small and $C' > 0$ sufficiently large we obtain

$$\sum_{x\in[B_\delta^\varepsilon(x_0)]^c} e^{-\frac{q(x-x_0)}{\varepsilon}} \leqslant C' e^{-\frac{\gamma}{\varepsilon}}.$$

The estimate (31) for $m = 0$ follows then using (30) with $m = 0$. The case of positive m can be proven in the same way. □

The following proposition concerns more general, not necessarily quadratic phase functions.

Proposition 3.5. *Let* $x_0 \in \mathbb{R}^d$, $\delta > 0$, $k \in \{3, 4\}$ *and* $\varphi \in C^k(\overline{B_\delta(x_0)})$ *s.t.*

$$\varphi(x_0) = 0, \ \operatorname{Hess}\varphi(x_0) > 0 \textit{ and } \varphi(x) > 0 \textit{ for every } x \in \overline{B_\delta(x_0)}. \tag{34}$$

Moreover let $m \in \mathbb{N}_0$. *Then for* $\varepsilon \in (0,1]$ *it holds*

$$\varepsilon^{\frac{d}{2}} \sum_{x \in B_\delta^\varepsilon(x_0)} |x - x_0|^{2m} e^{-\frac{\varphi(x)}{\varepsilon}} = \varepsilon^m \int_{\mathbb{R}^d} |x - x_0|^{2m} e^{-q(x-x_0)}\, dx \left(1 + \mathcal{O}(\varepsilon^{\frac{k-2}{2}})\right), \tag{35}$$

where $q(x) = \frac{1}{2} \operatorname{Hess} \varphi(x_0) x \cdot x$ *for all* $x \in \mathbb{R}^d$.

Remark 3.6. Finer asymptotic expansions for Laplace-type sums have been proven in [16, Appendix C] under the stronger regularity assumption $\varphi \in C^\infty(B_\delta(x_0))$.

Proof. We reduce the problem to the quadratic case of Proposition 3.3. For $x \in \overline{B_\delta(x_0)}$ let for short $r(x) = \varphi(x) - q(x - x_0)$ and note that there exist $\alpha, \delta' > 0$ such that $\tilde{q}(x) := \alpha |x|^2$ satisfies

$$\tilde{\varphi}(x) := q(x - x_0) - |r(x)| \geqslant \tilde{q}(x - x_0) \quad \forall x \in \overline{B_{\delta'}(x_0)}, \tag{36}$$

and also $\varphi(x) \geqslant \tilde{q}(x - x_0)$ for all $x \in \overline{B_\delta(x_0)}$. Indeed, the assumption $\varphi \in C^3(\overline{B_\delta(x_0)})$ implies the existence of a constant $C > 0$ such that $|r(x)| \leqslant C|x - x_0|^3$ for all $x \in \overline{B_\delta(x_0)}$. It follows that, denoting by $\lambda > 0$ the smallest eigenvalue of $\operatorname{Hess}\varphi(x_0)$ and taking e.g. $\delta' = \frac{\lambda}{4C}$ and $\alpha' = \frac{\lambda}{4}$,

$$\tilde{\varphi}(x) \geqslant (\tfrac{\lambda}{2} - C\delta')|x - x_0|^2 \geqslant \tfrac{\lambda}{4}|x - x_0|^2 \quad \forall x \in \overline{B_{\delta'}(x_0)}.$$

Note that, a fortiori, also $\varphi(x) \geqslant \tilde{q}(x)$ for every $x \in B_{\delta'}(x_0)$. Moreover, since $\frac{\varphi(x)}{|x|^2}$ is continuous and stricly positive on the compact set $\overline{B_\delta(x_0)} \setminus B_{\delta'}(x_0)$ we can take e.g.

$$\alpha = \min\{\alpha', \inf_{x \in \overline{B_\delta(x_0)} \setminus B_{\delta'}(x_0)} \tfrac{\varphi(x)}{|x|^2}\}.$$

It will be enough to prove (35) with the sum on the left hand side restricted to $B_{\delta'}^\varepsilon(x_0)$, since by Proposition 3.3 there exists a $\gamma > 0$ s.t. for $\varepsilon \in (0,1]$

$$\sum_{x \in B_\delta^\varepsilon(x_0) \setminus B_{\delta'}^\varepsilon(x_0)} |x - x_0|^{2m} e^{-\frac{\varphi(x)}{\varepsilon}} \leqslant \sum_{x \in [B_{\delta'}^\varepsilon(x_0)]^c} |x - x_0|^{2m} e^{-\frac{\tilde{q}(x - x_0)}{\varepsilon}} = \mathcal{O}(e^{-\gamma/\varepsilon}).$$

We shall consider the decomposition

$$\varepsilon^{\frac{d}{2}} \sum_{x \in B_{\delta'}^\varepsilon(x_0)} |x - x_0|^{2m} e^{-\frac{\varphi(x)}{\varepsilon}} = I_0(\varepsilon) + I_1(\varepsilon) + I_3(\varepsilon), \tag{37}$$

with, setting for short $u_\varepsilon(x) = |x - x_0|^{2m} e^{-\frac{q(x)}{\varepsilon}}$,

$$I_0(\varepsilon) = \varepsilon^{\frac{d}{2}} \sum_{x \in B_{\delta'}^\varepsilon(x_0)} u_\varepsilon(x), \quad I_1(\varepsilon) = \varepsilon^{\frac{d}{2}} \sum_{x \in B_{\delta'}^\varepsilon(x_0)} \varepsilon^{-1} r(x) u_\varepsilon(x)$$

and

$$I_2(\varepsilon) = \varepsilon^{\frac{d}{2}} \sum_{x \in B_{\delta'}^\varepsilon(x_0)} \left(e^{-\frac{r(x)}{\varepsilon}} - 1 - \varepsilon^{-1} r(x)\right) u_\varepsilon(x).$$

It follows from Proposition 3.3 that there exists a $\gamma > 0$ s.t. for $\varepsilon \in (0, 1]$

$$I_0(\varepsilon) = \varepsilon^m \int_{\mathbb{R}^d} |x - x_0|^{2m} e^{-q(x-x_0)}\, dx + \mathcal{O}(e^{-\frac{\gamma}{\varepsilon}}). \tag{38}$$

Moreover, using $|r(x)| \leqslant C|x - x_0|^3$ for all $x \in \overline{B_\delta(x_0)}$ and (36) gives

$$\begin{aligned} |I_2(\varepsilon)| &\leqslant \tfrac{1}{2}\varepsilon^{\frac{d}{2}-2} \sum_{x\in B^{\varepsilon}_{\delta'}(x_0)} |r(x)|^2 e^{\frac{|r(x)|}{\varepsilon}} u_\varepsilon(x) \\ &\leqslant \tfrac{C}{2}\varepsilon^{\frac{d}{2}-2} \sum_{x\in B^{\varepsilon}_{\delta'}(x_0)} |x - x_0|^{2m+6} e^{-\frac{\tilde{q}(x-x_0)}{\varepsilon}} = \mathcal{O}(\varepsilon^{m+1}), \end{aligned} \tag{39}$$

with the last estimate being a consequence of Proposition 3.3. Finally, in order to analyze the term $I_1(\varepsilon)$, we consider first the case $k = 3$. We then have by (32)

$$|I_1(\varepsilon)| \leqslant \varepsilon^{\frac{d}{2}-1} C \sum_{x\in B^{\varepsilon}_{\delta'}(x_0)} |x - x_0|^{2m+3} e^{-\frac{q(x-x_0)}{\varepsilon}} = \mathcal{O}(\varepsilon^{m+\frac{1}{2}}),$$

which together with (37), (38) and (39) finishes the proof for $k = 3$. For the case $k = 4$ we write $r(x) = t_3(x) + \rho(x)$, where $t_3 : \overline{B_{\delta'}(x_0)} \to \mathbb{R}$ is the cubic term in the Taylor expansion of φ around x_0, thus satisfying $t_3(x_0 + x) = t_3(x_0 - x)$, and $\rho : \overline{B_{\delta'}(x_0)} \to \mathbb{R}$ satisfies $|\rho(x)| \leqslant C'|x - x_0|^4$ for some $C' > 0$. We then have

$$I_1(\varepsilon) = \varepsilon^{\frac{d}{2}-1} \sum_{x\in B^{\varepsilon}_{\delta'}(x_0)} (t_3(x) + \rho(x))\, u_\varepsilon(x) = \varepsilon^{\frac{d}{2}-1} \sum_{x\in B^{\varepsilon}_{\delta'}(x_0)} \rho(x) u_\varepsilon(x),$$

and therefore by Proposition 3.3

$$|I_1(\varepsilon)| \leqslant \varepsilon^{\frac{d}{2}-1} C' \sum_{x\in B^{\varepsilon}_{\delta'}(x_0)} |x - x_0|^{2m+4} e^{-\frac{q(x-x_0)}{\varepsilon}} = \mathcal{O}(\varepsilon^{m+1}),$$

which finishes the proof in the case $k = 4$. □

4. Proof of Theorem 2.2

Recall the definition of V_ε given in (6). To prove Theorem 2.2 we shall reduce to suitable localized problems and then exploit basic pointwise estimates on V_ε as stated in the following two complementary lemmata. The first one gives a uniform strictly positive lower bound on V_ε away from critical points. The second one concerns the local behavior of V_ε around critical points. Note that these bounds are almost immediate to obtain, even under weaker assumptions, if instead of V_ε one considers the corresponding continuous space potential $\frac{1}{4}|\nabla f|^2 - \frac{\varepsilon}{2}\Delta f$ appearing in (3). The discrete case follows from straightforward Taylor expansions and elementary estimates. We shall give the details of the arguments at the end of this section for completeness.

Lemma 4.1. *Assume $f \in C^2(\mathbb{R}^d)$ and that* Hess f *is bounded on $\mathbb{R}^d$. Let $S \subset \mathbb{R}^d$ and $a > 0$ such that $|\nabla f(x)| > a$ for every $x \in S$. Then there exist constants $\varepsilon_0, C > 0$ such that*

$$V_\varepsilon(x) \geqslant C \quad \forall x \in S \quad \textit{and} \quad \forall \varepsilon \in (0, \varepsilon_0].$$

Lemma 4.2. *Assume $f \in C^3(\mathbb{R}^d)$. Let $z \in \mathbb{R}^d$ such that $\nabla f(z) = 0$, $R > 0$ and*

$$U(x) := \frac{1}{4}\langle [\mathrm{Hess}\, f(z)]^2\,(x-z), (x-z)\rangle.$$

Then there exists a constant $C > 0$ such that for all $x \in B_R(z)$ and $\varepsilon > 0$

$$|V_\varepsilon(x) - U(x) + \frac{\varepsilon}{2}\Delta f(z)| \leqslant C\left(|x-z|^3 + \varepsilon\,|x-z| + \varepsilon^2\right).$$

After these preliminary estimates on V_ε we turn to the proof of Theorem 2.2. We first show that the essential spectrum of H_ε is bounded from below by a constant, as claimed in Theorem 2.2 (i).

Proposition 4.3 (Localization of the essential spectrum). *Under Assumption **H1** there exist constants $\varepsilon_0, C > 0$ such that*

$$\mathrm{Spec}_{ess}(H_\varepsilon) \subset [C, \infty) \quad \forall \varepsilon \in (0, \varepsilon_0].$$

Remark 4.4. The proof given below shows that the claim of Proposition 4.3 still holds without assuming that the critical points of f are nondegenerate. Also the regularity assumption on f can be relaxed by assuming $f \in C^2(\mathbb{R}^d)$ instead of $f \in C^3(\mathbb{R}^d)$.

Proof. Let $\chi := \alpha \mathbf{1}_K$, where $\mathbf{1}_K$ is the indicator function of a bounded set $K \subset \mathbb{R}^d$ and $\alpha \in \mathbb{R}$. Then χ, seen as a multiplication operator in $\ell^2(\varepsilon\mathbb{Z}^d)$, is of finite rank (in particular compact) for every $\varepsilon > 0$. It follows from Weyl's theorem that for fixed $\varepsilon > 0$,

$$\inf \mathrm{Spec}_{\mathrm{ess}}\left(H_\varepsilon\right) = \inf \mathrm{Spec}_{\mathrm{ess}}\left(H_\varepsilon + \chi\right). \tag{40}$$

Moreover

$$\begin{aligned}
&\inf\ \mathrm{Spec}_{\mathrm{ess}}\left(H_\varepsilon + \chi\right) \geqslant \inf \mathrm{Spec}\left(H_\varepsilon + \chi\right) \\
&= \inf_{\substack{\psi \in \mathrm{Dom}(V_\varepsilon) \\ \psi \neq 0}} \frac{\langle (H_\varepsilon + \chi)\psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\langle \psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}} \geqslant \inf_{\substack{\psi \in \mathrm{Dom}(V_\varepsilon) \\ \psi \neq 0}} \frac{\langle (V_\varepsilon + \chi)\psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\langle \psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}.
\end{aligned}$$

The claim follows by chosing α and K large enough so that for some constants $\varepsilon_0, C > 0$ the inequality $V_\varepsilon(x) + \chi(x) \geqslant C$ holds for every $x \in \mathbb{R}^d$ and $\varepsilon \in (0, \varepsilon_0]$. To see that this choice is possible recall the uniform bound $V_\varepsilon \geqslant -2d$ and note that by Assumption **H**1 (i) there exist $a > 0$, $R > 0$ such that $|\nabla f(x)| > a$ for $|x| > R$. It follows then by Lemma 4.1 that for suitable $C, \varepsilon_0 > 0$ it holds $V_\varepsilon(x) \geqslant C$ for $|x| > R$ and $\varepsilon \in (0, \varepsilon_0)$. □

The next proposition provides the crucial estimate for the proof of statement (ii) in Theorem 2.2.

Proposition 4.5. *Assume **H1** and denote by $N_0 \in \mathbb{N}_0$ the number of local minima of f. Then there exist constants $\varepsilon_0, C > 0$ and, for every $\varepsilon > 0$, functions $\Psi_{1,\varepsilon}, \dots, \Psi_{N_0,\varepsilon} \in \ell^2(\varepsilon\mathbb{Z}^d)$ such that for every $\psi \in \mathrm{Dom}(V_\varepsilon)$ it holds*

$$\langle H_\varepsilon\psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant C\varepsilon\,\|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} - \sum_{k=1}^{N_0}\langle \psi, \Psi_{k,\varepsilon}\rangle^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \varepsilon_0]. \tag{41}$$

As shown next, Statement (ii) in Theorem 2.2 is then a simple consequence of the Max-Min principle (see e.g. [25, Theorem 11.7]). Recall that the latter implies the following: considering increasing order and counting multiplicity, if it exists, the N-th eigenvalue of H_ε below the bottom of the essential spectrum equals $\sup_{\mathcal{V}} \inf_\psi \langle H_\varepsilon \psi, \psi \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}$, with the supremum taken over all N-dimensional subspaces $\mathcal{V}$ of $\ell^2(\varepsilon\mathbb{Z}^d)$ and the infimum taken over all normalized $\psi \in \mathcal{V}^\perp \cap \mathrm{Dom}(V_\varepsilon)$.

Corollary 4.6. *Assume* ***H1*** *and denote by* $N_0 \in \mathbb{N}_0$ *the number of local minima of* f. *Then there exist constants* $\varepsilon_0, C > 0$ *such that*

$$|\operatorname{Spec}_{disc}(H_\varepsilon) \cap [0, C\varepsilon]| \leqslant N_0 \quad \forall \varepsilon \in (0, \varepsilon_0].$$

Proof of Corollary 4.6. By Propositions 4.3 and 4.5 we can find $\varepsilon_0, C > 0$ such that

$$\operatorname{Spec}_{\mathrm{ess}}(H_\varepsilon) \subset [C\varepsilon_0, \infty) \quad \forall \varepsilon \in (0, \varepsilon_0] \tag{42}$$

and such that (41) holds. If for every $\varepsilon \in (0, \varepsilon_0)$ it happens that

$$|\operatorname{Spec}_{\mathrm{disc}}(H_\varepsilon) \cap [0, \tfrac{C\varepsilon}{2}]| \leqslant N_0,$$

the claim is proven. Thus, we only have to check the case in which there exists $\varepsilon_* \in (0, \varepsilon_0)$ such that

$$|\operatorname{Spec}_{\mathrm{disc}}(H_{\varepsilon_*}) \cap [0, \tfrac{C\varepsilon_*}{2}]| > N_0. \tag{43}$$

But this case is impossible. Indeed (43) implies that there exist at least $N_0 + 1$ distinct eigenvalues of H_{ε_*} in $[0, \frac{C\varepsilon_*}{2}]$ and thus in particular the N_0+1-th eigenvalue $\lambda_{N_0+1}(\varepsilon_*)$(in increasing order and counting multiplicity) exists and satisfies

$$\lambda_{N_0+1}(\varepsilon_*) \leqslant \frac{C\varepsilon_*}{2}. \tag{44}$$

In particular $\lambda_{N_0+1}(\varepsilon_*) \leqslant \frac{C\varepsilon_0}{2}$ and therefore, by (42), $\lambda_{N_0+1}(\varepsilon_*)$ is smaller than the bottom of the essential spectrum. From this, the Max-Min principle and (41) it follows that

$$\lambda_{N_0+1}(\varepsilon_*) \geqslant \inf_\psi \langle H_{\varepsilon_*} \psi, \psi \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant C\varepsilon_*, \tag{45}$$

where the infimum is taken over all normalized $\psi \in \mathcal{V}_\varepsilon^\perp \cap \mathrm{Dom}(\mathrm{V}_\varepsilon)$, with $\mathcal{V}_\varepsilon$ being the linear span of the set $\{\Psi_{1,\varepsilon}, \ldots, \Psi_{N_0,\varepsilon}\} \subset \ell^2(\varepsilon\mathbb{Z}^d)$ appearing in (41). But (44) and (45) are in contradiction. □

Proof of Proposition 4.5. We label by $z_1, \ldots, z_N$ the critical points of f, the ordering being chosen such that $z_1, \ldots, z_{N_0}$ are the local minima. Then we take a function $\chi \in C^\infty(\mathbb{R}^d; [0, 1])$ which equals 1 on $\{x : |x| \leqslant 1\}$ and vanishes on $\{x : |x| \geqslant 2\}$. We shall consider a smooth quadratic partition of unity by defining with $s = \frac{2}{5}$

$$\chi_{j,\varepsilon}(x) := \chi\left(\varepsilon^{-s}(x - z_j)\right), \quad \chi_{0,\varepsilon}(x) := \left(1 - \sum_j \chi^2_{j,\varepsilon}(x)\right)^{\frac{1}{2}}$$

for $j = 1, \dots, N$ and $\varepsilon \in (0, \overline{\varepsilon}]$, where $\overline{\varepsilon} \in (0, 1]$ is sufficiently small so that $\chi_{0,\varepsilon} \in C^\infty(\mathbb{R}^d)$. We set moreover for $x \in \mathbb{R}^d$ and $j = 1, \dots, N$

$$U_j(x) := \tfrac{1}{4}\langle \big[\mathrm{Hess}\, f(z_j)\big]^2 (x - z_j), (x - z_j)\rangle.$$

Let $\psi \in \mathrm{Dom}(V_\varepsilon)$. It follows from $\sum_{j=0}^N \chi_{j,\varepsilon}^2 \equiv 1$ that we can write

$$\begin{aligned} \langle H_\varepsilon \psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = & \sum_{j=1}^N \langle \Big(-\varepsilon^2\Delta_\varepsilon + U_j - \tfrac{\varepsilon}{2}\Delta f(z_j)\Big)\chi_{j,\varepsilon}\psi, \chi_{j,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \\ & + \langle \Big(-\varepsilon^2\Delta_\varepsilon + V_\varepsilon\Big)\chi_{0,\varepsilon}\psi, \chi_{0,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} + \mathcal{E}_1 + \mathcal{E}_2, \end{aligned} \tag{46}$$

with the localization errors given by

$$\mathcal{E}_1 = \mathcal{E}_1(\varepsilon) := \sum_{j=1}^N \langle \big(V_\varepsilon - U_j + \tfrac{\varepsilon}{2}\Delta f(z_j)\big)\chi_{j,\varepsilon}\psi, \chi_{j,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)},$$

$$\mathcal{E}_2 = \mathcal{E}_2(\varepsilon) := -\varepsilon^2 \sum_{j=0}^N \langle \big(\chi_{j,\varepsilon}\Delta_\varepsilon - \Delta_\varepsilon\chi_{j,\varepsilon}\big)\psi, \chi_{j,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}.$$

The four terms in the right hand side of (46) are now analyzed separately.

(1) *Analysis of the first term in the right hand side of* (46).

We apply Proposition 3.2: let $\kappa_1(z_j)\dots, \kappa_d(z_j)$ be the eigenvalues of $\frac{1}{2}\,\mathrm{Hess}\, f(z_j)$, so that in particular $\frac{1}{2}\Delta f(z_j) = \sum_i \kappa_i(z_j)$ and $\kappa_1^2(z_j)\dots, \kappa_d^2(z_j)$ are the eigenvalues of $\frac{1}{4}\big[\mathrm{Hess}\, f(z_j)\big]^2$.

Case 1: $j = 1, \dots, N_0$ (i.e. z_j *is a local minimum of* f)

In this case $\sum_i \big(|\kappa_i(z_j)| - \kappa_i(z_j)\big) = 0$ and according to Prop. 3.2 (ii) there exist for every $\varepsilon > 0$, $j = 1, \dots, N_0$ a function $\Phi_{j,\varepsilon} \in \ell^2(\varepsilon\mathbb{Z}^d)$ and constants $\varepsilon_0', C' > 0$ such that for every $\varepsilon \in (0, \varepsilon_0']$, $j = 1, \dots, N_0$ and $\psi \in C_c(\varepsilon\mathbb{Z}^d)$

$$\begin{aligned} & \langle \Big(-\varepsilon^2\Delta_\varepsilon + U_j - \tfrac{\varepsilon}{2}\Delta f(z_j)\Big)\chi_{j,\varepsilon}\psi, \chi_{j,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \\ & \geqslant C'\varepsilon\|\chi_{j,\varepsilon}\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} - \langle \chi_{j,\varepsilon}\psi, \Phi_{j,\varepsilon}\rangle^2_{\ell^2(\varepsilon\mathbb{Z}^d)}. \end{aligned} \tag{47}$$

Case 2: $j = N_0 + 1, \dots, N$ (i.e. z_j *is not a local minimum of* f)

In this case $\sum_i \big(|\kappa_i(z_j)| - \kappa_i(z_j)\big) > 0$ and according to Prop. 3.2 (i), possibly taking the constants $\varepsilon_0', C' > 0$ smaller, the following holds: for every $\varepsilon \in (0, \varepsilon_0']$, $j = N_0 + 1, \dots, N$ and $\psi \in C_c(\varepsilon\mathbb{Z}^d)$

$$\langle \Big(-\varepsilon^2\Delta_\varepsilon + U_j - \tfrac{\varepsilon}{2}\Delta f(z_j)\Big)\chi_{j,\varepsilon}\psi, \chi_{j,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant C'\varepsilon\,\|\chi_{j,\varepsilon}\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}. \tag{48}$$

(2) *Analysis of the second term in the right hand side of* (46).

According to Lemma 4.2 there exist constants $r, C'' > 0$ and $\varepsilon_0'' \in (0, \overline{\varepsilon}]$ such that for every $j = 1, \dots, N$

$$V_\varepsilon(x) \geqslant C''|x - z|^2 - \tfrac{\varepsilon}{C''} \qquad \forall x \in B_r(z_j) \text{ and } \forall \varepsilon \in (0, \varepsilon_0'']. \tag{49}$$

Moreover, according to Lemma 4.1, possibly taking the constants $\varepsilon_0'', C'' > 0$ smaller, it holds also

$$V_\varepsilon(x) \geqslant C'' \quad \forall x \in \mathbb{R}^d \setminus \bigcup_{j=1}^{N} B_r(z_j) \text{ and } \forall \varepsilon \in (0, \varepsilon_0'']. \tag{50}$$

Since $\operatorname{supp} \chi_{0,\varepsilon} \subset \{x \in \mathbb{R}^d : |x - z_j| \geqslant 2\varepsilon^{\frac{2}{5}} \text{ for all } j = 1, \dots, N\}$, the lower bounds (49), (50) imply (with possibly reducing further the constant $\varepsilon_0'' > 0$)

$$\langle V_\varepsilon \chi_{0,\varepsilon}\psi, \chi_{0,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant C''\varepsilon^{\frac{4}{5}} \|\chi_{0,\varepsilon}\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \varepsilon_0''].$$

Using $-\Delta_\varepsilon \geqslant 0$ we conclude that

$$\langle\left(-\varepsilon^2\Delta_\varepsilon + V_\varepsilon\right) \chi_{0,\varepsilon}\psi, \chi_{0,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant C''\varepsilon \|\chi_{0,\varepsilon}\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \varepsilon_0'']. \tag{51}$$

(3) *Analysis of the localization error* $\mathcal{E}_1$.
Let $R_{j,\varepsilon}(x) := V_\varepsilon(x) - U_j(x) + \frac{\varepsilon}{2}\Delta f(z_j)$. By Lemma 4.2 there exist constants $C''', \varepsilon_0''' > 0$ such that

$$\sup_{x:|x-z_j|\leqslant 2\varepsilon^{\frac{2}{5}}} |R_{j,\varepsilon}(x)| \leqslant C'''\varepsilon^{\frac{6}{5}} \quad \forall \varepsilon \in (0, \varepsilon_0'''] \text{ and } \forall j = 1, \dots, N.$$

Thus, since $\operatorname{supp} \chi_{j,\varepsilon} \subset \{x \in \mathbb{R}^d : |x - z_j| \leqslant 2\varepsilon^{\frac{2}{5}}\}$ for all $j = 1, \dots, N$,

$$|\mathcal{E}_1(\varepsilon)| = \left|\sum_{j=1}^{N} \langle R_{j,\varepsilon}\chi_{j,\varepsilon}\psi, \chi_{j,\varepsilon}\psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}\right| \leqslant C'''\,\varepsilon^{\frac{6}{5}} \sum_{j=1}^{N} \|\chi_{j,\varepsilon}\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \varepsilon_0'''],$$

and we conclude that

$$\mathcal{E}_1(\varepsilon) \geqslant -C'''\varepsilon^{\frac{6}{5}} \|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \varepsilon_0''']. \tag{52}$$

(4) *Analysis of the localization error* $\mathcal{E}_2$.
Using $\sum_{j=0}^{N} \chi^2_{j,\varepsilon} \equiv 1$ gives

$$\mathcal{E}_2(\varepsilon) = -\varepsilon^2 \left\langle \left(\Delta_\varepsilon - \sum_{j=0}^{N} \chi_{j,\varepsilon}\Delta_\varepsilon\chi_{j,\varepsilon}\right)\psi, \psi\right\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}.$$

Since there is a constant $K > 0$ such that $\sup_{x\in\mathbb{R}^d} |\operatorname{Hess} \chi_{j,\varepsilon}(x)| \leqslant K\varepsilon^{-2s}$ for every $\varepsilon \in (0, \overline{\varepsilon}]$ and $j = 0, \dots, N$, it follows from Lemma 3.1 that there exists a constant $C'''' > 0$ such that

$$|\mathcal{E}_2(\varepsilon)| \leqslant C''''\,\varepsilon^{2-2s} \|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)} = C''''\,\varepsilon^{\frac{6}{5}} \|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \overline{\varepsilon}].$$

In particular we shall use that

$$\mathcal{E}_2(\varepsilon) \geqslant -C''''\,\varepsilon^{\frac{6}{5}} \|\psi\|_{\ell^2(\varepsilon\mathbb{Z}^d)} \quad \forall \varepsilon \in (0, \overline{\varepsilon}]. \tag{53}$$

Final step.

Taking $\Psi_{j,\varepsilon} := \chi_{j,\varepsilon}\Phi_{j,\varepsilon}, \tilde{\varepsilon}_0 := \min\{\varepsilon_0', \varepsilon_0'', \varepsilon_0'''\}$ and $\tilde{C} := \min\{C', C''\}$ gives, according to (46), (47), (48), (51), (52), (53) the lower bound

$$\begin{aligned}&\langle H_\varepsilon \psi, \psi\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}\\ &\quad \geqslant \left(\tilde{C}\varepsilon - (C'''' + C''''')\,\varepsilon^{\frac{6}{5}}\right)\,\|\psi\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} - \sum_{j=1}^{N_0}\langle \psi, \Psi_{j,\varepsilon}\rangle^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \qquad \forall \varepsilon \in (0, \tilde{\varepsilon}_0],\end{aligned}$$

which implies the desired estimate (41), by taking $C = \tilde{C}/2$ and a sufficiently small $\varepsilon_0 \in (0, \tilde{\varepsilon}_0)$. □

It remains to show part (iii) of Theorem 2.2 to complete the proof. In order to do so, we can assume $N_0 \neq 0$, since otherwise there is nothing to prove. By the Max–Min principle [25, Theorem 11.7 and Proposition 11.9] together with the bound on the essential spectrum given by Proposition 4.3 it is sufficient to show that for each $\varepsilon > 0$ there exist N_0 orthonormal functions in the domain $\mathrm{Dom}(V_\varepsilon)$ of H_ε such that the quadratic form associated with H_ε is exponentially small for each of these functions. We shall now exhibit such a family of orthonormal functions.

Let $\{z_1, \ldots, z_{N_0}\}$ be the set of local minima of f. We fix $\delta > 0$ such that $B_{3\delta}(z_k) \cap B_{3\delta}(z_j)$ is the empty set for $k \neq j$ and such that $f > f(z_k)$ on $B_{3\delta}(z_k)\backslash\{z_k\}$. Moreover we fix for each $k = 1, \ldots, N_0$ a cutoff function $\chi_k \in C^\infty(\mathbb{R}^d; [0, 1])$, satisfying $\chi \equiv 1$ on $B_\delta(z_k)$ $\chi \equiv 0$ on $\mathbb{R}^d\backslash B_{2\delta}(z_k)$. We consider then for each $\varepsilon > 0$ and for each $k = 1, \ldots, N_0$ the functions $\psi_{k,\varepsilon} : \mathbb{R}^d \to \mathbb{R}$ given by

$$\psi_{k,\varepsilon}(x) = \frac{\chi_k(x)e^{-f(x)/(2\varepsilon)}}{\|\chi_k e^{-f/(2\varepsilon)}\|_{\ell^2(\varepsilon\mathbb{Z}^d)}}. \tag{54}$$

Then for each $\varepsilon > 0$ the (restrictions to $\varepsilon\mathbb{Z}^d$ of the) functions $\psi_{1,\varepsilon}, \ldots, \psi_{N_0,\varepsilon}$ are in the domain of H_ε and orthonormal in $\ell^2(\varepsilon\mathbb{Z}^d)$. Moreover the following proposition shows that the quadratic form associated with H_ε is exponentially small for each of these functions and thus concludes the proof of Theorem 2.2.

Proposition 4.7. *Assume* ***H1*** *and that the set* $\{z_1, \ldots, z_{N_0}\}$ *of local minima of* f *is not empty. Then there exist* $C, \varepsilon_0 > 0$ *such that for each* $\varepsilon \in (0, \varepsilon_0]$ *the functions* $\psi_{1,\varepsilon}, \ldots, \psi_{N_0,\varepsilon}$ *defined in* (54) *satisfy the estimate*

$$\langle H_\varepsilon \psi_{k,\varepsilon}, \psi_{k,\varepsilon}\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \leqslant e^{-C/\varepsilon}.$$

Proof. Fix $k = 1, \ldots, N_0$. Then, applying Proposition 3.5 with $\varphi = f - f(z_k)$, $k = 3$ and $m = 0$, gives for a suitable constant $K > 0$ and for every $\varepsilon \in (0, 1]$

$$\|\chi_k e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \geqslant \varepsilon^d e^{-f(z_k)/\varepsilon} \sum_{x\in B^\varepsilon_\delta(z_k)} e^{-(f(x)-f(z_k)/(2\varepsilon)} \geqslant K\varepsilon^{\frac{d}{2}} e^{-f(z_k)/\varepsilon}. \tag{55}$$

Further, using (7) and the notation $F_\varepsilon(x, v) = \frac{1}{2}[f(x) + f(x + \varepsilon v)]$,

$$\langle H_\varepsilon(\chi_k e^{-f/(2\varepsilon)}), \chi_k e^{-f/(2\varepsilon)}\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \varepsilon^2\|e^{-F_\varepsilon/(2\varepsilon)}\nabla_\varepsilon \chi_k\|^2_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})}. \tag{56}$$

We take $\varepsilon_0' \in (0, 1]$ small enough such that for all $\varepsilon \in (0, \varepsilon_0]$ it holds

$$\nabla_\varepsilon \chi_k(x, v) = 0 \quad \forall x \in B_{\delta/2}(z_k) \quad \text{and} \quad \forall v \in \mathcal{N}.$$

Moreover we take $\gamma > 0$ small enough such that for all $\varepsilon \in (0, \varepsilon_0]$ and for all $k = 1, \dots, N_0$ it holds

$$F_\varepsilon(x, v) - f(z_k) \geqslant \gamma \quad \forall x \in \Omega_\varepsilon := B_{3\delta}(z_k) \setminus B_{\delta/2} \quad \text{and} \quad \forall v \in \mathcal{N}.$$

It follows then from (56), the uniform bound $\varepsilon^2 |\nabla_\varepsilon \chi_k| \leqslant 2$ and the existence of a $\tilde{K} > 0$ with $\varepsilon^d |\Omega_\varepsilon| \leqslant \tilde{K}$ that

$$\langle H_\varepsilon(\chi_k e^{-f/(2\varepsilon)}), \chi_k e^{-f/(2\varepsilon)} \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \leqslant 2^{d+1} \tilde{K} e^{-[f(z_k)+\gamma]/\varepsilon}. \tag{57}$$

Putting together (55) and (57) gives the claim with e.g. $C = \gamma/2$ and $\varepsilon_0 \in (0, \varepsilon_0']$ sufficiently small. □

In the remainder of this section we provide the proofs of the basic estimates on V_ε given in Lemmas 4.1 and 4.2.

Proof of Lemma 4.1. A Taylor expansion gives for every $x \in \mathbb{R}^d$ the representation

$$V_\varepsilon(x) = 2 \sum_{v \in \mathcal{N}} \sinh^2 \tfrac{\nabla f(x) \cdot v}{4} + \varepsilon \sum_{v \in \mathcal{N}} e^{-\frac{\nabla f(x) \cdot v}{2}} R_\varepsilon(x, v), \tag{58}$$

where, thanks to the boundedness of Hess f,

$$\exists R > 0 \ \text{ s.t. } \ |R_\varepsilon(x, v)| \leqslant R \ \ \forall x \in \mathbb{R}^d, v \in \mathcal{N} \text{ and } \varepsilon \in (0, 1].$$

In fact, one may write

$$V_\varepsilon(x) = \sum_{v \in \mathcal{N}} \left[e^{-\frac{\nabla f(x) \cdot v}{2}} - 1 \right] + \varepsilon \sum_{v \in \mathcal{N}} e^{-\frac{\nabla f(x) \cdot v}{2}} \, \tfrac{1}{\varepsilon} \left[e^{-\frac{f(x+\varepsilon v) - f(x) - \varepsilon \nabla f(x) \cdot v}{2\varepsilon}} - 1 \right],$$

and, using $\cosh 2t - 1 = 2\sinh^2 t$,

$$\begin{aligned} \sum_{v \in \mathcal{N}} \left[e^{-\frac{\nabla f(x) \cdot v}{2}} - 1 \right] &= \sum_{v \in \mathcal{N}} \left[\tfrac{1}{2} e^{\frac{\nabla f(x) \cdot v}{2}} + \tfrac{1}{2} e^{-\frac{\nabla f(x) \cdot v}{2}} - 1 \right] \\ &= \sum_{v \in \mathcal{N}} \left[\cosh \tfrac{\nabla f(x) \cdot v}{2} - 1 \right] \\ &= 2 \sum_{v \in \mathcal{N}} \sinh^2 \tfrac{\nabla f(x) \cdot v}{4}. \end{aligned}$$

Moreover, for

$$R_\varepsilon(x, v) := \tfrac{1}{\varepsilon} \left[e^{-\frac{f(x+\varepsilon v) - f(x) - \varepsilon \nabla f(x) \cdot v}{2\varepsilon}} - 1 \right],$$

using $|e^t - 1| \leqslant |t| e^{|t|}$ with

$$t := -\tfrac{f(x+\varepsilon v) - f(x) - \varepsilon \nabla f(x) \cdot v}{2\varepsilon},$$

and noting that, due to the boundedness of Hess f, there exists a constant $A > 0$ such that

$$|t| \leqslant \tfrac{\varepsilon}{4} \sup_x |\operatorname{Hess} f(x) v \cdot v| \leqslant \tfrac{\varepsilon}{4} A |v|^2,$$

one gets for $\varepsilon \in (0,1]$ and every $x \in \mathbb{R}^d$

$$|R_\varepsilon(x,v)| \leqslant \frac{A|v|^2}{4} e^{\frac{A|v|^2}{4}} \leqslant \frac{\max_{v\in\mathcal{N}} A|v|^2}{4} e^{\frac{\max_{v\in\mathcal{N}} A|v|^2}{4}} =: R > 0. \tag{59}$$

It follows from (58) and (59) that for $\varepsilon \in (0,1]$ and every $x \in \mathbb{R}^d$

$$\begin{aligned} V_\varepsilon(x) &\geqslant \sum_{v\in\mathcal{N}} \left[\cosh \frac{\nabla f(x)\cdot v}{2} - 1\right] - \varepsilon R \sum_{v\in\mathcal{N}} e^{-\frac{\nabla f(x)\cdot v}{2}} = \\ &= \sum_{v\in\mathcal{N}} \left[(1-\varepsilon R)\left(\cosh \frac{\nabla f(x)\cdot v}{2} - 1\right) - \varepsilon R\right]. \end{aligned}$$

Using that $\cosh t - 1 \geqslant t^2$ with $t = \frac{\nabla f(x)\cdot v}{2}$ and $\sum_{v\in\mathcal{N}} |\nabla f(x)\cdot v|^2 = 2|\nabla f(x)|^2$ we get for $\varepsilon \in (0, \min\{1, \frac{1}{R}\})$ and every $x \in \mathbb{R}^d$ the lower bound

$$V_\varepsilon(x) \geqslant \left[\frac{(1-\varepsilon R)}{2} s|\nabla f(x)|^2 - \varepsilon R\right].$$

In particular

$$V_\varepsilon(x) \geqslant \frac{a^2}{2} - \varepsilon\left(\frac{Ra^2}{2} + R\right) \qquad \forall x \in S \text{ and } \forall \varepsilon \in (0, \min\{1, \tfrac{1}{R}\}).$$

The claim follows by chosing an $\varepsilon_0 \in (0, \min\{1, \frac{1}{R}, \frac{a^2}{Ra^2+2R}\})$ and $C = \frac{a^2}{2} - \varepsilon_0 \left(\frac{Ra^2}{2} + R\right)$. □

Proof of Lemma 4.2. This follows from a straightforward Taylor expansion. Indeed, fixing $z \in \mathbb{R}^d$ such that $\nabla f(z) = 0$ and $R > 0$, we have on $B_R(z)$ the uniform estimate

$$-\tfrac{1}{2\varepsilon}\left[f(\cdot + \varepsilon v) - f\right] = -\tfrac{1}{2}\nabla f \cdot v - \tfrac{\varepsilon}{4} \operatorname{Hess} f v \cdot v + \mathcal{O}(\varepsilon^2).$$

Using the inequality $|e^t - 1 - t| \leqslant \frac{1}{2}t^2 e^{|t|}$ with $t = \frac{\varepsilon}{4} \operatorname{Hess} f\, v \cdot v + \mathcal{O}(\varepsilon^2)$ then gives

$$\begin{aligned} V_\varepsilon &= \sum_{v\in\mathcal{N}} \left\{e^{-\frac{1}{2}\nabla f\cdot v} - 1 - e^{-\frac{1}{2}\nabla f\cdot v} \tfrac{\varepsilon}{4} \operatorname{Hess} f\, v\cdot v + \mathcal{O}(\varepsilon^2)\right\} \\ &= \sum_{v\in\mathcal{N}} \left\{\cosh\left[\tfrac{1}{2}\nabla f\cdot v\right] - 1 - \cosh\left[\tfrac{1}{2}\nabla f\cdot v\right] \tfrac{\varepsilon}{4} \operatorname{Hess} f\, v\cdot v + \mathcal{O}(\varepsilon^2)\right\}. \end{aligned}$$

The expansion $\cosh x = 1 + \frac{1}{2}x^2 + \mathcal{O}(x^4)$ and the equalities $\sum_v |\nabla f\cdot v|^2 = 2|\nabla f|^2$ and $\sum_v \operatorname{Hess} f\, v\cdot v = 2\Delta f$ give

$$V_\varepsilon = \frac{1}{4}|\nabla f|^2 + \mathcal{O}\Big(\sum_k |\partial_k f|^4\Big) - \tfrac{\varepsilon}{2}\Delta f + \mathcal{O}(\varepsilon|\nabla f|^2) + \mathcal{O}(\varepsilon^2).$$

Expanding all terms in x around z, which gives in particular $|\nabla f(x)|^2 = [\operatorname{Hess} f(z)]^2(x-z)\cdot(x-z) + \mathcal{O}(|x-z|^3)$ and $\Delta f(x) = \Delta f(z) + \mathcal{O}(|x-z|)$, finishes the proof. □

5. Proof of Theorem 2.3

5.1. General strategy. In order to compute the precise asymptotics of the smallest non-zero eigenvalue $\lambda(\varepsilon)$ of H_ε we shall consider a suitable choice of an ε-dependent test function ψ_ε. The latter will be referred to as quasimode and its precise construction will be given in Sect. 5.2. Since ψ_ε will be chosen orthogonal to the ground state $e^{-f/(2\varepsilon)}$ for every ε, the upper bound on $\lambda(\varepsilon)$ given in Theorem 2.3 will follow immediately from the Max–Min principle, giving

$$\lambda(\varepsilon) \leqslant \frac{\langle H_\varepsilon \psi_\varepsilon, \psi_\varepsilon \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\|\psi_\varepsilon\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}}, \tag{60}$$

and from the precise computation of the right hand side in the above formula by using the Laplace asymptotics on $\varepsilon\mathbb{Z}^d$ given in Sect. 3.3. The result of these computations is the content of Propositions 5.2 and 5.3 (see also Remark 5.5 for the improved error bound under the assumption $f \in C^4(\mathbb{R}^d)$).

The proof of the lower bound on $\lambda(\varepsilon)$ given in Theorem 2.3 is more subtle. We shall derive it as a corollary of Theorem 2.2 and the following abstract Kato–Temple type estimate.

Proposition 5.1. *Let $(T, \mathcal{D}(T))$ be a nonnegative selfadjoint operator on a Hilbert space with scalar product denoted by $\langle \cdot, \cdot \rangle$. Further let $\tau > 0$ such that $(0, \tau) \cap \mathrm{Spec}(T) \neq \emptyset$ and set $\lambda = \sup((0, \tau) \cap \mathrm{Spec}(T))$. Then for every normalized $u \in \mathcal{D}(T)$ it holds*

$$\lambda \geqslant \langle Tu, u \rangle - \frac{1}{\tau} \langle Tu, Tu \rangle.$$

Proof. We fix a $u \in \mathcal{D}(T)$ and denote by $P = \mathbf{1}_{[0,\tau)}(T)$ the spectral projector of T corresponding to the interval $[0, \tau)$. Then

$$\begin{aligned}
\lambda \geqslant \lambda \|Pu\|^2 &\geqslant \langle TPu, Pu \rangle = \langle Tu, Pu \rangle \\
&\geq \langle Tu, u \rangle - |\langle Tu, u - Pu \rangle| \\
&\geq \langle Tu, u \rangle - \|Tu\| \|u - Pu\|,
\end{aligned}$$

with $\|\cdot\|$ the Hilbert space norm. The claim follows now from the Chebyshev-type estimate

$$\|u - Pu\|^2 \leqslant \tau^{-2} \langle Tu, Tu \rangle,$$

which is a simple consequence of the spectral theorem:

$$\begin{aligned}
\|u - Pu\|^2 = \|\mathbf{1}_{[\tau,\infty)}(T)u\|^2 &= \int_{-\infty}^{\infty} \mathbf{1}_{[\tau,\infty)}(\lambda)\, d\langle \mathbf{1}_{(-\infty,\lambda]}(T)u, u \rangle \\
&\leq \int_{-\infty}^{\infty} \frac{\lambda^2}{\tau^2} \mathbf{1}_{[\tau,\infty)}(\lambda)\ d\langle \mathbf{1}_{(-\infty,\lambda]}(T)u, u \rangle \\
&\leq \tau^{-2} \langle Tu, Tu \rangle.
\end{aligned}$$

□

We shall apply Proposition 5.1 to the case $T = H_\varepsilon$, $\tau = C\varepsilon$, where C is the constant appearing in Theorem 2.2 and $u = (\|\psi_\varepsilon\|_{\ell^2(\varepsilon\mathbb{Z}^d)})^{-1}\psi_\varepsilon$, where ψ_ε is the same quasimode used for the upper bound on $\lambda(\varepsilon)$. By Theorem 2.2 (ii) we thus obtain a lower bound on $\lambda(\varepsilon)$. The fact that this lower bound coincides with the lower bound given in Theorem 2.3 is a consequence of the precise computation of the right hand side of (60), which we already mentioned (see Propositions 5.2 and 5.3), and the estimate

$$(C\varepsilon)^{-1}\frac{\langle H_\varepsilon\psi_\varepsilon, H_\varepsilon\psi_\varepsilon\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\langle H_\varepsilon\psi_\varepsilon, \psi_\varepsilon\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}} = \mathcal{O}(\varepsilon).$$

The latter estimate will be a consequence of Propositions 5.3 and 5.4, which is proven again by analyzing the Laplace asymptotics of a sum over $\varepsilon\mathbb{Z}^d$.
We shall assume throughout the rest of this section that the Assumption **H**2 is satisfied.

5.2. Definition of the quasimode ψ_ε. In the semiclassical approach of [26] the eigenfunction corresponding to $\lambda(\varepsilon)$ is approximated by two distinct quasimodes: the first quasimode is a generic smoothed version of the function equal to one on the basin of attraction of m_0 and equal to -1 on the basin of attraction of m_1. This quasimode turns out to be a good global approximation, except possibly in vicinity of the relevant saddle points, where the transition from 1 to -1 takes place. Around the relevant saddle points, a second quasimode is constructed: it is actually a vector field and used as approximation of the gradient of the eigenfunction. This second quasimode is obtained via a WKB Ansatz and fails to be an exact vector field in general. The relevant estimates are then obtained exploiting the Witten complex structure and computing interaction integrals over the regions where the two quasimodes overlap.

In this paper we use a single global quasimode obtained by a suitable gluing procedure: instead of the mentioned WKB solution, we consider just its quadratic approximation around each saddle point and only in the direction of the unstable manifold. In this way, the vector field becomes exact, and still retains sufficient information to precisely compute leading asymptotics. We then consider a primitive of this exact vector field and use it to prescribe the transition from 1 to -1 around the saddle points, see the definition of κ_ε in (62) below.
Before giving the details, it might be useful to observe that a similar need of constructing good test functions arises also in the approach based on potential theory [7]: in that approach test functions approximate the so-called equilibrium potential which can be characterized as minimizer of the Dirichlet form (or capacity) under suitable boundary conditions. There is however a difference, which is worth to emphasize: in dimension one the variational problem for the equilibrium potential can be solved explicitly by a simple integration of the Euler–Lagrange equations. In higher dimensions this is still very useful, because the test function can be modelled on the 1-d case, exploiting the fact that the metastable transition occurs on the one-dimensional instanton path joining the minima. This is no longer possible for the eigenfunctions, where even in one dimension no explicit representation is available for the solution of the variational problem.

We provide now the details for the definition of the quasimode used in this paper: let $s_1, \dots, s_n$ be the relevant saddle points of f, i.e. the critical points of index one of f appearing in formula (10) defining the prefactor A. Given $x \in \mathbb{R}^d$ we associate to it a linear "reaction coordinate" $\xi_k = \xi_k(x)$ around the saddle point s_k, which parametrizes the unstable direction of Hess $f(s_k)$. More precisely, we choose one of the two normalized eigenvectors corresponding to the only negative eigenvalue $\mu(s_k)$ of Hess $f(s_k)$,

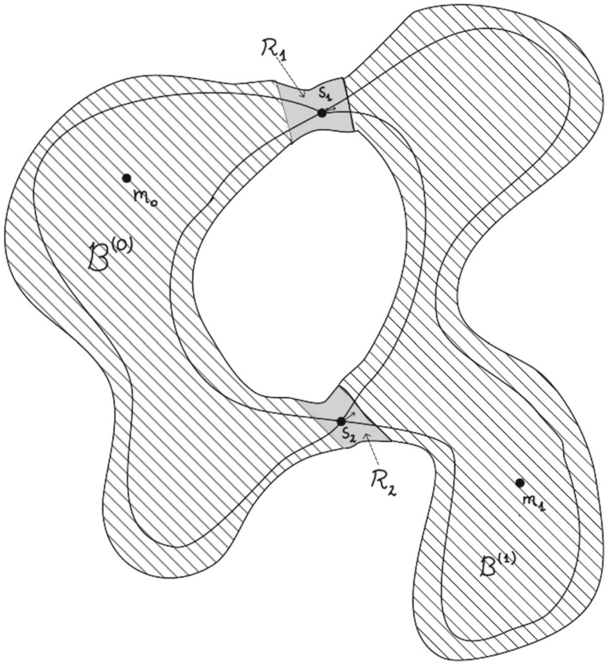

Fig. 2. Decomposition of the set $\mathcal{B}$ for an energy with two relevant saddle points

denote it by τ_k, and set

$$\xi_k(x) = \langle x - s_k, \tau_k \rangle \quad \forall k = 1, \ldots, n. \tag{61}$$

Recalling our notation $\mathcal{S}_f(h) = f^{-1}((-\infty, h))$ for the open sublevel set of f corresponding to the height $h \in \mathbb{R}$ and the definition of the height h^* given in (9), we consider for $\rho > 0$ and $k = 1, \ldots, n$ the closed set

$$\mathcal{R}_k = \left\{ x \in \overline{\mathcal{S}_f(h^* + \rho)} : |\xi_k(x)| \leqslant \rho \right\},$$

and the open set $\mathcal{B} = \mathcal{S}_f(h^* + \rho) \setminus \left(\bigcup_k \mathcal{R}_k \right)$.
Henceforth the parameter $\rho > 0$ appearing in the definition of $\mathcal{R}_k$ and $\mathcal{B}$ is fixed sufficiently small such that the following properties hold (Fig. 2):

- the set $\mathcal{B}$ has exactly two connected components $\mathcal{B}^{(0)}$ and $\mathcal{B}^{(1)}$, containing respectively m_0 and m_1. Moreover $f > h_*$ on $\bigcup_k \mathcal{R}_k$, where we recall that we have set $h_* = \max\{f(m_0), f(m_1)\}$.
- $\mathcal{R}_k$ is disjoint from $\mathcal{R}_{k'}$ for $k \neq k'$.
- For each $k = 1, \ldots, n$ the function $\varphi_k = f + |\mu(s_k)| \xi_k^2$ satisfies $\varphi_k(x) > f(s_k)$ for every $x \in \mathcal{R}_k \setminus \{s_k\}$.

Note that $\operatorname{Hess} \varphi_k(s_k) = |\operatorname{Hess} f(s_k)|$. In other terms the quadratic approximation of φ_k around s_k is obtained from that of f by flipping the sign of the only negative eigenvalue of $\operatorname{Hess} f(s_k)$.

Let $\varepsilon \in (0, 1]$. The quasimode ψ_ε for the spectral gap is defined as follows. We define first on the sublevel set $\mathcal{S}_f(h^* + \rho)$

$$\kappa_\varepsilon(x) = \begin{cases} +1 & \text{for} \quad x \in \mathcal{B}^{(1)}, \\ -1 & \text{for} \quad x \in \mathcal{B}^{(0)}, \\ C_{k,\varepsilon} \int_0^{\xi_k(x)} \chi(\eta)\, e^{-\frac{|\mu(s_k)|\eta^2}{2\varepsilon}}\, d\eta & \text{for} \quad x \in \bigcup_k \mathcal{R}_k. \end{cases} \tag{62}$$

The constant $C_{k,\varepsilon}$ appearing above is defined as

$$C_{k,\varepsilon} := \left[\frac{1}{2} \int_{-\infty}^{\infty} \chi(\eta)\, e^{-\frac{|\mu(s_k)|\eta^2}{2\varepsilon}}\, d\eta \right]^{-1},$$

and $\chi \in C^\infty(\mathbb{R}; [0, 1])$ satisfies $\chi \equiv 1$ on $[-\frac{\rho}{3}, \frac{\rho}{3}]$, $\chi(\eta) = 0$ for $|\eta| \geqslant \frac{2}{3}\rho$ and $\chi(\eta) = \chi(-\eta)$. Note that

$$\exists \gamma > 0 \;\text{ such that }\; C_{k,\varepsilon} = 2\sqrt{\frac{|\mu(s_k)|}{2\pi\varepsilon}} \left(1 + \mathcal{O}(e^{-\frac{\gamma}{\varepsilon}})\right). \tag{63}$$

Note also that for each $k = 1, \ldots n$ the sign of the vector τ_k defining ξ_k (see (61)) can be chosen such that κ_ε is C^∞ on $\mathcal{S}_f(h^* + \rho)$, which we shall assume in the sequel. In order to extend κ to a smooth function defined on the whole $\mathbb{R}^d$ we introduce another cutoff function $\theta \in C^\infty(\mathbb{R}^d; [0, 1])$ by setting for $x \in \mathbb{R}^d$

$$\theta(x) = \begin{cases} 1 & \text{for} \quad x \in \mathcal{S}_f(h^* + \frac{\rho}{2}) \\ 0 & \text{for} \quad x \in \mathbb{R}^d \setminus \mathcal{S}_f(h^* + \frac{3}{4}\rho) \end{cases}. \tag{64}$$

Finally we define the quasimode ψ_ε by setting for $x \in \mathbb{R}^d$

$$\psi_\varepsilon(x) = \left(\frac{1}{2}\theta(x)\, \kappa_\varepsilon(x) - \frac{1}{2} \frac{\langle \theta\kappa_\varepsilon, e^{-f/\varepsilon} \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\|e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}} \right) e^{-f(x)/(2\varepsilon)}. \tag{65}$$

Note that $\psi_\varepsilon \in C^\infty(\mathbb{R}^d)$ with compact support. In particular its restiction to $\varepsilon\mathbb{Z}^d$, which we still denote by ψ_ε, is in $C_c(\varepsilon\mathbb{Z}^d) \subset \mathrm{Dom}(V_\varepsilon)$. Moreover, it follows from its very definition that ψ_ε is orthogonal to the ground state $e^{-f/(2\varepsilon)}$ with respect to the scalar product $\langle \cdot, \cdot \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}$.

5.3. Quasimode estimates. We now state the crucial estimates concerning the quasimode ψ_ε. The proofs follow from straightforward computations exploiting the results of Sect. 3.3 on the Laplace asymptotics for sums over $\varepsilon\mathbb{Z}^d$. We shall give the details in Sect. 5.4.

Proposition 5.2. *Assume **H2** and let $\varepsilon \in (0, 1]$. The function ψ_ε defined in (65) satisfies*

$$\|\psi_\varepsilon\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} = (2\pi\varepsilon)^{\frac{d}{2}}\, J e^{-h_*/\varepsilon} \left(1 + \mathcal{O}(\sqrt{\varepsilon})\right),$$

where $h_* = \max\{f(m_0), f(m_1)\}$ and

$$J = \begin{cases} \left((\det \operatorname{Hess} f(m_1))^{\frac{1}{2}} + (\det \operatorname{Hess} f(m_0))^{\frac{1}{2}} \right)^{-1} & \textit{if } f(m_0) = f(m_1), \\ (\det \operatorname{Hess} f(m_1))^{-\frac{1}{2}} & \textit{if } f(m_0) < f(m_1). \end{cases}$$

Proposition 5.3. *Assume* ***H****2 and let* $\varepsilon \in (0, 1]$. *The function* ψ_ε *defined in* (65) *satisfies*

$$\langle H_\varepsilon \psi_\varepsilon, \psi_\varepsilon \rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \varepsilon \sum_{k=1}^{n} \frac{|\mu(s_k)|}{2\pi} \frac{(2\pi\varepsilon)^{\frac{d}{2}}}{|\det \operatorname{Hess} f(s_k)|^{\frac{1}{2}}} e^{-h^*/\varepsilon} \left(1 + \mathcal{O}(\sqrt{\varepsilon})\right),$$

where $\mu(s_k)$ *is the only negative eigenvalue of* Hess $f(s_k)$ *and* h^* *is defined in* (9).

Proposition 5.4. *Assume* ***H****2 and let* $\varepsilon \in (0, 1]$. *The function* ψ_ε *defined in* (65) *satisfies*

$$\| H_\varepsilon \psi_\varepsilon \|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} = \mathcal{O}(\varepsilon^3)\, e^{-h^*/\varepsilon},$$

where h^* *is defined in* (9).

Remark 5.5. With the stronger assumption $f \in C^4(\mathbb{R}^d)$ the $\mathcal{O}(\sqrt{\varepsilon})$ error terms appearing in Propositions 5.2 and 5.3 can be shown to be actually $\mathcal{O}(\varepsilon)$. Indeed it is enough to apply Proposition 3.5 with $k = 4$ instead of $k = 3$ each time it is used in the proofs given below.

5.4. Proofs of the quasimode estimates.

Proof of Proposition 5.2. Let $\varepsilon \in (0, 1]$. We first consider the case $f(m_0) < f(m_1)$ for which $h_* = f(m_1)$. It is then convenient to write

$$\psi_\varepsilon = \left(\frac{1}{2}\theta\kappa_\varepsilon + \frac{1}{2} - \frac{1}{2}D_\varepsilon\right) e^{-f/(2\varepsilon)}, \ \text{with } D_\varepsilon = \frac{\langle 1+\theta\kappa_\varepsilon, e^{-f/\varepsilon}\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\|e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}}. \tag{66}$$

Recalling the definitions (62), (64) of κ_ε and θ, we observe that there exist $\alpha, \delta > 0$ such that $\theta\kappa_\varepsilon \equiv -1$ on $B_\delta(m_0)$, $\theta\kappa_\varepsilon \equiv +1$ on $B_\delta(m_1)$ and

(i) $f \geqslant f(m_0) + \alpha$ on $[B_\delta(m_0)]^c$,
(ii) $f \geqslant f(m_1) + \alpha$ on $[B_\delta(m_1)]^c \bigcap \operatorname{supp}(1 + \theta\kappa_\varepsilon)$.

As a preliminary step we claim that

$$D_\varepsilon = \mathcal{O}(e^{-[f(m_1) - f(m_0)]/\varepsilon}). \tag{67}$$

Indeed, from (i) it follows that

$$\begin{aligned}
&\|e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \\
&\quad = \varepsilon^d \sum_{x \in B^\varepsilon_\delta(m_0)} e^{-f(x)/\varepsilon} + e^{-[f(m_0)+\alpha]/\varepsilon}\, \varepsilon^d \sum_{x \in [B^\varepsilon_\delta(m_0)]^c} e^{-[f(x) - f(m_0) - \alpha]/\varepsilon} \\
&\quad \leq \varepsilon^d \sum_{x \in B^\varepsilon_\delta(m_0)} e^{-f(x)/\varepsilon} + e^{-[f(m_0)+\alpha]/\varepsilon}\, \varepsilon^d \sum_{x \in \varepsilon\mathbb{Z}^d} e^{-[f(x) - f(m_0) - \alpha]} \\
&\quad = \varepsilon^d \sum_{x \in B^\varepsilon_\delta(m_0)} e^{-f(x)/\varepsilon} + \mathcal{O}(e^{-[f(m_0)+\alpha]/\varepsilon}),
\end{aligned}$$

where for the last estimate we have used that, by Hypothesis **H**2 (i), the sum $\varepsilon^d \sum_{x \in \varepsilon\mathbb{Z}^d} e^{-f(x)}$ is uniformly bounded in ε. Proposition 3.5 gives then

$$\|e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} = (2\pi\varepsilon)^{\frac{d}{2}} \left(\det \operatorname{Hess} f(m_0)\right)^{-\frac{1}{2}} e^{-f(m_0)/\varepsilon} \left(1 + \mathcal{O}(\sqrt{\varepsilon})\right). \tag{68}$$

Following the same reasoning, but using (ii) instead of (i), yields

$$\langle 1+\theta\kappa_\varepsilon, e^{-f/\varepsilon}\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = -(2\pi\varepsilon)^{\frac{d}{2}} \,(\det \operatorname{Hess} f(m_1))^{-\frac{1}{2}}\, e^{-f(m_1)/\varepsilon}\left(1+\mathcal{O}(\sqrt{\varepsilon})\right). \tag{69}$$

The claim (67) is thus obtained by taking the quotient between (68) and (69).
Next we set $\mathcal{B}_\varepsilon^{(1)} = \mathcal{B}^{(1)} \cap \varepsilon\mathbb{Z}^d$ and write

$$\|\psi_\varepsilon\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} = \varepsilon^d \sum_{x\in\mathcal{B}_\varepsilon^{(1)}} \psi_\varepsilon^2(x) + \varepsilon^d \sum_{x\in[\mathcal{B}_\varepsilon^{(1)}]^c} \psi_\varepsilon^2(x). \tag{70}$$

In order to compute the first sum we consider $\alpha, \delta > 0$ as above and write

$$\varepsilon^d \sum_{x\in\mathcal{B}_\varepsilon^{(1)}} \psi_\varepsilon^2(x) = \varepsilon^d \sum_{x\in B_\delta^\varepsilon(m_1)} \psi_\varepsilon^2(x) + \varepsilon^d \sum_{x\in\mathcal{B}_\varepsilon^{(1)}\cap[B_\delta^\varepsilon(m_1)]^c} \psi_\varepsilon^2(x). \tag{71}$$

Since $\kappa_\varepsilon \equiv 1$ on $B_\delta^\varepsilon(m_1)$, recalling (66) and (67), another application of Proposition 3.5 yields

$$\varepsilon^d \sum_{x\in B_\delta^\varepsilon(m_1)} \psi_\varepsilon^2(x) = (2\pi\varepsilon)^{\frac{d}{2}} \,(\det \operatorname{Hess} f(m_1))^{-\frac{1}{2}}\, e^{-f(m_1)/\varepsilon}\left(1+\mathcal{O}(\sqrt{\varepsilon})\right).$$

For the second sum in (71) it is enough to note that $\mathcal{B}_\varepsilon^{(1)} \subset \operatorname{supp}(1+\theta\kappa_\varepsilon)$ and use (ii), which, arguing as above, gives

$$\varepsilon^d \sum_{x\in\mathcal{B}_\varepsilon^{(1)}\cap[B_\delta^\varepsilon(m_1)]^c} \psi_\varepsilon^2(x) = \mathcal{O}(e^{-[f(m_1)+\alpha]/\varepsilon}).$$

In order to estimate the second sum in (70), note that

$$\psi_\varepsilon^2 \le \left(\frac{1}{2}\theta\kappa_\varepsilon + \frac{1}{2} - \frac{1}{2}D_\varepsilon\right)^2 e^{-f/\varepsilon} \le \frac{1}{2}\left((1+\theta\kappa_\varepsilon)^2 + D_\varepsilon^2\right) e^{-f/\varepsilon}.$$

Using (67) and (68) and setting $\Omega_\varepsilon = [\mathcal{B}_\varepsilon^{(1)}]^c \cap \operatorname{supp}(1+\theta\kappa_\varepsilon)$ gives then

$$\varepsilon^d \sum_{x\in[\mathcal{B}_\varepsilon^{(1)}]^c} \psi_\varepsilon^2(x) \le \varepsilon^d \sum_{x\in\Omega_\varepsilon} e^{-f(x)/\varepsilon} + \mathcal{O}(e^{-[f(m_1)-f(m_0)]/\varepsilon})\, e^{-f(m_1)/\varepsilon}.$$

The claim of the proposition in the case $f(m_0) < f(m_1)$ thus follows by observing that there exists $\alpha' > 0$ such that $f > f(m_1) + \alpha'$ on Ω_ε, yielding

$$\varepsilon^d \sum_{x\in\Omega_\varepsilon} e^{-f(x)/\varepsilon} \le e^{-[f(m_1)+\alpha']/\varepsilon}\, \varepsilon^d \sum_{x\in\varepsilon\mathbb{Z}^d} e^{-f(x)} = \mathcal{O}(e^{-[f(m_1)+\alpha']/\varepsilon}).$$

We now consider the case $h_* = f(m_0) = f(m_1)$. It follows from the definition of ψ_ε that

$$\|\psi_\varepsilon\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} = \frac{1}{4}\|\theta\kappa_\varepsilon e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} - \frac{1}{4}\frac{\langle\theta\kappa_\varepsilon, e^{-f/\varepsilon}\rangle^2_{\ell^2(\varepsilon\mathbb{Z}^d)}}{\|e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)}}. \tag{72}$$

Let $\alpha, \delta > 0$ such that $f \geqslant f(m_0)+\alpha$ on $[B_\delta(m_0) \cup B_\delta(m_1)]^c$ and $\theta\kappa_\varepsilon \equiv -1$ on $B_\delta(m_0)$, $\theta\kappa_\varepsilon \equiv 1$ on $B_\delta(m_1)$. With arguments as above one gets

$$\begin{aligned}
&\|e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} = \|\theta\kappa_\varepsilon e^{-f/(2\varepsilon)}\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} \left(1 + \mathcal{O}(\sqrt{\varepsilon})\right) \\
&\quad = (2\pi\varepsilon)^{\frac{d}{2}} \left[(\det \mathrm{Hess}\, f(m_1))^{-\frac{1}{2}} + (\det \mathrm{Hess}\, f(m_0))^{-\frac{1}{2}}\right] e^{-h_*/\varepsilon} \left(1 + \mathcal{O}(\sqrt{\varepsilon})\right), \\
&\langle \theta\kappa, e^{-f/\varepsilon}\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} \\
&\quad = (2\pi\varepsilon)^{\frac{d}{2}} \left[(\det \mathrm{Hess}\, f(m_1))^{-\frac{1}{2}} - (\det \mathrm{Hess}\, f(m_0))^{-\frac{1}{2}}\right] e^{-h_*/\varepsilon} \left(1 + \mathcal{O}(\sqrt{\varepsilon})\right).
\end{aligned}$$

Putting these expressions into (72), the desired result (5.2) follows after some algebraic manipulations. □

Proof of Proposition 5.3. Let $\varepsilon \in (0, 1]$. Using (7) and the notation $F_\varepsilon(x, v) = \frac{1}{2}[f(x)+f(x+\varepsilon v)]$ gives

$$\langle H_\varepsilon \psi_\varepsilon, \psi_\varepsilon\rangle_{\ell^2(\varepsilon\mathbb{Z}^d)} = \frac{\varepsilon^2}{4} \|e^{-F_\varepsilon/(2\varepsilon)} \nabla_\varepsilon(\theta\kappa_\varepsilon)\|^2_{\ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R}^{\mathcal{N}})}.$$

Since the function θ has support in the closure of $\mathcal{S}_f(h^* + \frac{3}{4}\rho)$, we can restrict (for ε sufficiently small) the sum running over $\varepsilon\mathbb{Z}^d$ to the bounded set $\varepsilon\mathbb{Z}^d \cap \mathcal{S}_f(h^* + \rho)$. Note that $\mathcal{S}_f(h^*+\rho)$ is the union of the disjoint sets $\mathcal{B}$ and $\bigcup_k(\mathcal{R}_k\backslash[\mathcal{S}_f(h^*+\rho)]^c)$. We write in the sequel for short $\mathcal{R}_{k,\varepsilon} := \varepsilon\mathbb{Z}^d \cap (\mathcal{R}_k\backslash[\mathcal{S}_f(h^*+\rho)]^c)$ and $\mathcal{B}_\varepsilon := \varepsilon\mathbb{Z}^d \cap \mathcal{B}$ and discuss below separately the sum over $\bigcup_{k=1}^n \mathcal{R}_{k,\varepsilon}$, which will give the main contribution, and the sum over $\mathcal{B}_\varepsilon$, which will give a negligible contribution.
Below we shall use the Taylor expansion

$$e^{-F_\varepsilon(x,v)/\varepsilon} = e^{-f(x)/\varepsilon} e^{-\nabla f(x)\cdot v/2} \left(1 + \mathcal{O}(\varepsilon)\right). \tag{73}$$

(1) *Analysis on* $\bigcup_{k=1}^n \mathcal{R}_{k,\varepsilon}$.
In order to get rid of θ we take $\delta > 0$ small enough such that for each k it holds $B_\delta(s_k) \subset \mathcal{R}'_k := \mathcal{R}_k \cap \mathcal{S}_f(h^* + \frac{1}{4}\rho)$. Since θ and κ_ε are uniformly bounded in ε and $f \geqslant h^* + \frac{1}{4}\rho$ on $\mathcal{R}_k\backslash B_\delta(s_k)$, we get using (73) that, for $\varepsilon > 0$ sufficiently small (and thus also for $\varepsilon \in (0, 1]$), it holds

$$\begin{aligned}
&\frac{\varepsilon^d}{2} \sum_{x\in\mathcal{R}_{k,\varepsilon}} \sum_{v\in\mathcal{N}} \frac{1}{4} \left[\theta\kappa_\varepsilon(x+\varepsilon v) - \theta\kappa_\varepsilon(x)\right]^2 e^{-F_\varepsilon(x,v)/\varepsilon} \\
&\quad = \frac{\varepsilon^d}{2} \sum_{x\in B^\varepsilon_\delta(s_k)} \sum_{v\in\mathcal{N}} \frac{1}{4} \left[\kappa_\varepsilon(x+\varepsilon v) - \kappa_\varepsilon(x)\right]^2 e^{-F_\varepsilon(x,v)/\varepsilon} + \mathcal{O}(e^{-(h^*+\frac{\rho}{4})/\varepsilon}),
\end{aligned} \tag{74}$$

where we have used also that for ε sufficiently small $\theta(x) = \theta(x+\varepsilon v) = 1$ for $x \in B_\delta(s_k)$. We discuss now in detail the behavior of $x \mapsto \kappa_\varepsilon(x+\varepsilon v) - \kappa_\varepsilon(x)$ near s_k. For $k = 1, \ldots, n$ and $x \in \mathcal{R}'_k$, $v \in \mathcal{N}$ and $\varepsilon \in (0, 1]$ consider the function $G = G_{k,x,v,\varepsilon} : [0, 1] \to \mathbb{R}$ defined by

$$G(\delta) = C^{-1}_{k,\varepsilon} \left[\kappa_\varepsilon(x+\delta v) - \kappa_\varepsilon(x)\right] = \int_{\xi_k(x)}^{\xi_k(x+\delta v)} \chi(\eta)\, e^{-|\mu(s_k)|\eta^2/(2\varepsilon)}\, d\eta. \tag{75}$$

Note that $G(0) = 0$, $G'(0) = e^{-|\mu(s_k)|\xi_k^2(x)/(2\varepsilon)}\chi(\xi_k(x))\tau_k \cdot v$,

$$G''(0) = e^{-|\mu(s_k)|\xi_k^2(x)/(2\varepsilon)}|\tau_k \cdot v|^2 \left[\chi'(\xi_k(x)) - |\mu(s_k)|\frac{\xi_k(x)}{\varepsilon}\chi(\xi_k(x))\right],$$

and for every $\delta \in [0, 1]$

$$\begin{aligned}&\varepsilon^3 G'''(\delta)\\ &\quad = \varepsilon e^{-|\mu(s_k)|\xi_k^2(x+\delta v)/(2\varepsilon)}(\tau_k \cdot v)^3 \left[|\mu(s_k)|^2\xi_k^2(x+\delta v)\chi(\xi_k(x+\delta v) + \varepsilon R\right],\end{aligned}$$

where R is not depending on ε and bounded in k, x, v. By Taylor expansion it follows that

$$\begin{aligned}G(\varepsilon) = \varepsilon e^{-|\mu(s_k)|\xi_k^2(x)/(2\varepsilon)}\chi(\xi_k(x))\\ \times \left[\tau_k \cdot v - \frac{1}{2}|\mu(s_k)|\,\xi_k(x)|\tau_k \cdot v|^2 + \mathcal{O}(|x - s_k|^2)\right](1 + \mathcal{O}(\varepsilon)).\end{aligned} \tag{76}$$

It follows from (75), (76), (73), (63) and the two identities

$$\begin{aligned}\sum_{v\in\mathcal{N}} |\tau_k \cdot v|^2 e^{-\nabla f(x)\cdot v/2} &= 2\sum_{j=1}^{d}(e_j \cdot \tau_k)^2 \cosh \tfrac{\partial_j f(x)}{2},\\ \sum_{v\in\mathcal{N}} (\tau_k \cdot v)^3\, e^{-\nabla f(x)\cdot v/2} &= -2\sum_{j}(e_j \cdot \tau_k)^3 \sinh \tfrac{\partial_j f(x)}{2}\end{aligned} \tag{77}$$

that for $k = 1, \ldots, n$ and $x \in \mathcal{R}'_k$ and $\varepsilon > 0$ small enough

$$\begin{aligned}&\frac{1}{2}\sum_{v\in\mathcal{N}}\frac{1}{4}\left[\kappa_\varepsilon\,(x + \varepsilon v) - \kappa_\varepsilon(x)\right]^2 e^{-F_\varepsilon(x,v)/\varepsilon}\\ &\quad = \varepsilon e^{-f(s_k)/\varepsilon}\frac{|\mu(s_k)|}{2\pi}\, e^{-\varphi_k(x)/\varepsilon}\alpha_k(x)\left(1 + \mathcal{O}(\varepsilon) + \mathcal{O}\left(|x - s_k|^2\right)\right),\end{aligned} \tag{78}$$

where for shortness we have set $\varphi_k(x) = f(x) - f(s_k) + |\mu(s_k)|\xi_k^2(x)$ and

$$\begin{aligned}&\alpha_k(x)\\ &= \chi^2(\xi_k(x))\sum_{j=1}^{d}\left\{(e_j \cdot \tau_k)^2 \cosh\frac{\partial_j f(x)}{2} + |\mu(s_k)|\xi_k(x)(e_j \cdot \tau_k)^3 \sinh\frac{\partial_j f(x)}{2}\right\}\\ &= 1 + \mathcal{O}(|x - s_k|^2).\end{aligned}$$

Putting together (74), (78), using Proposition 3.5, summing over k and using the fact that $f(s_k) = h^*$ for every k finally gives

$$\begin{aligned}&\frac{\varepsilon^d}{2}\sum_{x\in\bigcup_k \mathcal{R}_{k,\varepsilon}}\sum_{v\in\mathcal{N}}\frac{1}{4}\left[\kappa_\varepsilon\,(x + \varepsilon v) - \kappa_\varepsilon(x)\right]^2 e^{-F_\varepsilon(x,v)/\varepsilon}\\ &\quad = \varepsilon\sum_{k=1}^{n}\frac{|\mu(s_k)|}{2\pi}\frac{(2\pi\varepsilon)^{\frac{d}{2}}}{|\det \operatorname{Hess} f(s_k)|^{\frac{1}{2}}}\, e^{-\frac{h^*}{\varepsilon}}\left(1 + \mathcal{O}(\sqrt{\varepsilon})\right).\end{aligned}$$

(2) *Analysis on $\mathcal{B}_\varepsilon$.*
As in Step 1) we get rid of θ by considering the set $\mathcal{B}' = \mathcal{B} \cap \mathcal{S}_f(h^* + \frac{1}{4}\rho)$. Arguing as before and now using that $\kappa_\varepsilon(x) = \kappa_\varepsilon(x+\varepsilon v)$ for every $x \in \mathcal{B}'$, $v \in \mathcal{N}$ and ε sufficiently small, gives then, with the notation $\mathcal{B}'_\varepsilon = \mathcal{B}' \cap \varepsilon\mathbb{Z}^d$,

$$\begin{aligned}
&\frac{\varepsilon^d}{2} \sum_{x\in\mathcal{B}_\varepsilon} \sum_{v\in\mathcal{N}} \frac{1}{4} \left[\theta\kappa_\varepsilon\left(x+\varepsilon v\right) - \theta\kappa_\varepsilon(x)\right]^2 e^{-F_\varepsilon(x,v)/\varepsilon} \\
&= \frac{\varepsilon^d}{2} \sum_{x\in\mathcal{B}'_\varepsilon} \sum_{v\in\mathcal{N}} \frac{1}{4} \left[\kappa_\varepsilon\left(x+\varepsilon v\right) - \kappa_\varepsilon(x)\right]^2 e^{-F_\varepsilon(x,v)/\varepsilon} + \mathcal{O}(e^{-(h^*+\frac{\rho}{4})/\varepsilon}) \\
&= \mathcal{O}(e^{-(h^*+\frac{\rho}{4})/\varepsilon}).
\end{aligned}$$

□

Proof of Proposition 5.4. The isomporphism (12) gives the identity

$$\begin{aligned}
\|H_\varepsilon\psi_\varepsilon\|^2_{\ell^2(\varepsilon\mathbb{Z}^d)} &= \|\varepsilon\Phi_\varepsilon\left[L_\varepsilon\Phi_\varepsilon^{-1}[\psi]\right]\|^2_{\ell^2(\rho_\varepsilon)} \\
&= \tfrac{\varepsilon^d}{4} \sum_{x\in\varepsilon\mathbb{Z}^d} \left(\sum_{v\in\mathcal{N}} e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)} \varepsilon\nabla_\varepsilon(\theta\kappa_\varepsilon)(x,v)\right)^2 e^{-\frac{f(x)}{\varepsilon}}.
\end{aligned}$$

Since the function θ has support in the closure of $\mathcal{S}_f(h^* + \frac{3}{4}\rho)$, we can restrict (for ε sufficiently small) the sum over $\varepsilon\mathbb{Z}^d$ to the bounded set $\varepsilon\mathbb{Z}^d \cap \mathcal{S}_f(h^* + \rho)$. As in the proof of Proposition 5.3 we shall split the latter into the disjoint sets $\bigcup_k \mathcal{R}_{k,\varepsilon}$,with $\mathcal{R}_{k,\varepsilon} := \varepsilon\mathbb{Z}^d \cap (\mathcal{R}_k \backslash [\mathcal{S}_f(h^*+\rho)]^c)$, and $\mathcal{B}_\varepsilon := \varepsilon\mathbb{Z}^d \cap \mathcal{B}$.
We discuss here in detail only the contribution coming from the sets $\mathcal{R}_{k,\varepsilon}$. Indeed the sum over $\mathcal{B}_\varepsilon$ can be neglected arguing exactly as in Step 2) of Proposition 5.3 and using, instead of (73), that by Taylor expansion

$$e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)} = e^{-\nabla f(x)\cdot v/2}\left(1 + \mathcal{O}(\varepsilon)\right). \tag{79}$$

Analysis on $\bigcup_{k=1}^n \mathcal{R}_{k,\varepsilon}$.
As in the proof of Proposition 5.3 we first get rid of θ by taking a $\delta > 0$ small enough such that for each k it holds $B_\delta(s_k) \subset \mathcal{R}_k \cap \mathcal{S}_f(h^* + \frac{1}{4}\rho)$. Since θ and κ_ε are uniformly bounded in ε and $f \geqslant h^* + \frac{1}{4}\rho$ on $\mathcal{R}_k \setminus B_\delta(s_k)$, we get using (79) that, for $\varepsilon > 0$ sufficiently small (and thus also for $\varepsilon \in (0, 1]$), it holds

$$\begin{aligned}
&\tfrac{\varepsilon^d}{4} \sum_{x\in\mathcal{R}_{k,\varepsilon}} \left(\sum_{v\in\mathcal{N}} e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)} \varepsilon\nabla_\varepsilon(\theta\kappa_\varepsilon)(x,v)\right)^2 e^{-f(x)/\varepsilon} \\
&= \tfrac{\varepsilon^d}{4} \sum_{x\in B^\varepsilon_\delta(s_k)} \left(\sum_{v\in\mathcal{N}} e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)} \varepsilon\nabla_\varepsilon\kappa_\varepsilon(x,v)\right)^2 e^{-f(x)/\varepsilon} + \mathcal{O}(e^{-(h^*+\frac{\rho}{4})/\varepsilon}).
\end{aligned} \tag{80}$$

A computation already used in the proof of Proposition 5.3 (see (76)) yields

$$e^{|\mu(s_k)|\xi_k^2(x)/(2\varepsilon)} C_{k,\varepsilon}^{-1}\, \varepsilon\nabla_\varepsilon\kappa_\varepsilon(x,v)$$

$$= \varepsilon\chi(\xi_k(x))\left[\tau_k\cdot v - \frac{1}{2}|\mu(s_k)|\,\xi_k(x)|\tau_k\cdot v|^2 + \mathcal{O}(|x-s_k|^2)\right](1+\mathcal{O}(\varepsilon))\,.$$

Hence, using (63), (79), the identity (77) and the identity

$$\sum_{v\in\mathcal{N}}\tau_k\cdot v e^{-\nabla f(x)\cdot v/2} = -2\sum_j e_j\cdot\tau_k \sinh\tfrac{\partial_j f(x)}{2},$$

one obtains

$$e^{|\mu(s_k)|\xi_k^2(x)/(2\varepsilon)}\sum_{v\in\mathcal{N}} e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)}\varepsilon\nabla_\varepsilon\kappa_\varepsilon(x,v) = \sqrt{\varepsilon}\alpha_k(x)\,(1+\mathcal{O}(\varepsilon))\,, \tag{81}$$

with

$$\alpha_k(x) = -\sqrt{\tfrac{2|\mu(s_k)|}{\pi}}\chi(\xi_k(x)) \times\sum_{j=1}^d\left[2e_j\cdot\tau_k\sinh\tfrac{\partial_j f(x)}{2} + |\mu(s_k)|\xi_k(x)(e_j\cdot\tau_k)^2\cosh\tfrac{\partial_j f(x)}{2} + \mathcal{O}(|x-s_k|^2)\right]. \tag{82}$$

Observing that

$$\sum_{j=1}^d 2e_j\cdot\tau_k\sinh\tfrac{\partial_j f(x)}{2} = \langle \text{Hess}\, f(s_k)\tau_k, x-s_k\rangle + \mathcal{O}(|x-s_k|^2) = -|\mu(s_k)|\,\xi_k(x) + \mathcal{O}(|x-s_k|^2),$$

and that

$$\sum_{j=1}^d (e_j\cdot\tau_k)^2\cosh\tfrac{\partial_j f(x)}{2} = 1+\mathcal{O}(|x-s_k|^2)$$

shows that the first order terms in (82) cancel out and thus $\alpha_k(x) = \mathcal{O}(|x-s_k|^2)$. It follows then from (80), (81) that there exists a constant $C>0$ such that for every $\varepsilon\in(0,1]$ and every $k=1,\dots,n$

$$\tfrac{\varepsilon^d}{4}\sum_{x\in\mathcal{R}_{k,\varepsilon}}\left(\sum_{v\in\mathcal{N}} e^{-\frac{1}{2}\nabla_\varepsilon f(x,v)}\varepsilon\nabla_\varepsilon(\theta\kappa_\varepsilon)(x,v)\right)^2 e^{-f(x)/\varepsilon} \leqslant C\varepsilon^{d+1}e^{-f(s_k)/\varepsilon}\sum_{x\in B_\delta^\varepsilon(s_k)}|x-s_k|^4 e^{-\varphi_k(x)/\varepsilon} = \mathcal{O}(\varepsilon^3)e^{-h^*/\varepsilon},$$

with $\varphi_k(x) = f(x) + |\mu(s_k)|\xi_k^2(x) - f(s_k)$ and with the last estimate following from Proposition 3.5 by taking $m=2$. □

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