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Geometric analysis for the metropolis algorithm on Lipschitz domains

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Abstract This paper gives geometric tools: comparison, Nash and Sobolev inequalities for pieces of the relevant Markov operators, that give useful bounds on rates of convergence for the Metropolis algorithm. As an example, we treat the random placement of N hard discs in the unit square, the original application of the Metropolis algorithm.

1 Introduction and results

Let Ω be a bounded, connected open subset of $\mathbb{R}^d$. We assume that its boundary, $\partial\Omega$, has Lipschitz regularity. Let B_1 be the unit ball of $\mathbb{R}^d$ and $\varphi(z) = \frac{1}{\mathrm{vol}(B_1)} 1_{B_1}(z)$ so that $\int \varphi(z)\,dz = 1$. Let $\rho(x)$ be a measurable positive bounded function on $\overline{\Omega}$ such that $\int_\Omega \rho(x)\,dx = 1$. For $h \in]0,1]$, set

$$K_{h,\rho}(x,y) = h^{-d}\varphi\left(\frac{x-y}{h}\right)\min\left(\frac{\rho(y)}{\rho(x)}, 1\right), \tag{1.1}$$

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and let $T_{h,\rho}$ be the Metropolis operator associated with these data, that is,

$$T_{h,\rho}(u)(x) = m_{h,\rho}(x)u(x) + \int_\Omega K_{h,\rho}(x, y)u(y)\,dy,$$
$$m_{h,\rho}(x) = 1 - \int_\Omega K_{h,\rho}(x, y)\,dy \geq 0. \tag{1.2}$$

Then the Metropolis kernel $T_{h,\rho}(x, dy) = m_{h,\rho}(x)\delta_{x=y} + K_{h,\rho}(x, y)\,dy$ is a Markov kernel, the operator $T_{h,\rho}$ is self-adjoint on $L^2(\Omega, \rho(x)\,dx)$, and thus the probability measure $\rho(x)\,dx$ on Ω is stationary. For $n \geq 1$, we denote by $T^n_{h,\rho}(x, dy)$ the kernel of the iterated operator $(T_{h,\rho})^n$. For any $x \in \Omega$, $T^n_{h,\rho}(x, dy)$ is a probability measure on Ω, and our main goal is to get some estimates on the rate of convergence, when $n \to +\infty$, of the probability $T^n_{h,\rho}(x, dy)$ toward the stationary probability $\rho(y)\,dy$.

A good example to keep in mind is the random placement of N non-overlapping discs of radius $\varepsilon > 0$ in the unit square. This was the original motivation for the work of Metropolis et al. [8]. One version of their algorithm goes as follows: from a feasible configuration, pick a disc (uniformly at random) and a point within distance h of the center of the chosen disc (uniformly at random). If recentering the chosen disc at the chosen point results in a feasible configuration, the change is made. Otherwise, the configuration is kept as it started. If N is fixed and ε and h are small, this gives a Markov chain with a uniform stationary distribution over all feasible configurations. The state space consists of the N centers corresponding to feasible configurations. It is a bounded domain with a Lipschitz boundary when $N\epsilon$ is small (see Sect. 4, Proposition 4.1). The scientific motivation for the study of random packing of hard discs as a way of understanding the apparent existence of a liquid/solid phase transition for arbitrarily large temperatures (for suitably large pressure) is clearly described in Uhlenbeck [12, Sect. 5, p. 18]. An overview of the large literature is in Lowen [7]. Entry to the zoo of modern algorithms to do the simulation (particularly in the dense case) with many examples is in Krauth [5]. Further discussion, showing that the problem is still of current interest, is in Radin [9].

We shall denote by $g(h, \rho)$ the spectral gap of the Metropolis operator $T_{h,\rho}$. It is defined as the largest constant such that the following inequality holds true for all $u \in L^2(\rho) = L^2(\Omega, \rho(x)\,dx)$.

$$\|u\|^2_{L^2(\rho)} - \langle u, 1\rangle^2_{L^2(\rho)} \leq \frac{1}{g(h, \rho)}\langle u - T_{h,\rho}u, u\rangle_{L^2(\rho)}, \tag{1.3}$$

or equivalently,

$$\int_{\Omega\times\Omega} |u(x) - u(y)|^2 \rho(x)\rho(y)\,dx\,dy$$
$$\leq \frac{1}{g(h, \rho)} \int_{\Omega\times\Omega} K_{h,\rho}(x, y)|u(x) - u(y)|^2 \rho(x)\,dx\,dy. \tag{1.4}$$

Definition 1 We say that an open set $\Omega \subset \mathbb{R}^d$ is Lipschitz if it is bounded and for all $a \in \partial\Omega$ there exists an orthonormal basis $\mathcal{R}_a$ of $\mathbb{R}^d$, an open set $V = V' \times]-\alpha, \alpha[$ and a Lipschitz map $\eta : V' \to]-\alpha, \alpha[$ such that in the coordinates of $\mathcal{R}_a$, we have

$$\begin{aligned} V \cap \Omega &= \big\{(y', y_d < \eta(y')),\ (y', y_d) \in V' \times]-\alpha, \alpha[\big\}, \\ V \cap \partial\Omega &= \big\{(y', \eta(y')),\ y' \in V'\big\}. \end{aligned} \tag{1.5}$$

Our first result is the following:

Theorem 1.1 *Let Ω be an open, connected, bounded, Lipschitz subset of $\mathbb{R}^d$. Let $0 < m \le M < \infty$ be given numbers. There exists $h_0 > 0$, $\delta_0 \in]0, 1/2[$ and constants $C_i > 0$ such that for any $h \in]0, h_0]$, and any probability density ρ on Ω which satisfies for all x, $m \le \rho(x) \le M$, the following holds true.*

(i) *The spectrum of $T_{h,\rho}$ is a subset of $[-1+\delta_0, 1]$, 1 is a simple eigenvalue of $T_{h,\rho}$, and $\mathrm{Spec}(T_{h,\rho}) \cap [1-\delta_0, 1]$ is discrete. Moreover, for any $0 \le \lambda \le \delta_0 h^{-2}$, the number of eigenvalues of $T_{h,\rho}$ in $[1-h^2\lambda, 1]$ (with multiplicity) is bounded by $C_1(1+\lambda)^{d/2}$.*

(ii) *The spectral gap $g(h, \rho)$ satisfies*

$$C_2 h^2 \le g(h, \rho) \le C_3 h^2 \tag{1.6}$$

and the following estimates hold true for all integer n:

$$(1 - g(h, \rho))^n \le \sup_{x \in \Omega} \|T^n_{h,\rho}(x, dy) - \rho(y)\, dy\|_{TV} \le C_4 e^{-ng(h,\rho)}. \tag{1.7}$$

The above results have to be understood as results for small h, other parameters of the problem being fixed. In particular, our estimates are certainly not sharp with respect to the dimension d of the space. For instance, a carefull look at the proof of estimate (1.7) shows that the constant C_4 depends badly on the dimension d (if one tracks the dependance with respect to d, the bound obtained by the Nash estimates can not be better than d^d, [4]). Proving estimate on C_4 with respect to the dimension would be of great interest.

The next result will give some more information on the behavior of the spectral gap $g(h, \rho)$ when $h \to 0$. To state this result, let

$$\alpha_d = \int \varphi(z) z_1^2\, dz = \frac{1}{d} \int \varphi(z) |z|^2\, dz = \frac{1}{d+2} \tag{1.8}$$

and let us define $\nu(\rho)$ as the largest constant such that the following inequality holds true for all u in the Sobolev space $H^1(\Omega)$:

$$\|u\|^2_{L^2(\rho)} - \langle u, 1\rangle^2_{L^2(\rho)} \le \frac{1}{\nu(\rho)} \frac{\alpha_d}{2} \int_\Omega |\nabla u|^2(x) \rho(x)\, dx, \tag{1.9}$$

or equivalently,

$$\int_{\Omega\times\Omega} |u(x)-u(y)|^2\rho(x)\rho(y)\,dx\,dy \le \frac{\alpha_d}{\nu(\rho)}\int_\Omega |\nabla u|^2(x)\rho(x)\,dx. \quad (1.10)$$

Observe that for a Lipschitz domain Ω, the constant $\nu(\rho)$ is well-defined thanks to Sobolev embedding. For a smooth density ρ, this number $\nu(\rho)>0$ is closely related to the unbounded operator L_ρ acting on $L^2(\rho)$.

$$\begin{aligned} L_\rho(u) &= \frac{-\alpha_d}{2}\left(\Delta u + \frac{\nabla\rho}{\rho}.\nabla u\right) \\ D(L_\rho) &= \left\{u\in H^1(\Omega),\ -\Delta u\in L^2(\Omega),\, \partial_n u|_{\partial\Omega}=0\right\}. \end{aligned} \quad (1.11)$$

We now justify and explain the choice of domain in (1.11). Background for the following discussion and tools for working in Lipschitz domains is in [1].

When Ω has smooth boundary, standard elliptic regularity results show that for any $u\in H^1(\Omega)$ such that $-\Delta u\in L^2(\Omega)$, the normal derivative of u at the boundary, $\partial_n u = \overrightarrow{n}(x).\nabla u|_{\partial\Omega}$ is well defined and belongs to the Sobolev space $H^{-1/2}(\partial\Omega)$. Here, we denote by $\overrightarrow{n}(x)$ the incoming unit normal vector to $\partial\Omega$ at a point x. In the case where $\partial\Omega$ has only Lipschitz regularity, the Sobolev spaces $H^s(\partial\Omega)$ are well defined for all $s\in[-1,1]$. The trace operator, $\gamma_0(u)=u|_{\partial\Omega}$ maps $H^1(\Omega)$ onto $H^{1/2}(\partial\Omega)=Ran(\gamma_0)$, and its kernel is $\mathrm{Ker}(\gamma_0)=H^1_0(\Omega)$. Equipped with the norm $\|u\|_{H^{1/2}}=\inf\{\|v\|_{H^1},\ \gamma_0(v)=u\}$ it is an Hilbert space. Then, for any $\varphi\in H^{1/2}(\partial\Omega)^*$, there exists a unique $v\in H^{-1/2}(\partial\Omega)$ such that $\varphi(u)=\int_{\partial\Omega} vud\sigma$ for all $u\in H^{1/2}(\partial\Omega)$ (where σ is the measure induced on the boundary). For $v\in H^{-1/2}(\partial\Omega)$, the support of v can be defined in a standard way. The trace operator acting on vector fields $u\in(L^2)^d$ with $\mathrm{div}(u)\in L^2$,

$$\gamma_1 : \left\{u\in(L^2(\Omega))^d, \mathrm{div}(u)\in L^2(\Omega)\right\}\to H^{-1/2}(\partial\Omega), \quad (1.12)$$

is then defined by the formula

$$\begin{aligned} &\int_\Omega \mathrm{div}(u)(x)v(x)\,dx \\ &\quad = -\int_\Omega u(x).\nabla v(x)\,dx - \int_{\partial\Omega}\gamma_1(u)v|_{\partial\Omega}\,d\sigma(x), \quad \forall v\in H^1(\Omega). \end{aligned} \quad (1.13)$$

In particular, for $u\in H^1(\Omega)$ satisfying $\Delta u=\mathrm{div}\nabla u\in L^2(\Omega)$ we can define $\partial_n u|_{\partial\Omega}=\gamma_1(\nabla u)\in H^{-1/2}(\partial\Omega)$ and the set $D(L_\rho)$ is well defined. From (1.13) we deduce that for any $u\in H^1(\Omega)$ with $\Delta u\in L^2$ and any $v\in H^1(\Omega)$

we have

$$\langle L_\rho u, v\rangle_{L^2(\rho)} = \frac{\alpha_d}{2}\big(\langle \nabla u, \nabla v\rangle_{L^2(\rho)} + \langle \partial_n u, \rho v\rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}\big). \quad (1.14)$$

Then, it is standard that L_ρ is the self-adjoint realization of the Dirichlet form

$$\frac{\alpha_d}{2}\int_\Omega |\nabla u(x)|^2 \rho(x)\,dx. \quad (1.15)$$

A standard argument [10, Sects. 13, 14] using Sobolev embedding show that L_ρ has a compact resolvant. Denote its spectrum by $\nu_0 = 0 < \nu_1 < \nu_2 < \cdots$ and by m_j the multiplicity of ν_j. In particular, $\nu(\rho) = \nu_1$. Observe also that $m_0 = 1$ since $\operatorname{Ker} L$ is spanned by the constant function equal to 1.

To state our theorem, we need a basic definition:

Definition 2 Let Ω be a Lipschitz open set of $\mathbb{R}^d$. We say that $\partial\Omega$ is quasi-regular if $\partial\Omega = \Gamma_{\mathrm{reg}} \cup \Gamma_{\mathrm{sing}}$, $\Gamma_{\mathrm{reg}} \cap \Gamma_{\mathrm{sing}} = \emptyset$ with Γ_{reg} a finite union of smooth hypersurfaces, relatively open in $\partial\Omega$, and Γ_{sing} a closed subset of $\mathbb{R}^d$ such that

$$v \in H^{-1/2}(\partial\Omega) \quad \text{and} \quad \operatorname{supp}(v) \subset \Gamma_{\mathrm{sing}} \quad \Longrightarrow \quad v = 0. \quad (1.16)$$

Observe that (1.16) is obviously satisfied if $\partial\Omega$ is smooth, since in that case one can take $\Gamma_{\mathrm{sing}} = \emptyset$. More generally, the boundary is quasi-regular if it is 'piece-wise smooth' in the following sense: suppose Ω is a Lipschitz open set of $\mathbb{R}^d$ such that $\partial\Omega = \Gamma_{\mathrm{reg}} \cup \Gamma_{\mathrm{sing}}$, $\Gamma_{\mathrm{reg}} \cap \Gamma_{\mathrm{sing}} = \emptyset$, where Γ_{reg} is a smooth hypersurface of $\mathbb{R}^d$, relatively open in $\partial\Omega$, and Γ_{sing} a closed subset of $\mathbb{R}^d$ such that $\Gamma_{\mathrm{sing}} = \bigcup_{j\geq 2} S_j$ where the S_j are smooth disjoint submanifolds of $\mathbb{R}^d$ such that

$$\operatorname{codim}_{\mathbb{R}^d} S_j \geq j, \quad \bigcup_{k\geq j} S_k = \overline{S_j}, \quad (1.17)$$

then Ω is quasi-regular, since in that case, if $v \in H^{-1/2}(\partial\Omega)$ is such that near a point x_0, the support of v is contained in a submanifold S of codimension ≥ 2 in $\mathbb{R}^d$, then $v = 0$ near x_0. This follows from the fact that the distribution $\langle u, \phi\rangle = \langle v, \phi|_{\partial\Omega}\rangle$ on $\mathbb{R}^d$ belongs to $H^{-1}(\mathbb{R}^d)$, and if $u \in \mathcal{D}'(\mathbb{R}^d)$ is such that $u \in H^{-1}(\mathbb{R}^d)$ and $\operatorname{supp}(u) \subset \{x_1 = x_2 = 0\}$, then $u = 0$. As an example, a cube in $\mathbb{R}^d$ is quasi-regular. This 'piece-wise smooth' condition (often called "stratified") is easy to visualize. In our applications (Sect. 4) it was hard to work with products of stratified sets. The definition we give works easily with products and is exactly what is needed in the proof.

Theorem 1.2 *Let Ω be an open, connected, bounded and Lipschitz subset of $\mathbb{R}^d$, such that $\partial\Omega$ is quasi-regular. Assume that the positive density ρ is* *continuous on $\overline{\Omega}$. Then*

$$\lim_{h\to 0} h^{-2} g(h,\rho) = \nu(\rho). \tag{1.18}$$

Moreover, if the density ρ is smooth on $\overline{\Omega}$, then for any $R>0$ and $\varepsilon>0$ such that $\nu_{j+1}-\nu_j > 2\varepsilon$ for $\nu_{j+2} < R$, there exists $h_1 > 0$ such that one has for all $h \in]0, h_1]$,

$$\mathrm{Spec}\left(\frac{1-T_{h,\rho}}{h^2}\right) \cap]0,R] \subset \bigcup_{j\geq 1} [\nu_j - \varepsilon, \nu_j + \varepsilon], \tag{1.19}$$

and the number of eigenvalues of $\frac{1-T_{h,\rho}}{h^2}$ in the interval $[\nu_j-\varepsilon, \nu_j+\varepsilon]$ is equal to m_j.

Theorem 1.1 is proved in Sect. 2. This is done from the spectrum of the operator by comparison with a 'ball walk' on a big box B containing Ω. One novelty is the use of 'normal extensions' of functions from Ω to B allowing comparison of the two Dirichlet forms. When the Dirichlet forms and stationary distributions for random walk on a compact group are comparable, the rates of convergence are comparable as well [3, Lemma 5]. Here, the Metropolis Markov chain is far from a random walk on a group. Indeed, because of the holding implicit in the Metropolis algorithm, the operator does not have any smoothing properties. The transfer of information is carried out by a Sobolev inequality for a spectrally-truncated part of the operator. This is transfered to a Nash inequality and then an inductive argument is used to obtain decay bounds on iterates of the kernel. A further technique is the use of crude Weyl type estimates to get bounds on the number of eigenvalues close to 1. All of these enter the proof of the total variation estimate (1.7). All of these techniques seem broadly applicable.

Theorem 1.2 is proved in Sect. 3. It gives rigorous underpinnings to a general picture of the spectrum of the Metropolis algorithm based on small steps. This was observed and proved in special cases [2, 6]. The picture is this: because of the holding (or presence of the multiplier $m_{h,\rho}$ in (1.2)) in the Metropolis algorithm, the operator always has continuous spectrum. This is well isolated from 1 and can be neglected in bounding rates of convergence. The spectrum near 1 is discrete and for h small, merges with the spectrum of an associated Neumann problem. This is an analytic version of the weak convergence of the discrete time Metropolis chain to the Langevin diffusion with generator (1.11).

In Sect. 4, we return to the hard disc problem showing that a suitable power of the operators and domains involved satisfies our hypothesis. Precisely, in Theorem 4.6 we shall prove that the results of Theorem 1.1 and Theorem 1.2 hold true in this case.

2 A proof of Theorem 1.1

Let us recall that

$$K_{h,\rho}(x,y) = h^{-d}\varphi\left(\frac{x-y}{h}\right)\min\left(\frac{\rho(y)}{\rho(x)},1\right), \tag{2.1}$$

so that

$$\begin{aligned} &T_{h,\rho}(u) = u - Q_{h,\rho}(u),\\ &Q_{h,\rho}(u)(x) = \int_\Omega K_{h,\rho}(x,y)(u(x)-u(y))\,dy,\\ &\langle (1-T_{h,\rho})u,u\rangle_{L^2(\rho)} = \frac{1}{2}\iint_{\Omega\times\Omega} |u(x)-u(y)|^2 K_{h,\rho}(x,y)\rho(x)\,dx\,dy. \end{aligned} \tag{2.2}$$

Observe that since Ω is Lipschitz, there exists $\delta_0 > 0$ such that for any density ρ with $0 < m \le \rho(x) \le M$ one has $\sup_{x\in\Omega} m_{h,\rho}(x) \le 1-2\delta_0$ for all $h \in]0,1]$. Indeed, it follows from (1.2) and (2.1) that

$$1 - m_{h,\rho}(x) \ge \frac{mh^{-d}}{M\,\mathrm{vol}(B_1)}\int_\Omega 1_{|x-y|<h}\,dy. \tag{2.3}$$

For $x \in \Omega$ such that $\mathrm{dist}(x,\partial\Omega) > 2h$, it follows that $1 - m_{h,\rho}(x) \ge 1 - m/M$. If $\mathrm{dist}(x,\partial\Omega) < 2h$, using a Lipschitz local parametrization of the boundary, one shows easily that there exists a constant $c > 0$, independent of h such that $\int_\Omega 1_{|x-y|<h}\,dy \ge ch^d$. Moreover, by a simple compactness argument, this constant c can be chosen independent of x.

Since $\sup_{x\in\Omega} m_{h,\rho}(x) \le 1-2\delta_0$, the essential spectrum of T_h is a subset of $[0,1-2\delta_0]$ and the spectrum of T_h in $[1-\delta_0,1]$ is discrete. From the last line of (2.2), we get that if $u \in L^2$ is such that $u = T_{h,\rho}(u)$, then $u(x) = u(y)$ for almost all $x, y \in \Omega$, $|x-y| < h$ and since Ω is connected, u is constant. Therefore, 1 is a simple eigenvalue of $T_{h,\rho}$. In particular, for any $h > 0$, the spectral gap satisfies

$$g(h,\rho) > 0. \tag{2.4}$$

For the proof of Theorem 1.1, we will not really care about the precise choice of the density ρ. In fact, if ρ_1, ρ_2 are two densities such that $m \le \rho_i(x) \le M$ for all x, then

$$\begin{aligned} &\rho_2(x) \le \rho_1(x)\left(1 + \frac{\|\rho_1-\rho_2\|_\infty}{m}\right),\\ &K_{h,\rho_1}(x,y)\rho_1(x) \le K_{h,\rho_2}(x,y)\rho_2(x)\left(1 + \frac{\|\rho_1-\rho_2\|_\infty}{m}\right), \end{aligned} \tag{2.5}$$

and this implies, using the definition (1.4) of the spectral gap and of $\nu(\rho)$,

$$\begin{aligned} \frac{g(h,\rho_1)}{g(h,\rho_2)} &\le \left(1+\frac{\|\rho_1-\rho_2\|_\infty}{m}\right)^3, \\ \frac{\nu(\rho_1)}{\nu(\rho_2)} &\le \left(1+\frac{\|\rho_1-\rho_2\|_\infty}{m}\right)^3. \end{aligned} \tag{2.6}$$

In particular, it is sufficient to prove (1.6) for a constant density.

The proof that for some $\delta_0>0$, independent of ρ, one has $\mathrm{Spec}(T_{h,\rho})\subset[-1+\delta_0,1]$ for all $h\in]0,h_0]$ is the following: one has

$$\begin{aligned} \langle u+T_{h,\rho}u,u\rangle_{L^2(\rho)} = \frac{1}{2}\int_{\Omega\times\Omega} K_{h,\rho}(x,y)|u(x)+u(y)|^2\rho(x)\,dx\,dy \\ +2\langle m_{h,\rho}u,u\rangle_{L^2(\rho)}. \end{aligned} \tag{2.7}$$

Therefore, it is sufficient to prove that there exists $h_0, C_0>0$ such that the following inequality holds true for all $h\in]0,h_0]$ and all $u\in L^2(\Omega)$:

$$\int_{\Omega\times\Omega} h^{-d}\varphi\left(\frac{x-y}{h}\right)|u(x)+u(y)|^2\,dx\,dy \ge C_0\|u\|^2_{L^2(\Omega)}. \tag{2.8}$$

Let $\omega_j\subset\Omega$, $\bigcup_j\omega_j=\Omega$ be a covering of Ω such that $\mathrm{diam}(\omega_j)<h$ and for some $C_i>0$ independent of h, $\mathrm{vol}(\omega_j)\ge C_1h^d$, and for any j, the number of k such that $\omega_j\cap\omega_k\ne\emptyset$ is less than C_2. Such a covering exists as Ω is Lipschitz. Then

$$\begin{aligned} &C_2\int_{\Omega\times\Omega} h^{-d}\varphi\left(\frac{x-y}{h}\right)|u(x)+u(y)|^2\,dx\,dy \\ &\quad\ge\sum_j\int_{\omega_j\times\omega_j} h^{-d}\varphi\left(\frac{x-y}{h}\right)|u(x)+u(y)|^2\,dx\,dy \\ &\quad\ge\sum_j h^{-d}\frac{1}{|B_1|}\int_{\omega_j\times\omega_j}|u(x)+u(y)|^2\,dx\,dy \\ &\quad\ge\sum_j 2h^{-d}\frac{1}{|B_1|}\mathrm{vol}(\omega_j)\|u\|^2_{L^2(\omega_j)} \\ &\quad\ge\frac{2C_1}{|B_1|}\|u\|^2_{L^2(\Omega)}. \end{aligned} \tag{2.9}$$

From (2.9), we get that (2.8) holds true.

For the proof of (1.6) we need a suitable covering of Ω. Given $\epsilon > 0$ small enough, there exists some open sets $\Omega_0, \dots, \Omega_N$ such that $\{x \in \mathbb{R}^d, \operatorname{dist}(x, \overline{\Omega}) \le \epsilon^2\} \subset \bigcup_{j=0}^N \Omega_j$, where the Ω_j's have the following properties:

1. $\Omega_0 = \{x \in \Omega, d(x, \partial\Omega) > \epsilon^2\}$.
2. For $j = 1, \dots, N$, there exists $r_j > 0$, an affine isometry R_j of $\mathbb{R}^d$ and a Lipschitz map $\varphi_j : \mathbb{R}^{d-1} \to \mathbb{R}$ such that, denoting $\tilde{\phi}_j(x', x_d) = (x', x_d + \varphi_j(x'))$ and $\phi_j = R_j \circ \tilde{\phi}_j$, we have

$$
\begin{aligned}
\phi_j \text{ is injective on } & B(0, 2r_j) \times]-2\epsilon, 2\epsilon[, \\
\Omega_j &= \phi_j(B(0, r_j) \times]-\epsilon, \epsilon[), \\
\Omega_j \cap \Omega &= \phi_j(B(0, r_j) \times]0, \epsilon[), \\
\phi_j(B(0, 2r_j) & \times]0, 2\epsilon[) \subset \Omega.
\end{aligned} \tag{2.10}
$$

We put our open set Ω in a large box $B =]-A/2, A/2[^d$ and define an extension map $E : L^2(\Omega) \to L^2(B)$. For $j = 0, \dots, N$ we let $\chi_j \in C_0^\infty(\Omega_j)$ be such that $\sum_j \chi_j(x) = 1$ for $\operatorname{dist}(x, \overline{\Omega}) \le \epsilon^2$. For any function $u \in L^2(\Omega)$, let u_j, $j = 0, \dots, N$ be defined in a neighborhood of Ω_j by $u_j = u \circ \phi_j \circ S \circ \phi_j^{-1}$, where $S(x', x_d) = (x', -x_d)$ if $x_d < 0$ and $S(x', x_d) = (x', x_d)$ if $x_d \ge 0$. For $x \in \Omega \cap \Omega_j$, one has $u_j(x) = u(x)$ and we define

$$
E(u)(x) = \sum_{j=0}^N \chi_j(x) u_j(x). \tag{2.11}
$$

We observe that $\tilde{\phi}_j^{-1}(x) = (x', x_d - \varphi_j(x'))$. Consequently, as φ_j is Lipschitz-continuous, then ϕ_j and ϕ_j^{-1} are also Lipschitz-continuous. Hence, formula (2.11), gives us an extension map from $L^2(\Omega)$ into $L^2(B)$, which is also bounded from $H^1(\Omega)$ into $H^1(B)$. For $u \in L^2(\Omega)$, $v \in L^2(B)$, set

$$
\begin{aligned}
\mathcal{E}_{h,\rho}(u) &= \langle (1 - T_{h,\rho}) u, u \rangle_{L^2(\rho)}, \\
\mathcal{E}_h(v) &= \iint_{B \times B, |x-y| \le h} h^{-d} |v(x) - v(y)|^2 \, dx \, dy.
\end{aligned} \tag{2.12}
$$

Since for A large, $E(u)$ vanishes near the boundary of B, we can extend $v = E(u)$ as an A-periodic function on $\mathbb{R}^d$, and write its Fourier series $v(x) = E(u)(x) = \sum_{k \in \mathbb{Z}^d} c_k(v) e^{2i\pi kx/A}$ with $c_k(v) = A^{-d} \int_B e^{-2i\pi kx/A} v(x) \, dx$.

Then

$$\|E(u)\|^2_{L^2(B)} = A^d \sum_k |c_k|^2,$$
$$\|E(u)\|^2_{H^1(B)} = A^d \sum_k (1+4\pi^2k^2/A^2)|c_k|^2 \tag{2.13}$$

and since E is bounded from $H^1(\Omega)$ into $H^1(B)$, then $\|u\|^2_{L^2(\Omega)} \simeq A^d\sum_k |c_k|^2$ and $\|u\|^2_{H^1(\Omega)} \simeq A^d\sum_k(1+4\pi^2k^2/A^2)|c_k|^2$, where $f(u) \simeq g(u)$ means that there exists some constant $C>0$ independent of u, such that $\frac{1}{C}f(u) \le g(u) \le Cf(u)$.

Moreover, one gets

$$\mathcal{E}_h(v) = A^d \sum_k |c_k|^2\theta(hk), \tag{2.14}$$

with

$$\theta(\xi) = \int_{|z|\le 1} |e^{2i\pi\xi z/A} - 1|^2\, dz.$$

Observe that the function θ is nonnegative, quadratic near 0. Moreover, it vanishes if and only if $\xi = 0$ and it has a positive lower bound for $|\xi| \ge 1$.

The next two lemmas show that the Dirichlet forms for $u \in L^2(\Omega)$ and its extension to $L^2(B)$ are comparable.

Lemma 2.1 *For all $\alpha > 1$, there exists $C > 0$ and $h_0 > 0$ such that*

$$\mathcal{E}_{\alpha h,\rho}(u) \le C\mathcal{E}_{h,\rho}(u) \quad \forall u \in L^2(\Omega),\ \forall h \in]0,h_0]. \tag{2.15}$$

Proof Using (2.2) and (2.5), we observe that it suffices to prove the lemma in the case where $\rho(x) = \rho$ is constant, and we first show the result when Ω is convex. In that case, since $|u(x)-u(y)| \le |u(x)-u(\frac{x+y}{2})| + |u(\frac{x+y}{2})-u(y)|$, one has

$$\begin{aligned}
\mathcal{E}_{\alpha h,\rho}(u) &= \frac{(h\alpha)^{-d}}{2\,\mathrm{vol}(B_1)}\int_\Omega\int_\Omega 1_{|x-y|\le\alpha h}|u(x)-u(y)|^2\rho\, dx\, dy\\
&\le \frac{2(h\alpha)^{-d}}{\mathrm{vol}(B_1)}\int_\Omega\int_\Omega 1_{|x-y|\le\alpha h}\left|u(x)-u\left(\frac{x+y}{2}\right)\right|^2\rho\, dx\, dy\\
&= \frac{2(h\alpha/2)^{-d}}{\mathrm{vol}(B_1)}\int_{\phi(\Omega\times\Omega)} 1_{|x-y|\le\frac{\alpha h}{2}}|u(x)-u(y)|^2\rho\, dx\, dy,
\end{aligned} \tag{2.16}$$

where $\phi(x,y) = (x,\frac{x+y}{2})$. As Ω is convex $\phi(\Omega\times\Omega) \subset \Omega\times\Omega$ and we get $\mathcal{E}_{\alpha h,\rho}(u) \le 4\mathcal{E}_{\frac{\alpha h}{2},\rho}(u)$. Iterating this process we obtain the announced result for convex domains.

In the general case, we use the local covering introduced in (2.10). Let $\Omega_i^+ = \Omega_i \cap \Omega$ (respectively $\Omega_i^- = \Omega_i \cap (\mathbb{R}^d \setminus \Omega)$) and $U_i(h) = \{(x, y) \in \Omega_i^+ \times \Omega, |x-y| \le \alpha h\}$. Since by (2.2), $\Omega \subset \bigcup_i \Omega_i^+$, we have $\mathcal{E}_{\alpha h,\rho}(u) \le \sum_{i=0}^N \mathcal{E}^i_{\alpha h,\rho}(u)$ with

$$\mathcal{E}^i_{\alpha h,\rho}(u) = \frac{(\alpha h)^{-d}}{2\,\mathrm{vol}(B_1)} \int_{U_i(h)} 1_{|x-y|\le\alpha h} |u(x) - u(y)|^2 \rho\, dx\, dy. \tag{2.17}$$

Let us estimate $\mathcal{E}^0_{\alpha h,\rho}(u)$. For $h \in]0, \epsilon^2/\alpha[$ and $(x, y) \in U_0(h)$, we have $[x, y] \subset \Omega$. Therefore, the change of variable $\phi(x, y) = (x, \frac{x+y}{2})$ maps $U_0(h)$ into $\Omega_0 \times \Omega$ and we get as above

$$\mathcal{E}^0_{\alpha h,\rho}(u) \le \frac{2(\alpha h)^{-d}}{\mathrm{vol}(B_1)} \int_{U_0(h)} 1_{|x-y|\le\alpha h} \times \left| u(x) - u\left(\frac{x+y}{2}\right)\right|^2 \rho\, dx\, dy \le 4\mathcal{E}_{\frac{\alpha h}{2},\rho}(u). \tag{2.18}$$

For $i \neq 0$ and $h > 0$ small enough, we remark that $U_i(h) \subset \tilde{\Omega}_i^+ \times \tilde{\Omega}_i^+$, where $\tilde{\Omega}_i^\pm = \phi_i(B(0, 2r_i) \times \{0 < \pm x_d < 2\epsilon\})$. Denoting $Q_i = B(0, r_i)\times]0, \epsilon[$, $\tilde{Q}_i = B(0, 2r_i)\times]0, 2\epsilon[$, we can use the Lipschitz-continuous change of variable $\phi_i : \tilde{Q}_i \to \tilde{\Omega}_i^+ \subset \Omega$ to get

$$\mathcal{E}^i_{\alpha h,\rho}(u) \le \frac{(\alpha h)^{-d}}{2\,\mathrm{vol}(B_1)} \int_{\tilde{Q}_i} \int_{\tilde{Q}_i} J_{\phi_i}(x) J_{\phi_i}(y) 1_{|\phi_i(x)-\phi_i(y)|\le\alpha h} \times |u \circ \phi_i(x) - u \circ \phi_i(y)|^2 \rho\, dx\, dy \tag{2.19}$$

where the Jacobian J_{ϕ_i} of ϕ_i is a bounded function defined almost everywhere. As both ϕ_i, ϕ_i^{-1} are Lipschitz-continuous, there exists $M_i, m_i > 0$ such that for all $x, y \in \tilde{Q}_i$ we have $m_i|x-y| \le |\phi_i(x) - \phi_i(y)| \le M_i|x-y|$. Therefore,

$$\mathcal{E}^i_{\alpha h,\rho}(u) \le Ch^{-d} \int_{\tilde{Q}_i} \int_{\tilde{Q}_i} 1_{|x-y|\le\frac{\alpha h}{m_i}} |u \circ \phi_i(x) - u \circ \phi_i(y)|^2 \rho\, dx\, dy, \tag{2.20}$$

where C denotes a positive constant changing from line to line. As $\tilde{Q}_i$ is convex, it follows from the study of the convex case that

$$\mathcal{E}^i_{\alpha h,\rho}(u) \le Ch^{-d} \int_{\tilde{Q}_i} \int_{\tilde{Q}_i} 1_{|x-y|\le\frac{h}{M_i}} |u \circ \phi_i(x) - u \circ \phi_i(y)|^2 \rho\, dx\, dy$$

$$\leq Ch^{-d}\int_{\tilde{Q}_i}\int_{\tilde{Q}_i} 1_{|\phi_i(x)-\phi_i(y)|\leq h}|u\circ\phi_i(x)-u\circ\phi_i(y)|^2\rho\,dx\,dy$$

$$\leq Ch^{-d}\int_{\tilde{\Omega}_i^+}\int_{\tilde{\Omega}_i^+} 1_{|x-y|\leq h}|u(x)-u(y)|^2\rho\,dx\,dy \leq C_i\mathcal{E}_{h,\rho}(u), \tag{2.21}$$

and the proof is complete. □

Lemma 2.2 *There exist $C_0, h_0>0$ such that the following holds true for any $h\in]0,h_0]$ and any $u\in L^2(\rho)$.*

$$\mathcal{E}_{h,\rho}(u)/C_0 \leq \mathcal{E}_h(E(u)) \leq C_0\big(\mathcal{E}_{h,\rho}(u)+h^2\|u\|_{L^2}^2\big). \tag{2.22}$$

As a byproduct, there exists C_1 such that for all $h\in]0,h_0]$ and any function $u\in L^2(\rho)$ such that

$$\|u\|_{L^2(\rho)}^2 + h^{-2}\langle(1-T_{h,\rho})u,u\rangle_{L^2(\rho)} \leq 1,$$

the function u admits a decomposition $u=u_L+u_H$ with $u_L\in H^1(\Omega)$, $\|u_L\|_{H^1}\leq C_1$, and $\|u_H\|_{L^2}\leq C_1 h$.

Proof Using the second line of (2.5), we may assume that the density ρ is constant equal to 1. The proof of the left inequality in (2.22) is obvious. For the upper bound, we remark that there exists $C>0$ such that $\mathcal{E}_h(E(u)) \leq C\sum_{j=0}^N(\mathcal{E}_h^{j,1}+\mathcal{E}_h^{j,2})$ with

$$\mathcal{E}_h^{j,1} = h^{-d}\int_{B\times B} 1_{|x-y|\leq h}|\chi_j(x)-\chi_j(y)|^2|u_j(x)|^2\,dx\,dy \tag{2.23}$$

and

$$\mathcal{E}_h^{j,2} = h^{-d}\int_{B\times B} 1_{|x-y|\leq h}|\chi_j(y)|^2|u_j(x)-u_j(y)|^2\,dx\,dy. \tag{2.24}$$

As the functions χ_j are regular, there exist some $\tilde{\chi}_j\in C_0^\infty(B)$ equal to 1 near the support of χ_j such that

$$\begin{aligned}\mathcal{E}_h^{j,1} &\leq Ch^{-d}\int_B \tilde{\chi}_j(x)|u_j(x)|^2\bigg(\int_B 1_{|x-y|\leq h}|x-y|^2\,dy\bigg)\,dx\\ &\leq Ch^2\|u\|_{L^2(\Omega)}^2.\end{aligned} \tag{2.25}$$

In order to estimate $\mathcal{E}_h^{j,2}$ one has to estimate the contribution of the points $x\in\Omega$, $y\notin\Omega$ and $x\notin\Omega$, $y\notin\Omega$. All the terms are treated in the same way and we only examine

$$\begin{aligned}\mathcal{E}_h^{j,3} &= h^{-d}\int_{\Omega\times(B\setminus\Omega)} 1_{|x-y|\le h}|\chi_j(y)|^2|u_j(x)-u_j(y)|^2\,dx\,dy\\ &= h^{-d}\int_{\tilde{\Omega}_j^+\times\Omega_j^-} 1_{|x-y|\le h}|\chi_j(y)|^2|u(x)-u\circ\phi_j\circ S\circ\phi_j^{-1}(y)|^2\,dx\,dy,\end{aligned} \tag{2.26}$$

with S defined below (2.10). Let $\sigma:\mathbb{R}^d\to\mathbb{R}^d$ be the symmetry with respect to $\{y_d=0\}$, so that $S\sigma=Id$ on $\{y_d<0\}$. We use the Lipschitz-continuous change of variable $\psi_j: y\in\Omega_j^+\mapsto\phi_j\circ\sigma\circ\phi_j^{-1}(y)\in\Omega_j^-$ to get

$$\mathcal{E}_h^{j,3}\le Ch^{-d}\int_{\tilde{\Omega}_j^+\times\Omega_j^+} 1_{|x-\psi_j(y)|\le h}|\chi_j\circ\psi_j(y)|^2|u(x)-u(y)|^2\,dx\,dy. \tag{2.27}$$

We claim that there exists $\beta>0$ such that

$$|\psi_j(y)-x|\ge\beta^{-1}|x-y|\qquad\forall(x,y)\in\tilde{\Omega}_j^+\times\Omega_j^+. \tag{2.28}$$

Indeed, as both ϕ_j and ϕ_j^{-1} are Lipschitz-continuous, (2.28) is equivalent to finding $\beta>0$ such that

$$|\sigma(y)-x|\ge\beta^{-1}|x-y|\qquad\forall(x,y)\in\phi_j^{-1}(\tilde{\Omega}_j^+\times\Omega_j^+), \tag{2.29}$$

which is obvious with $\beta=1$. From (2.28) it follows that for some $\alpha>1$, one has

$$\mathcal{E}_h^{j,3}\le Ch^{-d}\int_{\tilde{\Omega}_j^+\times\Omega_j^+} 1_{|x-y|\le\alpha h}|u(x)-u(y)|^2\,dx\,dy\le C\mathcal{E}_{\alpha h,\rho}(u), \tag{2.30}$$

and the upper bound is then a straightforward consequence of Lemma 2.1.

The proof of the decomposition of u goes as follows. Start from $u\in L^2(\rho)$ such that $\|u\|_{L^2(\rho)}^2+h^{-2}\langle(1-T_{h,\rho})u,u\rangle_{L^2(\rho)}\le 1$ and let $v=E(u)$. It follows from (2.14) and (2.22) that

$$\sum_{k\in\mathbb{Z}^d}|c_k|^2\theta(hk)\le C_0'h^2=A^{-d}C_0h^2. \tag{2.31}$$

Let $v_L=\sum_{|hk|\le 1}c_ke^{2i\pi kx/A}$ and $v_H=v-v_L$. Since θ is quadratic near 0 and only vanishes at the origin, there exists some constant $C>0$ such that $\theta(\xi)\ge C|\xi|^2$ and hence

$$Ch^2\sum_{|hk|\le 1}|c_k|^2|k|^2\le C_0'h^2. \tag{2.32}$$

Dividing by h^2, this shows that $\|v_L\|^2_{H^1(B)} \le C_0'/C$ and hence, $u_L = (v_L)_{|\partial\Omega}$ is bounded in $H^1(\Omega)$ uniformly with respect to h.

Similarly, since θ is bounded from below by some $C > 0$ on $|\xi| \ge 1$, it follows from (2.31) that

$$\|v_H\|^2_{L^2(B)} \le C \sum_{h|k|>1} |c_k|^2 \le C_0' h^2. \tag{2.33}$$

Setting $u_H = (v_H)_{|\partial\Omega}$, this shows that $\|u_H\|_{L^2(\Omega)} = O(h)$ and the proof of Lemma 2.2 is complete. □

We are in position to prove the estimate (1.6) on the spectral gap. Once again, using the second line of (2.5), we may assume that the density ρ is constant equal to 1. To show the right inequality, it suffices to plug a function $u \in C_0^\infty(\Omega)$ with support contained in a ball $Q \subset \Omega$ and such that $\int_\Omega u(x)\rho(x)\,dx = 0$ into (1.3). As Q is convex, it follows from Taylor's formula that for such u, we have $\langle u - T_h u, u\rangle = O(h^2)$.

To show the left inequality in (1.6), we first observe that it is clearly satisfied when Ω is convex. Indeed, given $u \in L^2(\Omega)$ we have by Cauchy-Schwarz

$$\begin{aligned}
&\int_{\Omega\times\Omega} |u(x) - u(y)|^2\,dx\,dy \\
&\quad \le C h^{-1} \sum_{k=0}^{K(h)-1} \int_{\Omega\times\Omega} \big| u(x + k\hbar(y-x)) \\
&\qquad - u(x + (k+1)\hbar(y-x))\big|^2\,dx\,dy,
\end{aligned} \tag{2.34}$$

where $K(h)$ is the greatest integer $\le h^{-1}$ and $\hbar = 1/K(h)$. With the new variables $x' = x + k\hbar(y-x)$, $y' = x + (k+1)\hbar(y-x)$, one has $dx'\,dy' = \hbar^d\,dx\,dy$ and we get

$$\begin{aligned}
&\int_{\Omega\times\Omega} |u(x) - u(y)|^2\,dx\,dy \\
&\quad \le C h^{-d-1} K(h) \int_{\Omega\times\Omega} 1_{|x'-y'|<\hbar\,\mathrm{diam}(\Omega)} |u(x') - u(y')|^2\,dx'\,dy',
\end{aligned} \tag{2.35}$$

By Lemma 2.1, this proves the left inequality in (1.6) in the case where Ω is convex.

In the general case, we can find some open sets contained in Ω, $\omega_j \sum \Subset \Omega_j^+ \Subset \tilde\Omega_j^+$, $j = 1, \ldots, N + M$ such that for $j = 1, \ldots, N$, $\Omega_j^+, \tilde\Omega_j^+$ are given in the proof of Lemma 2.1, $(\Omega_j^+)_{j=N+1,\ldots,N+M}$ are convex $\Omega_0 \subset$

$\bigcup_{j=N+1}^{M+N} \Omega_j^+$, $\Omega \subset \bigcup_{j=1}^{N+M} \omega_j$, and where $A \Subset B$ means that $\overline{A}^{\Omega} \subset B$. Hence for $h > 0$ small enough,

$$\begin{aligned}\mathcal{E}_{h,\rho}(u) &\geq C \sum_{j=1}^{N+M} h^{-d} \int_{\Omega_j^+ \times \tilde{\Omega}_j^+} 1_{|x-y|<h} (u(x) - u(y))^2 \, dx \, dy \\ &\geq C \sum_{j=1}^{N} h^{-d} \int_{Q_j \times \tilde{Q}_j} 1_{|\phi_j(x) - \phi_j(y)|<h} (u \circ \phi_j(x) - u \circ \phi_j(y))^2 \, dx \, dy \\ &\quad + C \sum_{j=N+1}^{N+M} h^{-d} \int_{\Omega_j^+ \times \tilde{\Omega}_j^+} 1_{|x-y|<h} (u(x) - u(y))^2 \, dx \, dy,\end{aligned} \tag{2.36}$$

where Q_j, $\tilde{Q}_j$ are as in the proof of Lemma 2.1. From the estimate proved above in the convex case, we know that there exists $a > 0$ independent of h such that the second sum in (2.36) is bounded from below by

$$\begin{aligned}&Ch^2 \sum_{j=N+1}^{N+M} \int_{\omega_j \times \Omega_j^+} (u(x) - u(y))^2 \, dx \, dy \\ &\quad \geq Ch^2 \sum_{j=N+1}^{N+M} \int_{\omega_j \times \Omega, |x-y|<a} (u(x) - u(y))^2 \, dx \, dy.\end{aligned} \tag{2.37}$$

On the other hand, thanks to the fact that ϕ_j is a Lipschitz diffeomorphism, there exists $\alpha > 0$ such that $1_{|x-y|<h/\alpha} \leq 1_{|\phi_j(x)-\phi_j(y)|<h} \leq 1_{|x-y|<\alpha h}$. Using the convexity of Q_i and Lemma 2.1 it follows that the first sum in the right hand side of (2.36) is bounded from below by

$$Ch^2 \sum_{j=1}^{N} \int_{\omega_j \times \Omega, |x-y|<a} (u(x) - u(y))^2 \, dx \, dy. \tag{2.38}$$

Combining (2.36), (2.37) and (2.38), we get

$$\mathcal{E}_{h,\rho}(u) \geq Ch^2 \int_{\Omega \times \Omega, |x-y|<a} (u(x) - u(y))^2 \, dx \, dy \tag{2.39}$$

for some fixed $a > 0$ independent of h. Since by (2.4) we have $g(a, \rho) > 0$, we get

$$\mathcal{E}_{h,\rho}(u) \geq Ch^2 \int_{\Omega \times \Omega} (u(x) - u(y))^2 \, dx \, dy. \tag{2.40}$$

The proof of (1.6) is complete.

Lemma 2.3 *There exists* $\delta_0 \in]0, 1/2[$ *and some constants* C_i *independent on* λ *and* h *such that* $\mathrm{Spec}(T_{h,\rho}) \cap [1-\delta_0, 1]$ *is discrete, and for any* $0 \le \lambda \le \delta_0/h^2$, *the number of eigenvalues of* $T_{h,\rho}$ *in* $[1-h^2\lambda, 1]$ (*with multiplicity*) *is bounded by* $C_1(1+\lambda)^{d/2}$. *Moreover, any eigenfunction* $T_{h,\rho}(u) = \lambda u$ *with* $\lambda \in [1-\delta_0, 1]$ *satisfies the bound*

$$\|u\|_{L^\infty} \le C_2 h^{-d/2} \|u\|_{L^2}. \tag{2.41}$$

Proof To get (2.41), we just write that since λ is not in the range of m_h, one has

$$u(x) = \frac{1}{\lambda - m_h(x)} \int_\Omega h^{-d} \varphi\left(\frac{x-y}{h}\right) \min\left(\frac{\rho(y)}{\rho(x)}, 1\right) u(y)\, dy,$$

and we apply Cauchy–Schwarz. The important point here is the estimate on the number of eigenvalues in $[1-h^2\lambda, 1]$ by a power of λ. This is obtained by the min-max and uses (2.22). The min-max gives: if for some closed subspace F of $L^2(\rho)$ with $\mathrm{codim}(F) = N$ one has for all $u \in F$, $h^{-2}\langle (1-T_{h,\rho})u, u\rangle_{L^2(\rho)} \ge \lambda \|u\|^2_{L^2(\rho)}$, then the number of eigenvalues of T_h in $[1-h^2\lambda, 1]$ (with multiplicity) is bounded by $\mathrm{codim}(F) = N$. Then, we fix $c > 0$ small enough, and we choose for F the subspace of functions u such that their extension $v = E(u)$ is such that the Fourier coefficients satisfy $c_k(E(u)) = 0$ for $|k| \le D$ with $hD \le c$. The codimension of this space F is exactly the number of $k \in \mathbb{Z}^d$ such that $|k| \le D$, since if p is a trigonometric polynomial such that $E^*(p) = 0$, we will have $\int_\Omega p(x)u(x)\, dx = 0$ for any function u with compact support in Ω and such that $E(u) = u$, and this implies $p = 0$. Thus $\mathrm{codim}(F) \simeq (1+D)^d$. On the other hand, the right inequality in (2.22) gives for $u \in F$, $h^{-2}\langle (1-T_{h,\rho})u, u\rangle_{L^2(\rho)} \ge C_0(D^2 - C_1)\|u\|^2_{L^2(\rho)}$ for universal C_0, C_1, since by (2.14), there exists $C > 0$ such that one has $\theta(hk)h^{-2} \ge CD^2$ for all $D \le c/h$ and all $|k| > D$. The proof of our lemma is complete. □

We are now ready to prove the total variation estimate (1.7). We use the notation $T_h = T_{h,\rho}$. Let Π_0 be the orthogonal projector in $L^2(\rho)$ on the space of constant functions

$$\Pi_0(u)(x) = 1_\Omega(x) \int_\Omega u(y)\rho(y)\, dy. \tag{2.42}$$

Then

$$2 \sup_{x_0 \in \Omega} \|T_h^n(x_0, dy) - \rho(y)\, dy\|_{TV} = \|T_h^n - \Pi_0\|_{L^\infty \to L^\infty}. \tag{2.43}$$

To show the left hand side, it suffices to consider an eigenfunction e_h associated to the eigenvalue $(1-g(h,\rho))$ and normalized in $L^\infty(\Omega)$. Since e_h is orthogonal to constant functions, we get immediately $2\sup_{x_0\in\Omega}\|T_h^n(x_0,dy)-\rho(y)\,dy\|_{TV}\geq \|T_h^n e_h-\Pi_0 e_h\|_{L^\infty}=(1-g(h,\rho))^n$.

Let us now prove the right inequality. We have to show that there exist C_0, h_0, such that for any n and any $h\in]0,h_0]$, one has

$$\|T_h^n-\Pi_0\|_{L^\infty\to L^\infty}\leq C_0 e^{-ng_{h,\rho}}. \tag{2.44}$$

Observe that since we know that for h_0 small, the estimate (1.6) holds true for any ρ, we may assume $n\geq Ch^{-2}$. In order to prove (2.44), we split T_h into three pieces, using spectral theory.

Let $0<\lambda_{1,h}\leq\cdots\leq\lambda_{j,h}\leq\lambda_{j+1,h}\leq\cdots\leq h^{-2}\delta_0$ be such that the eigenvalues of T_h in the interval $[1-\delta_0,1[$ are the $1-h^2\lambda_{j,h}$, with associated orthonormal eigenfunctions $e_{j,h}$,

$$T_h(e_{j,h})=(1-h^2\lambda_{j,h})e_{j,h},\qquad (e_{j,h}|e_{k,h})_{L^2(\rho)}=\delta_{j,k}. \tag{2.45}$$

Then we write $T_h-\Pi_0=T_{1,h}+T_{2,h}+T_{3,h}$ with

$$\begin{aligned}
T_{1,h}(x,y)&=\sum_{\lambda_{1,h}\leq\lambda_{j,h}\leq h^{-\alpha}}(1-h^2\lambda_{j,h})e_{j,h}(x)e_{j,h}(y),\\
T_{2,h}(x,y)&=\sum_{h^{-\alpha}<\lambda_{j,h}\leq h^{-2}\delta_0}(1-h^2\lambda_{j,h})e_{j,h}(x)e_{j,h}(y),\\
T_{3,h}&=T_h-\Pi_0-T_{1,h}-T_{2,h}.
\end{aligned} \tag{2.46}$$

Here $\alpha>0$ is a small constant that will be chosen later. One has $T_h^n-\Pi_0=T_{1,h}^n+T_{2,h}^n+T_{3,h}^n$, and we will get the bound (2.44) for each of the three terms. We start by very rough bounds. Since there are at most Ch^{-d} eigenvalues $\lambda_{j,h}$ and using the bound (2.41), we get that there exists C independent of $n\geq 1$ and h such that

$$\|T_{1,h}^n\|_{L^\infty\to L^\infty}+\|T_{2,h}^n\|_{L^\infty\to L^\infty}\leq Ch^{-3d/2}. \tag{2.47}$$

Since T_h^n is bounded by 1 on L^∞, we get from $T_h^n-\Pi_0=T_{1,h}^n+T_{2,h}^n+T_{3,h}^n$

$$\|T_{3,h}^n\|_{L^\infty\to L^\infty}\leq Ch^{-3d/2}. \tag{2.48}$$

Next we use (1.2) to write $T_h=m_h+R_h$ with

$$\begin{aligned}
\|m_h\|_{L^\infty\to L^\infty}&\leq\gamma<1,\\
\|R_h\|_{L^2\to L^\infty}&\leq C_0h^{-d/2}.
\end{aligned} \tag{2.49}$$

From this, we deduce that for any $p = 1, 2, \dots$, one has $T_h^p = A_{p,h} + B_{p,h}$, with $A_{1,h} = m_h$, $B_{1,h} = R_h$ and the recurrence relation $A_{p+1,h} = m_h A_{p,h}$, $B_{p+1,h} = m_h B_{p,h} + R_h T_h^p$. Thus one gets, since T_h^p is bounded by 1 on L^2,

$$\begin{aligned} &\|A_{p,h}\|_{L^\infty \to L^\infty} \leq \gamma^p, \\ &\|B_{p,h}\|_{L^2 \to L^\infty} \leq C_0 h^{-d/2}(1 + \gamma + \cdots + \gamma^p) \leq C_0 h^{-d/2}/(1-\gamma). \end{aligned} \tag{2.50}$$

Let $\theta = 1 - \delta_0 < 1$ so that $\|T_{3,h}\|_{L^2 \to L^2} \leq \theta$. Then one has

$$\|T_{3,h}^n\|_{L^\infty \to L^2} \leq \|T_{3,h}^n\|_{L^2 \to L^2} \leq \theta^n,$$

and for $n \geq 1$, $p \geq 1$, one gets, using (2.50) and (2.48),

$$\begin{aligned} \|T_{3,h}^{p+n}\|_{L^\infty \to L^\infty} &= \|T_h^p T_{3,h}^n\|_{L^\infty \to L^\infty} \\ &\leq \|A_{p,h} T_{3,h}^n\|_{L^\infty \to L^\infty} + \|B_{p,h} T_{3,h}^n\|_{L^\infty \to L^\infty} \\ &\leq C h^{-3d/2} \gamma^p + C_0 h^{-d/2} \theta^n/(1-\gamma). \end{aligned} \tag{2.51}$$

Taking $p = n$, we get $\|T_{3,h}^{2n}\|_{L^\infty \to L^\infty} \leq C h^{-\alpha} \tilde{\theta}^n$ for some $\alpha > 0$ and $0 < \tilde{\theta} < 1$. This shows that there exists some constants $C > 0$, $\mu > 0$, such that

$$\|T_{3,h}^n\|_{L^\infty \to L^\infty} \leq C e^{-\mu n}, \quad \forall h,\ \forall n \geq 1/h, \tag{2.52}$$

and thus the contribution of $T_{3,h}^n$ is far smaller than the bound we have to prove in (2.44).

Next, for the contribution of $T_{2,h}^n$, we just write, since there are at most Ch^{-d} eigenvalues $\lambda_{j,h}$ and using the bound (2.41),

$$\begin{aligned} &T_{2,h}^n(x, y) = \sum_{h^{-\alpha} < \lambda_{j,h} \leq h^{-2}\delta_0} (1 - h^2 \lambda_{j,h})^n e_{j,h}(x) e_{j,h}(y), \\ &\|T_{2,h}^n\|_{L^\infty \to L^\infty} \leq C h^{-3d/2} (1 - h^{2-\alpha})^n. \end{aligned} \tag{2.53}$$

Thus we get for some $C_\alpha > 0$,

$$\|T_{2,h}^n\|_{L^\infty \to L^\infty} \leq C_\alpha e^{-\frac{nh^{2-\alpha}}{2}}, \quad \forall h,\ \forall n \geq h^{-2+\alpha/2}, \tag{2.54}$$

and thus this contribution is still neglectible for $h \in]0, h_0]$ for h_0 small. It remains to study the contribution of $T_{1,h}^n$.

Let E_α be the (finite dimensional) subspace of $L^2(\rho)$ spanned by the eigenvectors $e_{j,h}, \lambda_{j,h} \leq h^{-\alpha}$. By Lemma 2.3, one has $\dim(E_\alpha) \leq Ch^{-d\alpha/2}$. We next prove a Sobolev-type inequality for the form $\mathcal{E}_{h,\rho}$. For background on Sobolev and the following Nash inequality, see [4, 11].

Lemma 2.4 *There exist $\alpha > 0$, $p > 2$ and C independent of h such that for all $u \in E_\alpha$, the following inequality holds true*:

$$\|u\|_{L^p}^2 \leq Ch^{-2}\big(\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2\big). \tag{2.55}$$

Proof Clearly, one has for $u = \sum_{\lambda_{1,h} \leq \lambda_{j,h} \leq h^{-\alpha}} a_j e_{j,h} \in E_\alpha$,

$$\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2 = \sum_{\lambda_{1,h} \leq \lambda_{j,h} \leq h^{-\alpha}} h^2(1 + \lambda_{j,h})|a_j|^2.$$

Take $u \in E_\alpha$ such that $h^{-2}(\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2) \leq 1$. Then by (2.22), one has $h^{-2}\mathcal{E}_h(E(u)) \leq C_0$. Let $\psi(t) \in C_0^\infty(\mathbb{R})$ be equal to 1 near $t = 0$, and for $v(x) = \sum_{k \in \mathbb{Z}^d} c_k(v) e^{2i\pi kx/A}$, set

$$v = v_L + v_H, \quad v_L(x) = \sum_{k \in \mathbb{Z}^d} \psi(h|k|) c_k(v) e^{2i\pi kx/A}. \tag{2.56}$$

Then $v = v_L + v_H$ is a decomposition of the extension $v = E(u)$ in low frequencies (v_L) and high frequencies (v_H). One has $v_L(x) = \int_{\mathbb{R}^d} h^{-d}\theta(\frac{x-y}{h}) v(y)\, dy$, where θ is the function in the Schwartz space defined by $\hat{\theta}(2\pi z/A) = \psi(|z|)$. Hence, the map $v \mapsto v_L$ is bounded uniformly in h on all the spaces L^q for $1 \leq q \leq \infty$. Using the definition of ψ, it follows from (2.32) that

$$\|v_L\|_{H^1(B)} \leq C. \tag{2.57}$$

Thus, with $u_L = v_L|_\Omega$ and $u_H = v_H|_\Omega$, we get $\|u_L\|_{H^1(\Omega)} \leq C$ so by Sobolev for $p < \frac{2d}{d-2}$,

$$\|u_L\|_{L^p} \leq C. \tag{2.58}$$

One the other hand, one has also by (2.22),

$$h^{-2}\mathcal{E}_h(E(e_{j,h})) \leq C_0(1 + \lambda_{j,h}), \tag{2.59}$$

and this implies, by (2.33),

$$h^{-2}\|E(e_{j,h})_H\|_{L^2}^2 \leq C_0(1 + \lambda_{j,h}) \leq C_0(1 + h^{-\alpha}). \tag{2.60}$$

Thus for $\alpha \leq 1$, we get $\|E(e_{j,h})_H\|_{L^2} \leq Ch^{1/2}$. On the other hand, since $\|e_{j,h}\|_{L^\infty} \leq Ch^{-d/2}$, using the definition of the low frequency cut-off we get

$$\begin{aligned}\|E(e_{j,h})_H\|_{L^\infty} &\leq \|E(e_{j,h})\|_{L^\infty} + \|E(e_{j,h})_L\|_{L^\infty}\\ &\leq C\|E(e_{j,h})\|_{L^\infty} \leq Ch^{-d/2}.\end{aligned}$$

By interpolation we can find some $p > 2$ such that

$$\|E(e_{j,h})_H\|_{L^p} \leq C_0 h^{1/4}. \tag{2.61}$$

Thus one gets, for $u = \sum_{\lambda_{1,h} \leq \lambda_{j,h} \leq h^{-\alpha}} a_j e_{j,h} \in E_\alpha$ with $h^{-2}(\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2) \leq 1$,

$$\begin{aligned}\|u_H\|_{L^p} &\leq \sum_{\lambda_{1,h} \leq \lambda_{j,h} \leq h^{-\alpha}} |a_j| \|E(e_{j,h})_H\|_{L^p} \\ &\leq C_0 h^{1/4} \dim(E_\alpha)^{1/2} \|u\|_{L^2} \leq C h^{1/4} h^{-d\alpha/4}.\end{aligned} \tag{2.62}$$

Our lemma follows from (2.58) and (2.62) if one takes α small. Observe that here, the estimate on the number of eigenvalues (i.e., the estimation of the dimension of E_α) is crucial. The proof of Lemma 2.4 is complete. □

From Lemma 2.4, using the interpolation inequality $\|u\|_{L^2}^2 \leq \|u\|_{L^p}^{\frac{p}{p-1}} \|u\|_{L^1}^{\frac{p-2}{p-1}}$, we deduce the Nash inequality, with $1/D = 2 - 4/p > 0$,

$$\|u\|_{L^2}^{2+1/D} \leq C h^{-2}\big(\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2\big)\|u\|_{L^1}^{1/D}, \quad \forall u \in E_\alpha. \tag{2.63}$$

For $\lambda_{j,h} \leq h^{-\alpha}$, one has $h^2\lambda_{j,h} \leq 1$, and thus for any $u \in E_\alpha$, one gets $\mathcal{E}_{h,\rho}(u) \leq \|u\|_{L^2}^2 - \|T_h u\|_{L^2}^2$ and thus we get, from (2.63),

$$\|u\|_{L^2}^{2+1/D} \leq C h^{-2}\big(\|u\|_{L^2}^2 - \|T_h u\|_{L^2}^2 + h^2\|u\|_{L^2}^2\big)\|u\|_{L^1}^{1/D}, \quad \forall u \in E_\alpha. \tag{2.64}$$

For $0 < \alpha \leq 2$, we deduce from (2.52), (2.54), and $T_h^n - \Pi_0 = T_{1,h}^n + T_{2,h}^n + T_{3,h}^n$, that there exists C_2 such that

$$\|T_{1,h}^n\|_{L^\infty \to L^\infty} \leq C_2, \quad \forall h,\ \forall n \geq h^{-2+\alpha/2}, \tag{2.65}$$

and thus since $T_{1,h}$ is self adjoint on L^2,

$$\|T_{1,h}^n\|_{L^1 \to L^1} \leq C_2, \quad \forall h,\ \forall n \geq h^{-2+\alpha/2}. \tag{2.66}$$

Fix $p \simeq h^{-2+\alpha/2}$. Take $g \in L^2$ such that $\|g\|_{L^1} \leq 1$ and consider the sequence c_n, $n \geq 0$,

$$c_n = \|T_{1,h}^{n+p} g\|_{L^2}^2. \tag{2.67}$$

Then $0 \leq c_{n+1} \leq c_n$, and from (2.64) and (2.66), we get

$$\begin{aligned}c_n^{1+\frac{1}{2D}} &\leq C h^{-2}(c_n - c_{n+1} + h^2 c_n)\|T_{1,h}^{n+p} g\|_{L^1}^{1/D} \\ &\leq C C_2^{1/D} h^{-2}(c_n - c_{n+1} + h^2 c_n).\end{aligned} \tag{2.68}$$

From this inequality, we deduce that there exist $A \simeq CC_2 \sup_{0\le n\le h^{-2}}(2+n)(1+h^2-(1-\frac{1}{n+2})^{2D})$ which depends only on $C,\ C_2,\ D$, such that for all $0\le n\le h^{-2}$, one has $c_n \le (\frac{Ah^{-2}}{1+n})^{2D}$, and thus there exist C_0 which depends only on $C,\ C_2,\ D$, such that for $N\simeq h^{-2}$, one has $c_N\le C_0$. This implies

$$\|T_{1,h}^{N+p} g\|_{L^2} \le C_0\|g\|_{L^1}, \tag{2.69}$$

and thus taking adjoints,

$$\|T_{1,h}^{N+p} g\|_{L^\infty} \le C_0\|g\|_{L^2}, \tag{2.70}$$

and so we get, for any n and with $N+p\simeq h^{-2}$,

$$\|T_{1,h}^{N+p+n} g\|_{L^\infty} \le C_0(1-h^2\lambda_{1,h})^n\|g\|_{L^2}. \tag{2.71}$$

And thus for $n\ge h^{-2}$,

$$\begin{aligned}\|T_{1,h}^{n}\|_{L^\infty\to L^\infty} &\le C_0 e^{-(n-h^{-2})h^2\lambda_{1,h}} = C_0 e^{\lambda_{1,h}} e^{-ng(h,\rho)}, \quad \forall h,\ \forall n\ge h^{-2}\\ &\le C_1 e^{-nC_2h^2}\end{aligned} \tag{2.72}$$

for some $C_1, C_2>0$ independant on h, by (1.6). This concludes the proof of Theorem 1.1.

Remark 1 We believe that (2.41) is true with a power of Λ instead of a power of h with $\lambda = 1-h^2\Lambda$. We have no proof for this which is why we use a Nash inequality for $T_{1,h}$.

Remark 2 The above proof seems to apply for a more general choice of the elementary Markov kernel $h^{-d}\varphi(\frac{x-y}{h})$. Replace φ by a positive symmetric measure of total mass 1 with support in the unit ball, and let T_h be the Metropolis algorithm with this data. Assume that one is able to prove that for some $\delta_0>0$ one has $\mathrm{Spec}(T_h)\subset[-1+\delta_0, 1]$ for all $h\le h_0$, and that for some power M, one has for some $C, c>0$,

$$T_h^M(x,dy) = \mu_h(x,dy) + Ch^{-d}1_{|x-y|\le ch}\rho(y)\,dy, \quad \mu_h(x,dy)\ge 0.$$

Then there exists $\gamma<1$ such that $\|\mu_h\|_{L^\infty}\le\gamma$. Moreover, the right inequality in (2.22) and (2.41) are still valid for T_h^M. Also, the spectral gap of T_h^M is given by formula (1.4) with $T_h^M(x,dy)$ in place of $K_{h,\rho}(x,y)\,dy$, and therefore the left inequality in (1.6) holds true, and the right one is true, since if ρ is constant, for any $\theta\in C_0^\infty(\Omega)$, one has $u-T_hu\in O(h^2)$.

We shall use these remarks in the study of the hard disc problem, in Sect. 4.

3 A proof of Theorem 1.2

In this section, we suppose additionally that Ω is quasi-regular (Definition 2). For a given continuous density ρ, using (2.6) and an approximation of ρ in L^∞ by a sequence of smooth densities ρ_k on $\overline{\Omega}$, one sees that the first assertion (1.18) of Theorem 1.2 is a consequence of the second one (1.19). Assume now that ρ is smooth.

Lemma 3.1 *Let* $\theta \in C^\infty(\overline{\Omega})$ *be such that* $\mathrm{supp}(\theta) \cap \Gamma_{\mathrm{sing}} = \emptyset$ *and* $\partial_n \theta|_{\Gamma_{\mathrm{reg}}} = 0$. *Then, with* $Q_{h,\rho}$ *defined in* (2.2) *and* L_ρ *defined in* (1.11), *we have*

$$Q_{h,\rho}(\theta) = h^2 L_\rho(\theta) + r, \quad \|r\|_{L^2} = O(h^{5/2}). \tag{3.1}$$

Proof For $\theta \in C^\infty(\overline{\Omega})$ and $x \in \Omega$, we can use the Taylor formula to get

$$\begin{aligned} Q_{h,\rho}(\theta)(x) = \frac{1}{\mathrm{vol}(B_1)} \int_{A(x,h)} & \min\left(1 + h\frac{\nabla\rho(x)}{\rho(x)}.z + O(h^2|z|^2), 1\right) \\ & \times \left(-h\nabla\theta(x).z - \frac{h^2}{2}\sum_{i,j} z_i z_j \partial_{x_i}\partial_{x_j}\theta(x) + O(h^3|z|^3)\right) dz, \end{aligned} \tag{3.2}$$

with $A(x,h) = \{z \in \mathbb{R}^d,\ |z| < 1,\ x + hz \in \Omega\}$. As $A(x,h) = A^+(x,h) \cup A^-(x,h)$, with $A^\pm(x,h) = \{z \in A(x,h),\ \pm(\rho(x+hz) - \rho(x)) \geq 0\}$, it follows by an easy computation that

$$\begin{aligned} Q_{h,\rho}(\theta)(x) = & -\frac{h}{\mathrm{vol}(B_1)}\nabla\theta(x).\int_{A(x,h)} z\,dz \\ & -\frac{h^2}{2\,\mathrm{vol}(B_1)}\sum_{i,j=1}^{d} \partial_{x_i}\partial_{x_j}\theta(x)\int_{A(x,h)} z_i z_j\,dz \\ & -\frac{h^2}{\mathrm{vol}(B_1)}\int_{A^-(x,h)} \frac{\nabla\rho(x)}{\rho(x)}.z\nabla\theta(x).z\,dz + r(x) \\ = & f_1(x) + f_2(x) + f_3(x) + r(x), \end{aligned} \tag{3.3}$$

with $\|r\|_{L^\infty(\Omega)} = O(h^3)$. Let $\chi = 1_{d(x,\partial\Omega)<2h}$, then for $j = 2, 3$,

$$\|\chi f_j\|_{L^2(\Omega)} \leq \|\chi\|_{L^2(\Omega)}\|f_j\|_{L^\infty}(\Omega) = O(h^{5/2}), \tag{3.4}$$

thanks to the support properties of χ. Moreover, for $x \in \mathrm{supp}(1-\chi)$, $A(x,h) = \{|z| < 1\}$ and the change of variable $z \mapsto -z$ shows that $(1-$

$\chi)f_2 = -(1-\chi)\frac{\alpha_d}{2}h^2\Delta\theta(x)$ thanks to (1.8). Hence,

$$f_2(x) = -\frac{\alpha_d}{2}h^2\Delta\theta(x) + r(x), \tag{3.5}$$

with $\|r\|_{L^2} = O(h^{5/2})$.

To compute $f_3(x)$ for $x \in \operatorname{supp}(1-\chi)$, we first observe that $|f_3(x)| \le Ch^2|\nabla\rho(x)||\nabla\theta(x)|$. We thus get $\|1_{|\nabla\rho|\le h^{1/2}} f_3\|_{L^\infty} \le Ch^{5/2}\|\nabla\theta\|_{L^\infty}$. At a point x where $|\nabla\rho(x)| \ge h^{1/2}$, we may write $z = t\frac{\nabla\rho(x)}{|\nabla\rho(x)|} + z^\perp$, $t = \frac{z.\nabla\rho(x)}{|\nabla\rho(x)|}$ and $z^\perp.\nabla\rho(x) = 0$. In these coordinates, one has $A^-(x,h) = \{|z| < 1, (t, z^\perp), t|\nabla\rho(x)| + O(h(t^2 + |z^\perp|^2)) \le 0\}$. From $|\nabla\rho(x)| \ge h^{1/2}$ we get that the symmetric difference R between $A^-(x,h)$ and $\{t \le 0\}$ satisfies $\operatorname{meas}(R) = O(h^{1/2})$ (the symmetric difference of two sets A, B is $A \cup B \setminus A \cap B$). Therefore

$$\begin{aligned}
&1_{|\nabla\rho|\ge h^{1/2}}(1-\chi)f_3(x)\\
&\quad= -h^2 1_{|\nabla\rho|\ge h^{1/2}}\frac{(1-\chi)(x)}{\operatorname{vol}(B_1)}\int_{\{|z|<1,\nabla\rho(x).z\le 0\}}\frac{\nabla\rho(x)}{\rho(x)}.z\nabla\theta(x).z\,dz + r(x),
\end{aligned} \tag{3.6}$$

with $\|r\|_{L^\infty} = O(h^{5/2})$. Using the change of variable $z \mapsto z - 2z^\perp$, we get

$$\begin{aligned}
&1_{|\nabla\rho|\ge h^{1/2}}(1-\chi)f_3(x)\\
&\quad= -h^2 1_{|\nabla\rho|\ge h^{1/2}}\frac{\alpha_d}{2}(1-\chi)(x)\frac{\nabla\rho(x)}{\rho(x)}.\nabla\theta(x) + r(x),
\end{aligned} \tag{3.7}$$

and therefore, using (3.4), we get

$$f_3(x) = -h^2\frac{\alpha_d}{2}\frac{\nabla\rho(x)}{\rho(x)}.\nabla\theta(x) + r(x), \tag{3.8}$$

with $\|r\|_{L^2} = O(h^{5/2})$. It remains to show that $\|f_1\|_{L^2(\Omega)} = O(h^{5/2})$. Using the change of variable $z \mapsto -z$ we easily obtain $(1-\chi)f_1 = 0$. Hence, it suffices to show that $f_1'(x,h) = \chi\int_{A(x,h)} z.\nabla\theta(x)\,dz$ satisfies $\|f_1'\|_{L^\infty(\Omega)} = O(h)$. As Γ_{sing} is compact and $\operatorname{supp}(\theta) \cap \Gamma_{\text{sing}} = \emptyset$, this is a local problem near any point x_0 of the regular part Γ_{reg} of the boundary. Let ψ be a smooth function such that near $x_0 = (0,0)$ one has $\Omega = \{x_d > \psi(x')\}$. For x close to x_0 one has

$$A(x,h) = \big\{z \in \mathbb{R}^d, |z| < 1,\ x_d + hz_d > \psi(x' + hz')\big\}. \tag{3.9}$$

Set

$$A_1(x,h) = \big\{z \in \mathbb{R}^d, |z| < 1,\ x_d + hz_d > \psi(x') + h\nabla\psi(x')z'\big\}, \tag{3.10}$$

then the symmetric difference R between $A(x,h)$ and $A_1(x,h)$ satisfies $\text{meas}(R) = O(h)$ uniformly in x close to x_0. This yields

$$f_1'(x,h) = \nabla\theta(x).v(x,h) + r(x), \quad v(x,h) = \int_{A_1(x,h)} z\,dz, \tag{3.11}$$

with $\|r\|_{L^\infty} = O(h)$. Let $\nu(x)$ be the vector field defined by $\nu(x) = (-\nabla\psi(x'), 1)$. Observe that $v(x,h) = \phi(\frac{\psi(x')-x_d}{h|\nu(x)|})\frac{\nu(x)}{|\nu(x)|}$ with $\phi(a) = \int_{|z|<1, z_1>a} z_1\,dz$, vanishes for $\text{dist}(x, \partial\Omega) > Ch$ and that for $x \in \partial\Omega$, $\nu(x)$ is collinear to the unit normal to the boundary $\overrightarrow{n}(x)$. Since $\partial_n\theta|_{\Gamma_{\text{reg}}} = 0$, we thus get $\|f_1'\|_{L^\infty} = O(h)$. The proof of our lemma is complete. □

Let us recall that we denote $1 = \nu_0 < \nu_1 < \cdots < \nu_j < \cdots$ the eigenvalues of L_ρ and m_j the associated multiplicities. We introduce the bilinear form

$$a_\rho(u,v) = \frac{\alpha_d}{2}\langle\nabla u, \nabla v\rangle_{L^2(\rho)} + \langle u, v\rangle_{L^2(\rho)}. \tag{3.12}$$

This defines an Hilbertian structure on $H^1(\Omega)$ which is equivalent to the usual one. We write $\|.\|_{H^1_\rho}$ for the norm induced by a_ρ. We denote

$$\mathcal{D}_0 = \left\{\theta \in C^\infty(\overline{\Omega}), \theta = 0 \text{ near } \Gamma_{\text{sing}}, \partial_n\theta_{|\Gamma_{\text{reg}}} = 0\right\}. \tag{3.13}$$

Lemma 3.2 *$\mathcal{D}_0$ is dense in $H^1(\Omega)$.*

Proof Let $f \in H^1(\Omega)$ be orthogonal to $\mathcal{D}_0$ for the inner product a_ρ defined above. Then, it is orthogonal to $C_0^\infty(\Omega)$ so that $(L_\rho + 1)f = 0$ in the sense of distributions. In particular $-\Delta f \in L^2(\Omega)$. Hence we can use the Green formula (1.14) to get for any $\theta \in \mathcal{D}_0$, since $a_\rho(f,\theta) = 0$,

$$\langle\partial_n f, \rho\theta\rangle_{H^{-1/2}, H^{1/2}} = 0. \tag{3.14}$$

For any $\psi \in C_0^\infty(\Gamma_{\text{reg}})$, using smooth local coordinates we can find $\tilde{\psi}$ in $\mathcal{D}_0$ such that $\tilde{\psi}_{|\partial\Omega} = \psi$. Consequently,

$$\langle\partial_n f, \rho\psi\rangle_{H^{-1/2}, H^{1/2}} = \langle\partial_n f, \rho\tilde{\psi}\rangle_{H^{-1/2}, H^{1/2}} = 0. \tag{3.15}$$

Hence, $\partial_n f_{|\Gamma_{\text{reg}}} = 0$. This shows that $\partial_n f_{|\partial\Omega} \in H^{-1/2}$ is supported in Γ_{sing}. From (1.16) this implies $\partial_n f_{|\partial\Omega} = 0$. This shows that $f \in D(L_\rho)$. As the operator $L_\rho + 1$ is strictly positive, this implies $f = 0$. The proof of our lemma is complete. □

We are now in position to complete the proof of Theorem 1.2. Let $K \in \mathbb{N}$ be fixed (independent of h). We first observe that if $\nu_h \in [0, M]$ and $\psi_{k,h} \in$

$L^2(\rho)$, $k = 1, \dots, K$ satisfy $\|\psi_{k,h}\|_{L^2} = 1$, $h^{-2}Q_{h,\rho}\psi_{k,h} = \nu_h\psi_{k,h}$ and $\psi_{i,h}$ orthogonal to $\psi_{j,h}$ for any $j \neq i$, then thanks to Lemma 2.2 the family $(\psi_{k,h})_{h\in]0,1]}$ is relatively compact in $L^2(\rho)$ for any k, so that we can suppose (extracting a subsequence h_n) that $\nu_h \to \nu$, $\psi_{k,h} \to \psi_k$ in $L^2(\rho)$, $\|\psi_k\|_{L^2} = 1$ and ψ_i orthogonal to ψ_j for any $j \neq i$. Moreover by Lemma 2.2, the limit ψ_k belongs to $H^1(\rho)$. Given $\theta \in \mathcal{D}_0$, it follows from self-adjointness of $Q_{h,\rho}$ and Lemma 3.1 that

$$0 = \langle (h^{-2}Q_{h,\rho} - \nu_h)\psi_{k,h}, \theta\rangle_{L^2(\rho)} = \langle \psi_{k,h}, (L_\rho - \nu_h)\theta\rangle_{L^2(\rho)} + O(h^{1/2}). \tag{3.16}$$

Making $h \to 0$ we obtain $\langle \psi_k, (L_\rho - \nu)\theta\rangle_{L^2(\rho)} = 0$ for all $\theta \in \mathcal{D}_0$. It follows that $(L_\rho - \nu)\psi_k = 0$ in the distribution sense, and integrating by parts that $\partial_n\psi_k$ vanish on Γ_{reg}. Since $\psi_k \in H^1(\rho)$, we get as above using (1.16) that $\partial_n\psi_k = 0$, and it follows that $\psi_k \in D(L_\rho)$. This shows that ν is an eigenvalue of L_ρ, and thus (1.19) is satisfied. Moreover, the inequality $\dim(\mathrm{Ker}(L_\rho - \nu)) \geq K$, shows that for any $\epsilon > 0$ small enough, there exists $h_\epsilon > 0$ small enough such that

$$\sharp\,\mathrm{Spec}(h^{-2}Q_{h,\rho}) \cap [\nu_j - \epsilon, \nu_j + \epsilon] \leq m_j, \tag{3.17}$$

for $h \in]0, h_\epsilon]$. It remains to show that there is equality in (3.17), and we shall proceed by induction on j.

Let $\epsilon > 0$, small, be given such that for $0 \leq \nu_j \leq M + 1$, the intervals $I_j^\epsilon = [\nu_j - \epsilon, \nu_j + \epsilon]$ are disjoint. Let $(\mu_j(h))_{j\geq 0}$ be the increasing sequence of eigenvalues of $h^{-2}Q_{h,\rho}$, $\sigma_N = \sum_{j=1}^N m_j$ and $(e_k)_{k\geq 0}$ the eigenfunctions of L_ρ such that for all $k \in \{1 + \sigma_N, \dots, \sigma_{N+1}\}$, one has $(L_\rho - \nu_{N+1})e_k = 0$. As 0 is a simple eigenvalue of both L_ρ and $Q_{h,\rho}$, we have clearly $\nu_0 = \mu_0 = 0$ and $m_0 = 1 = \sharp\,\mathrm{Spec}(h^{-2}Q_{h,\rho}) \cap [\nu_0 - \epsilon, \nu_0 + \epsilon]$.

Suppose that for all $n \leq N$, $m_n = \sharp\,\mathrm{Spec}(h^{-2}Q_{h,\rho}) \cap [\nu_n - \epsilon, \nu_n + \epsilon]$. Then, one has by (1.19), for $h \leq h_\varepsilon$,

$$\mu_{1+\sigma_N}(h) \geq \nu_{N+1} - \epsilon. \tag{3.18}$$

By the min-max principle, if G is a finite dimensional subspace of H^1 with $\dim(G) = 1 + \sigma_{N+1}$, one has

$$\mu_{\sigma_{N+1}}(h) \leq \sup_{\psi\in G, \|\psi\|=1} \langle h^{-2}Q_{h,\rho}\psi, \psi\rangle_{L^2(\rho)}. \tag{3.19}$$

Thanks to Lemma 3.2, for all e_k, $0 \leq k \leq \sigma_{N+1}$ and all $\alpha > 0$, there exists $e_{k,\alpha} \in \mathcal{D}_0$ such that $\|e_k - e_{k,\alpha}\|_{H^1_\rho} \leq \alpha$. Let G_α be the vector space spanned by the $e_{k,\alpha}$, $0 \leq k \leq \sigma_{N+1}$. For α small enough, one has $\dim(G_\alpha) = 1 + \sigma_{N+1}$. From Lemma 3.1, one has

$$\langle h^{-2}Q_{h,\rho}e_{k,\alpha}, e_{k',\alpha}\rangle_{L^2(\rho)} = \langle L_\rho e_{k,\alpha}, e_{k',\alpha}\rangle_{L^2(\rho)} + O_\alpha(h^{1/2}). \tag{3.20}$$

Since $e_{k,\alpha} \in \mathcal{D}_0$, one has $\langle L_\rho e_{k,\alpha}, e_{k',\alpha}\rangle_{L^2(\rho)} = \frac{\alpha_d}{2}\langle \nabla e_{k,\alpha}, \nabla e_{k',\alpha}\rangle_{L^2_\rho}$ and $\langle \nabla e_{k,\alpha}, \nabla e_{k',\alpha}\rangle_{L^2_\rho} = \langle \nabla e_k, \nabla e_{k'}\rangle_{L^2_\rho} + O(\alpha)$. Therefore, for $\psi \in G_\alpha$, $\|\psi\| = 1$, we get

$$\langle h^{-2} Q_{h,\rho}\psi, \psi\rangle_{L^2(\rho)} \leq \nu_{N+1} + C\alpha + O_\alpha(h^{1/2}). \tag{3.21}$$

Taking $\alpha > 0$ small enough and $h < h_\alpha \ll 1$, we obtain from (3.19) and (3.21), $\mu_{\sigma_{N+1}}(h) \leq \nu_{N+1} + \epsilon$. Combining this with (3.18) and (3.17), we get $m_{N+1} = \sharp\,\mathrm{Spec}(h^{-2}Q_{h,\rho}) \cap [\nu_{N+1} - \epsilon, \nu_{N+1} + \epsilon]$. The proof of Theorem 1.2 is complete.

4 Application to random placement of non-overlapping balls

In this section, we suppose that Ω is a bounded, Lipschitz, quasi-regular, connected, open subset of $\mathbb{R}^d$ with $d \geq 2$. Let $N \in \mathbb{N}$, $N \geq 2$ and $\epsilon > 0$ be given. Let $\mathcal{O}_{N,\epsilon}$ be the open bounded subset of $\mathbb{R}^{Nd}$,

$$\mathcal{O}_{N,\epsilon} = \left\{x = (x_1, \dots, x_N) \in \Omega^N, \forall\, 1 \leq i < j \leq N, |x_i - x_j| > \epsilon\right\}$$

and recall that B_1 denotes the unit ball in $\mathbb{R}^d$ and $\varphi(z) = \frac{1}{\mathrm{vol}(B_1)} 1_{B_1}(z)$. We introduce the kernel

$$\begin{aligned} K_h(x, dy) = \frac{1}{N}\sum_{j=1}^{N} \delta_{x_1} \otimes \cdots \otimes \delta_{x_{j-1}} \otimes h^{-d}\varphi\left(\frac{x_j - y_j}{h}\right) dy_j \\ \otimes\, \delta_{x_{j+1}} \otimes \cdots \otimes \delta_{x_N}, \end{aligned} \tag{4.1}$$

and the associated Metropolis operator on $L^2(\mathcal{O}_{N,\epsilon})$

$$T_h(u)(x) = m_h(x)u(x) + \int_{\mathcal{O}_{N,\epsilon}} u(y) K_h(x, dy), \tag{4.2}$$

with

$$m_h(x) = 1 - \int_{\mathcal{O}_{N,\epsilon}} K_h(x, dy). \tag{4.3}$$

The operator T_h is Markov and self-adjoint on $L^2(\mathcal{O}_{N,\epsilon})$. The configuration space $\mathcal{O}_{N,\epsilon}$ is the set of N disjoint closed balls of radius $\epsilon/2$ in $\mathbb{R}^d$, with centers at the $x_j \in \Omega$. The topology of this set, and the geometry of its boundary is generally hard to understand, but since $d \geq 2$, $\mathcal{O}_{N,\epsilon}$ is clearly non-void and connected for a given N if ϵ is small enough. The Metropolis kernel T_h is associated to the following algorithm: at each step, we choose uniformly at random a ball, and we move its center uniformly at random in $\mathbb{R}^d$ in a ball of radius h. If the new configuration is in $\mathcal{O}_{N,\epsilon}$, the change is made. Otherwise, the configuration is kept as it started.

In order to study the random walk associated to T_h, we will assume that N and ϵ are such that $N\epsilon$ is small enough. Under this condition, we prove in Proposition 4.1 that the open set $\mathcal{O}_{N,\epsilon}$ is connected, Lipschitz and quasi-regular, and in Proposition 4.4 we prove that the kernel of the iterated operator T_h^M (with M large, but independent of h) admits a suitable lower bound, so that we will be able to use Remark 2 at the end of Sect. 2. The main results are collected together in Theorem 4.6 below.

We define Γ_{reg} and Γ_{sing} the set of regular and singular points of $\partial\mathcal{O}_{N,\epsilon}$ as follows. Denote $\mathbb{N}_N = \{1, \dots, N\}$. For $x \in \overline{\mathcal{O}}_{N,\epsilon}$ set

$$\begin{aligned} &R(x) = \{i \in \mathbb{N}_N,\ x_i \in \partial\Omega\}, \\ &S(x) = \left\{\tau = (\tau_1, \tau_2) \in \mathbb{N}_N,\ \tau_1 < \tau_2 \text{ and } |x_{\tau_1} - x_{\tau_2}| = \epsilon\right\}, \\ &r(x) = \sharp R(x), \qquad s(x) = \sharp S(x). \end{aligned} \tag{4.4}$$

The functions r and s are lower semi-continuous and any $x \in \overline{\mathcal{O}}_{N,\epsilon}$ belongs to $\partial\mathcal{O}_{N,\epsilon}$ iff $r(x) + s(x) \geq 1$. Define

$$\begin{aligned} \Gamma_{\text{reg}} = &\left\{x \in \overline{\mathcal{O}}_{N,\epsilon},\ s(x) = 1 \text{ and } r(x) = 0\right\} \\ &\cup \left\{x \in \overline{\mathcal{O}}_{N,\epsilon},\ s(x) = 0,\ R(x) = \{j_0\} \text{ and } x_{j_0} \in \partial\Omega_{\text{reg}}\right\} \end{aligned} \tag{4.5}$$

and $\Gamma_{\text{sing}} = \partial\mathcal{O}_{N,\epsilon} \setminus \Gamma_{\text{reg}}$. Then Γ_{sing} is clearly closed, and the Γ_{reg} is the union of smooth disjoint hypersurfaces in $\mathbb{R}^{Nd}$.

Proposition 4.1 *There exists $\alpha > 0$ such that for $N\epsilon \leq \alpha$, the set $\mathcal{O}_{N,\epsilon}$ is arcwise connected, Lipschitz and quasi-regular.*

Remark 3 Observe that in the above Proposition, the smallness condition on ϵ is $N\epsilon \leq \alpha$ where $\alpha > 0$ depends only on Ω. The condition $N\epsilon^d \leq c$, which says that the density of the balls is sufficiently small, does not imply that the set $\mathcal{O}_{N,\epsilon}$ has Lipschitz regularity. As an example, if $\Omega =]0,1[^2$ is the unit square in the plane, then $x = (x_1, \dots, x_N),\ x_j = ((j-1)\epsilon, 0),\ j = 1, \dots, N$, with $\epsilon = \frac{1}{N-1}$ is a configuration point in the boundary $\partial\mathcal{O}_{N,\epsilon}$. However, $\partial\mathcal{O}_{N,\epsilon}$ is not Lipschitz at x: otherwise, there would exist $\nu_j = (a_j, b_j)$ such that $(x_1 + t\nu_1, \dots, x_N + t\nu_N) \in \mathcal{O}_{N,\epsilon}$ for $t > 0$ small enough, and this implies $a_1 > 0, a_{j+1} > a_j$ and $a_N < 0$ which is impossible.

Proof For $\nu \in S^{p-1},\ p \geq 1$ and $\delta \in]0,1[$, denote

$$\Gamma_{\pm}(\nu, \delta) = \left\{\xi \in \mathbb{R}^p,\ \pm\langle\xi, \nu\rangle > (1-\delta)|\xi|,\ |\langle\xi, \nu\rangle| < \delta\right\}. \tag{4.6}$$

We remark [1] that an open set $\mathcal{O} \subset \mathbb{R}^p$ is Lipschitz if and only if it satisfies the cone property: $\forall a \in \partial\mathcal{O}, \exists \delta > 0, \exists \nu_a \in S^{p-1}, \forall b \in B(a,\delta) \cap \partial\mathcal{O}$ we have

$$b + \Gamma_+(\nu_a, \delta) \subset \mathcal{O} \quad \text{and} \quad b + \Gamma_-(\nu_a, \delta) \subset \mathbb{R}^p \setminus \overline{\mathcal{O}}. \tag{4.7}$$

Let us first show that $\mathcal{O}_{N,\epsilon}$ is connected for $N\epsilon$ small. For $x \in \mathcal{O}_{N,\epsilon}$ define

$$I(x) = \inf_{i \neq j} |x_i - x_j|. \tag{4.8}$$

Then $I(x) > \epsilon$ and we have the following lemma.

Lemma 4.2 *There exists* $\alpha_0 > 0$ *such that for any* $N \in \mathbb{N}, \epsilon > 0$ *with* $N\epsilon \leq \alpha_0$, *there exists* $\delta_{N,\epsilon} > 0$ *such that for any* $x \in \mathcal{O}_{N,\epsilon}$ *with* $I(x) < \alpha_0/N$, *there exists a continuous path* $\gamma : [0,1] \to \mathcal{O}_{N,\epsilon}$ *such that* $\gamma(0) = x$ *and* $I(\gamma(1)) \geq I(x) + \delta_{N,\epsilon}$.

Proof As Ω is bounded and Lipschitz, a compactness argument shows that there exists $\delta_0 > 0, r_0 > 0$ such that

$$\begin{aligned} &\forall x_0 \in \overline{\Omega}, \exists \nu \in S^{d-1}, \forall x \in B(x_0, r_0) \cap \overline{\Omega}, \quad x + \Gamma_+(\nu, \delta_0) \subset \Omega, \\ &\forall x_0 \in \partial\Omega, \exists \nu \in S^{d-1}, \forall x \in B(x_0, r_0) \cap \partial\Omega, \quad x + \Gamma_-(\nu, \delta_0) \subset \mathbb{R}^d \setminus \overline{\Omega}. \end{aligned} \tag{4.9}$$

Let $0 < \alpha_0 < \min(\delta_0, r_0)/100$. For $K \in \mathbb{N}^*$ denote $\delta_K = \alpha_0/K^3$, $\rho_K = 10\alpha_0/K^2$. Observe that it suffices to show the following statement:

$$\begin{aligned} \forall K \in \mathbb{N}^*, \forall \epsilon \in]0, \alpha_0/K], \forall N \in \mathbb{N}_K, \forall x \in \mathcal{O}_{N,\epsilon} \quad &\text{s.t.} \quad I(x) < \alpha_0/K, \\ \exists \gamma \in C([0,1], \mathcal{O}_{N,\epsilon}),\ &\text{s.t.} \\ \gamma(0) = x, \qquad I(\gamma(1)) \geq I(x) + \delta_K \quad &\text{and} \quad \forall t \in [0,1], \\ |x - \gamma(t)|_\infty \leq N\rho_K&. \end{aligned} \tag{4.10}$$

Let $K \geq 1$ and $0 < \epsilon < \alpha_0/K$. We proceed by induction on $N \in \mathbb{N}_K$. (Recall that $\mathbb{N}_K = \{0, 1, \ldots, K\}$.) In the case $N = 1$, there is nothing to show. Suppose that the above property holds true at rank $N - 1$ and let $x \in \mathcal{O}_{N,\epsilon}$ be such that $I(x) < \alpha_0/K$ (this is possible since $\epsilon < \alpha_0/K$). Introduce the equivalence relation on $\mathbb{N}_N$ defined by $i \simeq_x j$ iff x_i and x_j can be connected by a path lying in $\bigcup_{k \in \mathbb{N}_N} \overline{B}(x_k, 40\alpha_0/K)$ and denote by $c(x)$ the number of equivalence class.

Suppose that $c(x) \geq 2$. Then there exists a partition $\mathbb{N}_N = I \cup J$, such that $N_I = \sharp I \geq 1$, $N_J = \sharp J \geq 1$ and for all $i \in I$, $j \in J$, $|x_i - x_j| > 40\alpha_0/K$. By induction, there exists a path $\gamma_I : [0,1] \to \Omega^{N_I} \cap \{(x_i)_{i\in I},\ \forall i \neq j, |x_i - x_j| > \epsilon\}$ such that $\gamma_I(0) = (x_i)_{i \in I}$, $I(\gamma_I(1)) \geq I(\gamma_I(0)) + \delta_K$ and $|\gamma_I(0) - \gamma_I(t)|_\infty < N_I\rho_K$. The same construction for the set J provides a path γ_J

with the same properties. Define the path $\tilde{\gamma}$ on $[0,1]$ by $(\tilde{\gamma}(t))_i = (\gamma_I(t))_i$ for $i \in I$ and $(\tilde{\gamma}(t))_j = (\gamma_J(t))_j$ for $j \in J$. Since $40\alpha_0/K - (N_I + N_J)\rho_K > \alpha_0/K + \delta_K > \epsilon$, $\tilde{\gamma}$ has values in $\mathcal{O}_{N,\epsilon}$ and we have $I(\tilde{\gamma}(1)) \geq I(x) + \delta_K$ as well as

$$|x - \gamma(t)|_\infty < \max(N_I, N_J)\rho_K \leq (N-1)\rho_K. \tag{4.11}$$

Suppose now that there is only one equivalence class. Then for all $k \in \mathbb{N}_N$, $|x_1 - x_k| \leq 40\alpha_0 N/K \leq 40\alpha_0 < r_0$, where r_0 is defined in (4.9). In particular, there exists $\nu \in S^{d-1}$ such that for all $y \in B(x_1, 40\alpha_0) \cap \Omega$, $y + \Gamma_+(\nu, \delta_0) \subset \Omega$. On the other hand, we can suppose without loss of generality that

$$\langle x_1, \nu\rangle \leq \cdots \leq \langle x_N, \nu\rangle. \tag{4.12}$$

For $j \in \{1, \ldots, N\}$ set $a_j = j\rho_K$ and

$$\gamma(t) = (x_1 + ta_1\nu, \ldots, x_N + ta_N\nu), \quad t \in [0,1]. \tag{4.13}$$

Then, one has $|x - \gamma(t)|_\infty \leq \sup a_j = N\rho_K$, $x_j + ta_j\nu \in \Omega$ since $N\rho_K \leq \delta_0$, and for $i < j$

$$\begin{aligned} &|(x_j + ta_j\nu) - (x_i + ta_i\nu)|^2 \\ &\quad = |x_j - x_i|^2 + 2t(a_j - a_i)\langle x_j - x_i, \nu\rangle + t^2|a_j - a_i|^2 \\ &\quad \geq |x_j - x_i|^2 + t^2|a_j - a_i|^2. \end{aligned} \tag{4.14}$$

Thus one has

$$I(\gamma(1))^2 \geq I(x)^2 + \rho_K^2 \geq (I(x) + \delta_K)^2. \tag{4.15}$$

The proof of Lemma 4.2 is complete. □

Using this lemma, it is easy to show that $\mathcal{O}_{N,\epsilon}$ is arcwise connected for $N\epsilon$ small. For $x \in \mathcal{O}_{N,\epsilon}$, define

$$\mathcal{I}_x = \left\{y \in \mathcal{O}_{N,\epsilon}, \exists\gamma \in C([0,1], \mathcal{O}_{N,\epsilon}), \gamma(0) = x, \gamma(1) = y\right\}. \tag{4.16}$$

We first show easily that there exists $y \in \mathcal{I}_x$ such that $I(y) \geq \alpha_0/N$ if $N\epsilon < \alpha_0$. Let $M = \max_{y\in\mathcal{I}_x} I(y)$. As I is a bounded function, M is finite and given $\gamma \in]0, \delta_{N,\epsilon}/2[$, there exists $y_1 \in \mathcal{I}_x$ such that $I(y_1) \geq M - \gamma$. If $I(y_1) < \alpha_0/N$, Lemma 4.2 shows that there exists $y_2 \in \mathcal{I}_x$ such that $I(y_2) \geq I(y_1) + \delta_{N,\epsilon} > M$ which is impossible. This shows that there exists $y \in \mathcal{I}_x$ such that $I(y) \geq \alpha_0/N$. Now by 4.9, for any $x \in \Omega$, there exists $\nu_x \in S^{d-1}$ such that $x + t\nu_x \in \Omega$ for $t \in [0, \delta_0]$ and $\mathrm{dist}(x + t\nu_x, \partial\Omega) \geq t\sin\theta_0$ with $\cos\theta_0 = 1 - \delta_0$. Let $\alpha_1 = \alpha_0 \sin\theta_0/20$. Then for $N\varepsilon \leq \alpha_1$, and $I(y) \geq$

α_0/N, $\gamma(t) = (y_1 + t(\alpha_0/4N)\nu_{y_1}, \dots, y_N + t(\alpha_0/4N)\nu_{y_N})$, $t \in [0,1]$ is a path in $\mathcal{O}_{N,\epsilon}$ and one has with $\gamma(1) = y' = (y'_1, \dots, y'_N)$, $I(y') \geq \alpha_0/2N$, and $\mathrm{dist}(y'_j, \partial\Omega) > 3\varepsilon$ for all j.

Let $\mathcal{C}_{N,\epsilon}$ be the set of $x \in \mathcal{O}_{N,\epsilon}$ such that $I(x) \geq \alpha_0/2N$ and $\mathrm{dist}(x_j, \partial\Omega) > 3\varepsilon$ for all j. It remains to show that for any $x, y \in \mathcal{C}_{N,\epsilon}$ there exists a continuous path γ from x to y, with values in $\mathcal{O}_{N,\epsilon}$ for $N\epsilon \leq \alpha_1$. Decreasing α_0 we may assume $6c_d\alpha_0^d < \mathrm{vol}(\Omega)$ with $c_d = \mathrm{vol}(B(0,1))$. Decreasing α_1, we get that for any $x, y \in \mathcal{C}_{N,\epsilon}$ with $N\epsilon \leq \alpha_1$, there exists $z \in \mathcal{C}_{N,\epsilon}$ such that

$$|x_p - z_q| \geq \alpha_0/2N \quad \text{and} \quad |y_p - z_q| \geq \alpha_0/2N \quad \forall p, q \in \mathbb{N}_N. \tag{4.17}$$

One can easily choose the z_j by induction, since for any $x, y \in \mathcal{O}_{N,\epsilon}$ and any $z_1, \dots, z_l \in \Omega$ with $0 \leq l \leq N-1$ we have $\mathrm{vol}(\bigcup_{j=1}^N B(x_j, \alpha_0/N) \bigcup_{j=1}^N B(y_j, \alpha_0/N) \bigcup_{j=1}^l B(z_j, \alpha_0/N)) \leq 3Nc_d\alpha_0^d N^{-d} < \mathrm{vol}(\Omega)/2 < \mathrm{vol}(\{x \in \Omega, \mathrm{dist}(x, \partial\Omega)\} > 3\epsilon)$.

Thus we are reduce to show that if $y, z \in \mathcal{C}_{N,\epsilon}$ satisfy (4.17), there exists a continuous path γ from y to z, with values in $\mathcal{O}_{N,\epsilon}$ if $N\epsilon \leq \alpha_1$. We look for a path γ of the form $\gamma = \gamma_N \circ \cdots \circ \gamma_1$, where the path γ_j moves only the jth ball from y_j to z_j. Let us explain how to choose γ_j. As Ω is connected, there exists an analytic path $\tilde{\gamma}_1$ which connect y_1 to z_1 in Ω. We have to modify the path $\tilde{\gamma}_1$ into a new path γ_1 in order that

$$|\gamma_1(t) - y_j| > \epsilon \quad \forall j \in \{2, \dots, N\}. \tag{4.18}$$

Let $K = \{t \in [0,1], \exists j_0 \in \{2, \dots, N\}, |\tilde{\gamma}_1(t) - y_{j_0}| \leq 2\epsilon\}$. If K is empty, we set $\gamma_1 = \tilde{\gamma}_1$. If K is non empty, since the path $\tilde{\gamma}_1$ is analytic and $I(y) \geq \alpha_0/2N > 4\epsilon$, K is a disjoint union of intervals, $K = [a_1, b_1] \cup \cdots \cup [a_L, b_L]$ and for any $l \in \{1, \dots, L\}$ there exists a unique j_l such that $|\tilde{\gamma}_1(t) - y_{j_l}| \leq 2\epsilon$ for $t \in [a_l, b_l]$. For $t \notin K$ we set $\gamma_1(t) = \tilde{\gamma}_1(t)$ and for $t \in [a_l, b_l]$ we replace $\tilde{\gamma}_1$ by a continuous path γ_1 connecting $\tilde{\gamma}_1(a_l)$ to $\tilde{\gamma}_1(b_l)$ on the sphere $|x - y_{j_l}| = 2\epsilon$ which is contained in Ω. Then $\gamma_1(t)$ is continuous. Moreover, as $I(y) > 4\epsilon$, for any $j \in \{2, \dots, N\}$ and $t \in [0,1]$ we have $|\gamma_1(t) - y_j| \geq 2\epsilon$. In particular, the path $t \in [0,1] \mapsto (\gamma_1(t), y_2, \dots, y_N)$ has values in $\mathcal{O}_{N,\epsilon}$ and connects y and $\tilde{y} := (z_1, y')$. From (4.17) it is clear that $\tilde{y} \in \mathcal{C}_{N,\epsilon}$ and that (4.17) holds true with y replace by $\tilde{y}$. This permits iterating the construction to build a continuous path from y to z. Thus $\mathcal{O}_{N,\epsilon}$ is connected for $N\epsilon < \alpha_1$.

Let us now prove that $\partial\mathcal{O}_{N,\epsilon}$ has Lipschitz regularity for $N\epsilon \leq r_0/2$, where r_0 is such that (4.9) holds. For a given ϵ, we will prove this fact by induction on $N \in [1, r_0/2\epsilon]$. The case $N = 1$ is obvious since $\partial\Omega$ is Lipschitz. Let $\overline{x} \in \partial\mathcal{O}_{N,\epsilon}$. The equivalence relation $i \simeq j$ iff $\overline{x}_i$ and $\overline{x}_j$ can be connected by a path lying in the union of closed balls of radius $\epsilon/2$, gives us a partition

$\{1,\dots,N\}=\bigcup_{k=1}^r F_k$ such that

$$\begin{aligned}
&|\overline{x}_i-\overline{x}_j|>\epsilon \quad \forall k\neq l, \forall i\in F_k, \forall j\in F_l;\\
&|\overline{x}_{n_l}-\overline{x}_{n_{l+1}}|=\epsilon \\
&\quad \forall k, \forall i\neq j\in F_k, \exists (n_l)\in F_k, 1\leq l\leq m, n_1=i, n_m=j.
\end{aligned} \tag{4.19}$$

The Cartesian product $\mathcal{O}_1\times\mathcal{O}_2$ of two bounded Lipschitz open subsets $\mathcal{O}_i\subset\mathbb{R}^{d_i}$ has Lipschitz regularity. Thus, if $r\geq 2$, the induction hypothesis on N shows that $\partial\mathcal{O}_{N,\epsilon}$ has Lipschitz regularity near $\overline{x}$. Thus we may assume $r=1$, and therefore, for all i,j one has $|\overline{x}_i-\overline{x}_j|\leq\epsilon(N-1)\leq r_0/2$.

Thus there exists $x_0\in\overline{\Omega}$ such that $\overline{x}_i\in B(x_0,r_0/2)$, and (4.9) gives us a unit vector ν and $\delta_0>0$. We set

$$\overline{\xi}_i=\alpha\overline{x}_i+\nu \tag{4.20}$$

with $\alpha>0$ small such that $t\overline{\xi}_i\in\Gamma_+(\nu,\delta_0/2)$ for $t>0$ small. We choose $\beta>0$, $\rho>0$, $t_0>0$ such that $\beta\ll\alpha\epsilon^2$, $\beta\ll\delta_0$, $\rho\ll\alpha\epsilon^2$, $\rho\ll r_0$, $t_0|\overline{\xi}_i|^2\ll\alpha\epsilon^2$, $t_0\ll\delta_0$.

Let $x\in\partial\mathcal{O}_{N,\epsilon}$ such that $|x_j-\overline{x}_j|\leq\rho$ and $\theta_i\in\mathbb{R}^d$ such that $|\theta_i|\leq\beta$. Let $\xi_i=\overline{\xi}_i+\theta_i$, and $\xi=(\xi_1,\dots,\xi_N)$. One has $t\xi_i\in\Gamma_+(\nu,\delta_0)$ for $t\in]0,t_0]$ and $t\xi_i\in\Gamma_-(\nu,\delta_0)$ for $t\in[-t_0,0[$. From

$$\begin{aligned}
\langle x_i-x_j,\xi_i-\xi_j\rangle&=\langle x_i-x_j,\overline{\xi}_i-\overline{\xi}_j\rangle+O(\beta)\\
&=\alpha|\overline{x}_i-\overline{x}_j|^2+O(\beta+\rho)
\end{aligned} \tag{4.21}$$

and

$$\begin{aligned}
&|(x_i+t\xi_i)-(x_j+t\xi_j)|^2\\
&\quad=|x_i-x_j|^2+2t\langle x_i-x_j,\xi_i-\xi_j\rangle+t^2|\xi_i-\xi_j|^2
\end{aligned} \tag{4.22}$$

we get that the function $t\in[-t_0,t_0]\mapsto g_{i,j}(t)=|(x_i+t\xi_i)-(x_j+t\xi_j)|^2$ is strictly increasing. Since by (4.9) we have $x_i+t\xi_i\in\Omega$ for $t\in]0,t_0]$, we get $x+t\xi\in\mathcal{O}_{N,\epsilon}$ for $t\in]0,t_0]$. It remains to show $x+t\xi\notin\overline{\mathcal{O}}_{N,\epsilon}$ for $t\in[-t_0,0[$. If there exists two indices i,j such that $|x_i-x_j|=\epsilon$, this follows from $g_{i,j}(t)<\epsilon^2$ for $t<0$. If there exists one indice i such that $x_i\in\partial\Omega$, this follows from $t\xi_i\in\Gamma_-(\nu,\delta_0)$ and the second line of (4.9) which implies $x_i+t\xi_i\notin\overline{\Omega}$ for $t\in[-t_0,0[$. Thus $\partial\mathcal{O}_{N,\epsilon}$ is Lipschitz.

Let us finally prove that $\mathcal{O}_{N,\epsilon}$ is quasi-regular. Let $u\in H^{-1/2}(\partial\mathcal{O}_{N,\epsilon})$ be supported in Γ_{sing}. We have to show that u is identically zero. This is a local problem near any point $\overline{x}\in\Gamma_{\text{sing}}$. Let $\overline{x}$ be such that $s(\overline{x})=0$, $R(\overline{x})=\{j_0\}$ (say $j_0=1$) and $\overline{x}_{j_0}\in\partial\Omega_{\text{sing}}$. Denote $\mathcal{D}_{N,\epsilon}=\{x\in(\mathbb{R}^d)^N,$

$|x_i - x_j| > \epsilon, \forall 1 \leq i < j \leq N\}$. Let χ be a cut-off function supported near $\overline{x}$ such that $\mathrm{supp}(\chi) \subset (\mathbb{R}^d \times \Omega^{N-1}) \cap \mathcal{D}_{N,\epsilon}$. Then, for any $\psi \in C_0^\infty(\Omega^{N-1})$ the linear form u_ψ defined on $H^{1/2}(\partial\Omega)$ by

$$\langle u_\psi, f\rangle = \langle \chi u, f(x_1)\psi(x_2,\dots,x_N)\rangle \tag{4.23}$$

is continuous and supported in $\partial\Omega_{\mathrm{sing}}$. As $\partial\Omega$ is quasi-regular, it follows that u_ψ is equal to zero for all ψ and hence, $\chi u = 0$. Therefore, we can suppose that u is supported in the set $\{r(x) + s(x) \geq 2\}$. Let v be the distribution on $\mathbb{R}^{Nd}$

$$\langle v, \varphi\rangle = \langle u, \varphi|_{\partial\mathcal{O}_{N,\epsilon}}\rangle. \tag{4.24}$$

Then $v \in H^{-1}(\mathbb{R}^{Nd})$ and its support is equal to $\mathrm{supp}(u)$. The Sobolev space H^{-1} is preserved by bi-Lipschitz maps. Therefore, if there exists a bi-Lipschitz map Φ defined near $\overline{x}$ such that locally one has $\Phi(\mathrm{supp}(u)) \subset \{y_1 = y_2 = 0\}$, then u is identically 0 near $\overline{x}$. For $n \in \mathbb{N}$, $n \geq 2$, introduce the following property:

$$\begin{aligned}(\mathcal{P}_n):\ &\text{for any } \overline{x} \in \Gamma_{\mathrm{sing}} \text{ with } r(\overline{x}) + s(\overline{x}) = n,\\ &\text{we have } u = 0 \text{ near } \overline{x}.\end{aligned} \tag{4.25}$$

This property is proved by induction on n. By lower semicontinuity of the functions r and s, we may assume in the proof that for $x \in \mathrm{supp}(u)$ closed to $\overline{x}$, one has $r(x) = r(\overline{x})$ and $s(x) = s(\overline{x})$ and hence $R(x) = R(\overline{x})$ and $S(x) = S(\overline{x})$. Therefore, we are reduced to prove that for $\overline{x} \in \Gamma_{\mathrm{sing}}$ with $r(\overline{x}) + s(\overline{x}) \geq 2$ and $u \in H^{-1/2}(\partial\mathcal{O}_{N,\epsilon})$ supported in $R(x) = R(\overline{x})$ and $S(x) = S(\overline{x})$, we have $u = 0$ near $\overline{x}$.

First assume $r(\overline{x}) = s(\overline{x}) = 1$. Then, we can suppose without losing generality, that u is supported near $\overline{x}$ in $G = (\partial\Omega \times \Omega^{N-1}) \cap \{|x_i - x_2| = \epsilon\}$ for some $i \in \{1, 3, \dots, N\}$. Denoting $x_i = (x_{i,1}, \dots, x_{i,d})$, we may assume that near $\overline{x}$, G is given by two equations,

$$\begin{aligned} x_{1,1} &= \alpha(x_1'), \qquad & x_1' &= (x_{1,2},\dots,x_{1,d}),\\ x_{2,k} &= \beta(x_2', x_i), \qquad & x_2' &= (x_{2,1},\dots,x_{2,k-1},x_{2,k+1},\dots,x_{2,d}),\end{aligned} \tag{4.26}$$

with α Lipschitz and β smooth. Then, $\nu(x) = (x_{1,1} - \alpha(x_1'), x_{2,k} - \beta(x_2', x_i), x_1', x_2', x_3, \dots, x_N)$ defines a local bi-Lipschitz homeomorphism of $\mathbb{R}^{Nd}$ such that $\nu \circ G \subset \{0\}^2 \times \mathbb{R}^{Nd-2}$. Therefore, $\nu_*(v)$ vanishes identically near $\nu(\overline{x})$ and hence u is null near $\overline{x}$.

We may thus assume that $s(\overline{x}) \geq 2$ or $r(\overline{x}) \geq 2$. In the case $s(\overline{x}) \geq 2$, the support of u near $\overline{x}$ is contained in a set A of the form $|x_1 - x_2| = |x_2 - x_3| = \epsilon$ or $|x_1 - x_2| = |x_3 - x_4| = \epsilon$. Since A is a subvariety of $\mathbb{R}^{Nd}$ of codimension 2, we get as above that u is null near $\overline{x}$. In the case $r(\overline{x}) \geq 2$, the support of u near $\overline{x}$ is contained in a set B of the form $\partial\Omega \times \partial\Omega \times \mathbb{R}^{(N-2)d}$ which is near $\overline{x}$ bi-Lipschitz homeomorphic to $(y_1 = y_2 = 0) \times \mathbb{R}^{Nd-2}$, and thus u is null near $\overline{x}$. The proof of Proposition 4.1 is complete. □

Define for $j \in \mathbb{N}_N$ the two functions π_j from $\mathbb{R}^{Nd}$ to $\mathbb{R}^{Nd}$ and σ_j from $\mathbb{R}^d$ to $\mathbb{R}^{Nd}$ by

$$\begin{aligned} \pi_j(x_1, \dots, x_j, \dots, x_N) = (x_1, \dots, 0, \dots, x_N), \\ \sigma_j(y) = (0, \dots, y, \dots, 0), \end{aligned} \tag{4.27}$$

so that $x = \pi_j(x) + \sigma_j(x_j)$. The following geometric lemma will be the main ingredient of the proof of Proposition 4.4.

Lemma 4.3 *Let $\alpha_0 = r_0/10$ with r_0 given by (4.9). For all $N \in \mathbb{N}$ and $\epsilon \in]0, \alpha_0/N]$, there exists $\delta_{N,\epsilon} > 0$ and a finite covering $(U_l)_l$ of $\overline{\mathcal{O}}_{N,\epsilon}$ such that for all l, there exists j and $\nu \in S^{d-1}$ such that*

$$x + \sigma_j(\Gamma_+(\nu, \delta_{N,\epsilon})) \subset \mathcal{O}_{N,\epsilon} \quad \forall x \in U_l \cap \mathcal{O}_{N,\epsilon}, \tag{4.28}$$

where Γ_+ is defined in (4.6)

Proof Since $\overline{\mathcal{O}}_{N,\epsilon}$ is compact, we have to prove that for any given $x^0 \in \overline{\mathcal{O}}_{N,\epsilon}$, there exist $r > 0$, $\delta = \delta_{N,\epsilon} > 0$, j and $\nu \in S^{d-1}$ such that (4.28) holds true for $x \in \mathcal{O}_{N,\epsilon} \cap B(x^0, r)$. This means that we can select one ball, and that moving only this ball by a vector in $\Gamma_+(\nu, \delta)$ while keeping the other balls fixed, results in an admissible configuration. We shall proceed by induction on $N \geq 1$. For $N = 1$, this is true since Ω is Lipschitz. Let $N \geq 2$. If one can write $\{1, \dots, N\}$ as the disjoint union $I \cup J$ with $\sharp I \geq 1, \sharp J \geq 1$, and

$$|x_i^0 - x_j^0| \geq 5\epsilon \quad \forall i \in I, \forall j \in J, \tag{4.29}$$

then, by the induction hypothesis, the result is true for some $\delta_{N,\epsilon} \in]0, 4\epsilon[$. Thus, using the definition of α_0, we may assume that all the x_i^0 are in a small neighborhood of a given point $y^0 \in \overline{\Omega}$ and $\sup_k |x_k^0 - y^0| \leq r_0/2$. By (4.9) there exist $\nu, \delta_0 > 0, r_0 > 0$ such that

$$y \in \overline{\Omega} \quad \text{and} \quad |y - y^0| \leq r_0 \quad \Longrightarrow \quad y + \Gamma_+(\nu, \delta_0) \in \Omega. \tag{4.30}$$

It remains to show that there exist $j, r_0' \in]0, r_0[$, and $\nu', \delta_0' > 0$, with $\Gamma_+(\nu', \delta_0') \subset \Gamma_+(\nu, \delta_0)$, such that for all $x = (x_1, \dots, x_N) \in \mathcal{O}_{N,\epsilon}$ with $\mathrm{dist}(x, x^0) \leq r_0'$, and all $z \in x_j + \Gamma_+(\nu', \delta_0')$, one has $|z - x_k| > \epsilon$ for all

$k \neq j$. This will be a consequence of the following property:

$$\begin{aligned} &\forall \beta > 0,\ \exists j,\ \exists \nu' \in S^{d-1} \quad \text{s.t.} \quad |\nu' - \nu| \leq \beta \\ &\text{and} \quad \nu'.(x_j^0 - x_k^0) > 0 \quad \forall k \neq j. \end{aligned} \tag{4.31}$$

In fact, if (4.31) holds true, first take β small enough, such that for all $\nu' \in S^{d-1}$ with $|\nu' - \nu| \leq \beta$ there exists $\delta_0' > 0$ with $\Gamma_+(\nu', \delta_0') \subset \Gamma_+(\nu, \delta_0)$; then (4.31) gives us a pair ν', j such that $\nu'.(x_j^0 - x_k^0) > 0\ \forall k \neq j$. For $r_0' > 0, \delta_0' > 0$ small enough, we get for all $\xi \in \Gamma_+(\nu', \delta_0')$ and all $x \in \mathcal{O}_{N,\epsilon}$, $\operatorname{dist}(x, x^0) \leq r_0'$, that $\inf_{k \neq j} \xi.(x_j - x_k) \geq \delta_0' |\xi|$, and thus there exists t_0 such that for $t \in [0, t_0]$ and $k \neq j$, the function $t \mapsto |x_k - (x_j + t\xi)|^2$ is strictly increasing for all $x \in \mathcal{O}_{N,\epsilon}$, $\operatorname{dist}(x, x^0) \leq r_0'$ and all $\xi \in \Gamma_+(\nu', \delta_0')$.

Let us show that (4.31) holds true. If $j \mapsto \nu.x_j^0$ achieves its maximum at a single j, then (4.31) is obvious with $\nu = \nu'$. Otherwise, the set $A = \{\nu' \in S^{d-1}, \exists j \neq k, \nu'.(x_j^0 - x_k^0) = 0\}$ is contained in a finite union of equators in the sphere S^{d-1}, with $\nu \in A$, and thus (4.31) is still obvious by taking $\nu' \in S^{d-1} \setminus A$ close to ν. The proof of Lemma 4.3 is complete. □

Proposition 4.4 *Let N, ϵ be such that Lemma 4.3 holds true. There exists $h_0 > 0, c_0, c_1 > 0$ and $M \in \mathbb{N}^*$ such that for all $h \in]0, h_0]$, one has*

$$T_h^M(x, dy) = \mu_h(x, dy) + c_0 h^{-Nd} \varphi\left(\frac{x - y}{c_1 h}\right) dy, \tag{4.32}$$

where for all $x \in \mathcal{O}_{N,\epsilon}$, $\mu_h(x, dy)$ is a positive Borel measure.

Proof For $k \in \mathbb{N}^*$ denote $B^k = B_{\mathbb{R}^k}(0, 1)$ the unit Euclidean ball and $\varphi_k(z) = \frac{1}{\operatorname{vol}(B^k)} 1_{B^k}(z)$. For $x, y \in \mathcal{O}_{N,\epsilon}$, we set $\operatorname{dist}(x, y) = \sup_{1 \leq i \leq N} |x_i - y_i|$. For $N \geq 1$, denote by $K_{h,N}$ the kernel given in (4.1). It is sufficient to prove the following: there exists $h_0 > 0, c_0, c_1 > 0$ and $M(N) \in \mathbb{N}^*$ such that for all $h \in]0, h_0]$, one has for all nonnegative function f,

$$K_{h,N}^{M(N)}(f)(x) \geq c_0 h^{-Nd} \int_{y \in \mathcal{O}_{N,\epsilon}, \operatorname{dist}(y,x) \leq c_1 h} f(y)\, dy. \tag{4.33}$$

First note that it is sufficient to prove the weaker version: for all $x^0 \in \overline{\mathcal{O}}_{N,\epsilon}$, there exist $M(N, x^0), r = r(x^0) > 0, c_0 = c_0(x_0) > 0, c_1 = c_1(x_0) > 0, h_0 = h_0(x_0) > 0$ such that for all $h \in]0, h_0]$, all $x \in \mathcal{O}_{N,\epsilon}$ and all nonnegative function f

$$\begin{aligned} \operatorname{dist}(x, x^0) \leq 2r \quad \Longrightarrow \quad & K_{h,N}^{M(N,x^0)}(f)(x) \\ & \geq c_0 h^{-Nd} \int_{y \in \mathcal{O}_{N,\epsilon}, \operatorname{dist}(y,x) \leq c_1 h} f(y)\, dy. \end{aligned} \tag{4.34}$$

Let us verify that (4.34) implies (4.33). Decreasing $r(x_0)$ if necessary, we may assume that any set $\{\mathrm{dist}(x,x^0)\le 2r(x_0)\}$ is contained in one of the open set U_l of Lemma 4.3. There exists a finite set F such that $\overline{\mathcal{O}}_{N,\epsilon}\subset\bigcup_{x^0\in F}\{\mathrm{dist}(x,x^0)\le r(x_0)\}$. Let $M(N)=\sup_{x^0\in F}M(N,x_0)$, $c_i'=\min_{x_0\in F}c_i(x_0)$ and $h_0'=\min_{x_0\in F}h_0(x_0)$. One has to check that for any $x^0\in F$ and any x with $\mathrm{dist}(x,x^0)\le r(x^0)$, the right inequality in (4.34) holds true with $M(N)=M(N,x^0)+n$ in place of $M(N,x^0)$ for some constants c_0,c_1,h_0. Let l be such that $\mathrm{dist}(x,x^0)\le r(x_0)$ implies $x\in U_l$. Let j and $\Gamma_+(\nu,\delta)$ be given by Lemma 4.3. Clearly, if f is nonnegative, one has

$$\begin{aligned}&K_{h,N}^{M(N,x^0)+1}(f)(x)\\&\quad\ge\frac{1}{N}h^{-d}\int_{x+\sigma_j(z)\in\mathcal{O}_{N,\epsilon}}\varphi(z/h)K_{h,N}^{M(N,x^0)}(f)(x+\sigma_j(z))\,dz.\end{aligned}\tag{4.35}$$

For $\mathrm{dist}(x,x^0)\le 2r(x^0)-c_1'h/2$, and $|z|\le c_1'h/2, z\in\Gamma_+(\nu,\delta)$, one has $\mathrm{dist}(x+\sigma_j(z),x^0)\le 2r(x^0)$ and by (4.28), $x+\sigma_j(z)\in\mathcal{O}_{N,\epsilon}$. Moreover, $\mathrm{dist}(y,x)\le c_1'h/2\Longrightarrow\mathrm{dist}(y,x+\sigma_j(z))\le c_1'h$. From (4.35) and (4.34) we thus get, with a constant C_δ depending only on the δ given by Lemma 4.3, and for $h\le h_0'$,

$$\begin{aligned}\mathrm{dist}(x,x^0)\le 2r(x^0)-c_1'h/2\quad&\Longrightarrow\quad K_{h,N}^{M(N,x^0)+1}(f)(x)\\&\ge\frac{C_\delta}{N}c_0'h^{-Nd}\int_{y\in\mathcal{O}_{N,\epsilon},\mathrm{dist}(y,x)\le c_1'h/2}f(y)\,dy.\end{aligned}\tag{4.36}$$

By induction on n, we thus get

$$\begin{aligned}\mathrm{dist}(x,x^0)\le 2r(x^0)-c_1'h\quad&\Longrightarrow\quad K_{h,N}^{M(N,x^0)+n}(f)(x)\\&\ge\left(\frac{C_\delta}{N}\right)^n c_0'h^{-Nd}\int_{y\in\mathcal{O}_{N,\epsilon},\mathrm{dist}(y,x)\le c_1'\frac{h}{2^n}}f(y)\,dy.\end{aligned}\tag{4.37}$$

Since n is bounded, we get the desired result with $h_0=\min(\min_{x^0\in F}r(x^0)/c_1',h_0')$.

To complete the proof, let us show (4.34) by induction on N. The case $N=1$ is obvious. Suppose that (4.34) holds for $N-1$ discs. Let $x^0\in\overline{\mathcal{O}}_{N,\epsilon}$ be fixed. Thanks to Lemma 4.3, we can suppose that there exists an open neighborhood U of x^0 a direction $\nu\in S^{d-1}$ and $\delta>0$ such that (4.28) holds with $j=1$. Let us denote $x=(x_1,x')$ and

$$K_{h,N}=K_{h,N,1}+K_{h,N,>}\tag{4.38}$$

with

$$K_{h,N,1}f(x) = \frac{h^{-d}}{N}\int_{(y_1,x')\in\mathcal{O}_{N,\epsilon}} \varphi\left(\frac{x_1-y_1}{h}\right) f(y_1,x')\,dy_1. \tag{4.39}$$

We also denote $G(\nu,\delta) = \{x_1 \in \Gamma_+(\nu,\delta), |x_1| > \frac{\delta}{2}\}$. Then, we have the following:

Lemma 4.5 *For any $\delta' \in]0,\delta/2]$, there exists $C > 0$, $\alpha > 0$, $h_0 > 0$ and $r_0 > 0$ such that $\forall r \in]0,r_0]$, $\forall h \in]0,h_0]$, $\forall x \in U \cap \mathcal{O}_{N,\epsilon}$, $\forall \tilde{x} \in x + h(G(\nu,\delta') \times B(0,r)^{N-1})$ with $\tilde{x}' \in \mathcal{O}_{N-1,\epsilon}$, we have $\tilde{x} \in \mathcal{O}_{N,\epsilon}$ and*

$$K_{h,N,>}f(\tilde{x}) \geq C K_{\alpha h,N-1}(f(\tilde{x}_1,.))(\tilde{x}'), \tag{4.40}$$

for any nonnegative function f. In particular, for all $M \in \mathbb{N}^*$, there exists C, r_0, h_0, α as above such that $\forall x \in U \cap \mathcal{O}_{N,\epsilon}$ and $\forall \tilde{x} \in x + h(G(\nu,\delta') \times B(0,r)^{N-1})$, we have

$$K^M_{h,N,>}f(\tilde{x}) \geq C K^M_{\alpha h,N-1}(f(\tilde{x}_1,.))(\tilde{x}'). \tag{4.41}$$

Proof Inequality (4.41) is obtained easily from (4.40) by induction on M. To prove (4.40), observe that for nonnegative f and $\alpha \in]0,1[$ we have

$$K_{h,N,>}f(\tilde{x}) \geq \frac{h^{-d}}{N}\sum_{j=2}^{N}\int_{A_{j,\alpha,h}(\tilde{x})} f(\tilde{x}_1,\dots,y_j,\dots,\tilde{x}_N)\,dy_j, \tag{4.42}$$

with $A_{j,\alpha,h}(\tilde{x}) = \{z \in \Omega, |\tilde{x}_j - z| < \alpha h \text{ and } \forall k \neq j, |\tilde{x}_k - z| > \epsilon\}$. Let $B_{j,\alpha,h}(\tilde{x}) = \{z \in \Omega, |\tilde{x}_j - z| < \alpha h \text{ and } \forall k \neq 1,j, |\tilde{x}_k - z| > \epsilon\}$. Then $A_{j,\alpha,h} \subset B_{j,\alpha,h}$ and we claim that for $\alpha, r > 0$ small enough and $\tilde{x} \in x + h(G(\nu,\delta') \times B(0,r)^{N-1})$ with $\tilde{x}' \in \mathcal{O}_{N-1,\epsilon}$, we have $B_{j,\alpha,h}(\tilde{x}) = A_{j,\alpha,h}(\tilde{x})$. Indeed, let $\tilde{x}_1 = x_1 + hu_1$ with $u_1 \in G(\nu,\delta')$ and $\tilde{x}' \in \mathcal{O}_{N-1,\epsilon}$ be such that $|\tilde{x}_j - x_j| < hr$. Then for $z \in B_{j,\alpha,h}(\tilde{x})$,

$$|\tilde{x}_1 - z| = |x_1 - x_j + hv_1|, \tag{4.43}$$

with $v_1 = u_1 + \frac{x_j-\tilde{x}_j}{h} + \frac{\tilde{x}_j - z}{h}$. Taking α, r small enough (w.r.t. δ) it follows that $v_1 \in \Gamma_+(\nu,\delta)$. Consequently, Lemma 4.3 shows that $|\tilde{x}_1 - z| > \epsilon$ and hence $z \in A_{j,\alpha,h}(\tilde{x})$ (the same argument shows that $\tilde{x} \in \mathcal{O}_{N,\epsilon}$). Therefore,

$$\begin{aligned}K_{h,N,>}f(\tilde{x}) &\geq \frac{h^{-d}}{N}\sum_{j=2}^{N}\int_{B_{j,\alpha,h}(\tilde{x})} f(\tilde{x}_1,\dots,y_j,\dots,\tilde{x}_N)\,dy_j\\ &= \frac{(N-1)\,\mathrm{vol}(B^d)}{N} K_{\alpha h,N-1}(f(\tilde{x}_1,.))(\tilde{x}'),\end{aligned} \tag{4.44}$$

and the proof of Lemma 4.5 is complete. □

Using this lemma we can complete the proof of (4.34). In the following computations, C denotes a strictly positive constant independent of h, whose value may change from line to line. Let $p \in \mathbb{N}$, $\alpha \in]0, \alpha_0]$ and $x \in \mathcal{O}_{N,\epsilon}$, then

$$\begin{aligned} K_{h,N}^{p+1} f(x) &\geq K_{h,N,1} K_{h,N,>}^{p} f(x) \\ &\geq \frac{h^{-d}}{N} \int_{(z_1,x')\in\mathcal{O}_{N,\epsilon}, z_1\in x_1+hG(\nu,\delta')} K_{h,N,>}^{p} f(z_1,x')\, dz_1 \\ &\geq C \frac{h^{-d}}{N} \int_{(z_1,x')\in\mathcal{O}_{N,\epsilon}, z_1\in x_1+hG(\nu,\delta')} K_{\alpha h,N-1}^{p} (f(z_1,.))(x')\, dz_1, \end{aligned} \tag{4.45}$$

thanks to Lemma 4.5. From the induction hypothesis we can choose $p \in \mathbb{N}$ so that

$$\begin{aligned} &K_{h,N}^{p+1} f(x) \\ &\quad \geq C h^{-Nd} \int_{(z_1,x')\in\mathcal{O}_{N,\epsilon}, z_1\in x_1+hG(\nu,\delta')} \int_{|x'-y'|<\alpha h, y'\in\mathcal{O}_{N-1,\epsilon}} f(z_1,y')\, dy'\, dz_1. \end{aligned} \tag{4.46}$$

Hence, for any $\beta \in]0,1]$ we get

$$\begin{aligned} K_{h,N}^{p+2} f(x) &\geq K_{h,N}^{p+1} K_{h,N,1} f(x) \\ &\geq C h^{-Nd} \int_{D_{\alpha,\beta,h}(x)} f(y_1,y')\gamma_h(x,y_1)\, dy_1\, dy', \end{aligned} \tag{4.47}$$

with

$$D_{\alpha,\beta,h}(x) = \left\{ y \in \mathcal{O}_{N,\epsilon},\ |x'-y'| < \alpha h,\ |x_1-y_1| < \beta h \right\} \tag{4.48}$$

and

$$\gamma_h(x,y_1) = h^{-d} \int_{(z_1,x')\in\mathcal{O}_{N,\epsilon}, z_1\in x_1+hG(\nu,\delta')} 1_{|z_1-y_1|<h}\, dz_1. \tag{4.49}$$

We have to show that γ_h is bounded from below by a positive constant, uniformly with respect to (x, y_1) when $|x_1 - y_1| < \beta h$. For $z_1 \in x_1 + hG(\nu,\delta')$, one has $|z_1 - y_1| \leq |z_1 - x_1| + |x_1 - y_1| \leq h\delta' + h\beta < h$ for β and δ' small.

Thus for $|x_1 - y_1| < \beta h$ one has

$$\gamma_h(x, y_1) = h^{-d} \int_{(z_1, x') \in \mathcal{O}_{N,\epsilon}, z_1 \in x_1 + hG(\nu, \delta')} dz_1$$
$$= \int_{u \in G(\nu, \delta')} 1_{(x_1 + hu, x') \in \mathcal{O}_{N,\epsilon}} du. \tag{4.50}$$

Using Lemma 4.3 again, we get for $|x_1 - y_1| < \beta h$

$$\gamma_h(x, y_1) = \int_{u \in G(\nu, \delta')} du = C_0 > 0. \tag{4.51}$$

Plugging this lower bound into (4.47), gives

$$K_{h,N}^{p+2} \geq C h^{-Nd} \int_{D_{\alpha,\beta,h}(x)} f(y)\, dy, \tag{4.52}$$

and the proof of (4.34) is complete. This completes the proof of Proposition 4.4. $\square$

By Proposition 4.1, we can consider the Neumann Laplacian $|\Delta|_N$ on $\mathcal{O}_{N,\epsilon}$ defined by

$$\begin{aligned} |\Delta|_N &= -\frac{\alpha_d}{2N}\Delta, \\ D(|\Delta|_N) &= \big\{u \in H^1(\mathcal{O}_{N,\epsilon}),\ -\Delta u \in L^2(\mathcal{O}_{N,\epsilon}), \partial_n u|_{\partial \mathcal{O}_{N,\epsilon}} = 0\big\}. \end{aligned} \tag{4.53}$$

We still denote $0 = \nu_0 < \nu_1 < \nu_2 < \cdots$ the spectrum of $|\Delta|_N$ and m_j the multiplicity of ν_j. Our main result is the following.

Theorem 4.6 *Let $N \geq 2$ be fixed. Let $\epsilon > 0$ be small enough such that Proposition 4.1 and Proposition 4.4 hold true. Let $R > 0$ be given and $\beta > 0$ such that the spectrum ν_j of the Neumann Laplacian (4.53) satisfies $\nu_{j+1} - \nu_j > 2\beta$ for all j such that $\nu_{j+2} \leq R$.*

There exists $h_0 > 0$, $\delta_0 \in]0, 1/2[$ and constants $C_i > 0$ such that for any $h \in]0, h_0]$, the following hold true:

(i) *The spectrum of T_h is a subset of $[-1 + \delta_0, 1]$, 1 is a simple eigenvalue of T_h, and $\mathrm{Spec}(T_h) \cap [1 - \delta_0, 1]$ is discrete. Moreover,*

$$\mathrm{Spec}\left(\frac{1 - T_h}{h^2}\right) \cap]0, R] \subset \bigcup_{j \geq 1} [\nu_j - \beta, \nu_j + \beta];$$

$$\sharp\, \mathrm{Spec}\left(\frac{1 - T_h}{h^2}\right) \cap [\nu_j - \beta, \nu_j + \beta] = m_j \quad \forall \nu_j \leq R; \tag{4.54}$$

and for any $0 \leq \lambda \leq \delta_0 h^{-2}$, *the number of eigenvalues of* T_h *in* $[1 - h^2\lambda, 1]$ (*with multiplicity*) *is bounded by* $C_1(1+\lambda)^{dN/2}$.

(ii) *The spectral gap* $g(h)$ *satisfies*

$$\lim_{h \to 0^+} h^{-2} g(h) = \nu_1 \tag{4.55}$$

and the following estimate holds true for all integer n:

$$\sup_{x \in \mathcal{O}_{N,\epsilon}} \left\| T_h^n(x, dy) - \frac{dy}{\mathrm{vol}(\mathcal{O}_{N,\epsilon})} \right\|_{TV} \leq C_4 e^{-ng(h)}. \tag{4.56}$$

The rest of this section is devoted to the proof of Theorem 4.6.

Let $\mu_h(x, dy)$ be given by (4.32) and $\mu_h(f)(x) = \int_{\mathcal{O}_{N,\epsilon}} f(y)\mu_h(x, dy)$. Thanks to the positivity of $\mu_h(x, dy)$, using the Markov property of T_h^M and Lipschitz-continuity of the boundary, we get for some $\delta_0' > 0$, independant of $h > 0$, small enough

$$\|\mu_h\|_{L^\infty, L^\infty} \leq 1 - \inf_{x \in \mathcal{O}_{N,\epsilon}} \int_{\mathcal{O}_{N,\epsilon}} c_0 h^{-Nd} \varphi_{Nd}\left(\frac{x-y}{c_1 h}\right) dy < 1 - \delta_0'. \tag{4.57}$$

Since by (4.32) μ_h is self-adjoint on $L^2(\mathcal{O}_{N,\epsilon})$, we also get

$$\|\mu_h\|_{L^1, L^1} \leq 1 - \delta_0', \tag{4.58}$$

and by interpolation it follows that $\|\mu_h\|_{L^2, L^2} \leq 1 - \delta_0'$. In particular the essential spectrum of T_h^M is contained in $[0, 1 - \delta_0']$ so that $\sigma_{\mathrm{ess}}(T_h) \subset [0, 1 - 2\delta_0]$ with $2\delta_0 = 1 - (1 - \delta_0')^{1/M}$. Thus $\mathrm{Spec}(T_h) \cap [1 - \delta_0, 1]$ is discrete. Let us verify that, decreasing $\delta_0 > 0$, we may also assume

$$\mathrm{Spec}(T_h) \subset [-1 + \delta_0, 1]. \tag{4.59}$$

Thanks to the Markov property of T_h^M, to prove this, it suffices to find $M \in 2\mathbb{N} + 1$ such that

$$\int_{\mathcal{O}_{N,\epsilon}} \int_{\mathcal{O}_{N,\epsilon}} (u(x) + u(y))^2 T_h^M(x, dy)\, dx \geq \delta_0 \|u\|_{L^2}^2, \tag{4.60}$$

for any $u \in L^2(\Omega)$. Thanks to the proof of Proposition 4.4, there exists $M \in 2\mathbb{N} + 1$ such that

$$\begin{aligned} &\int_{\mathcal{O}_{N,\epsilon}} \int_{\mathcal{O}_{N,\epsilon}} (u(x) + u(y))^2 T_h^M(x, dy)\, dx \\ &\quad \geq c_0 h^{-Nd} \int_{\mathcal{O}_{N,\epsilon} \times \mathcal{O}_{N,\epsilon}} (u(x) + u(y))^2 \varphi_{Nd}\left(\frac{x-y}{c_1 h}\right) dx\, dy. \end{aligned} \tag{4.61}$$

Hence, (4.59) follows from (4.61) and (2.8).

Following the strategy of Sect. 2 we put $\mathcal{O}_{N,\epsilon}$ in a large box $B =]-A/2, A/2[^{Nd}$ and, thanks to Proposition 4.1, there is an extension map $E : L^2(\mathcal{O}_{N,\epsilon}) \to L^2(B)$ which is also bounded from $H^1(\mathcal{O}_{N,\epsilon})$ into $H^1(B)$. Define

$$\mathcal{E}_{h,k}(u) = \langle (1 - T_h^k)u, u\rangle_{L^2(\mathcal{O}_{N,\epsilon})}, \tag{4.62}$$

and define $\mathcal{E}_h$ as in Sect. 2. Moreover, the identities (2.13) and (2.14) remain true with obvious modifications.

Lemma 4.7 *There exist $C_0, h_0 > 0$ such that the following holds true for any $h \in]0, h_0]$ and any $u \in L^2(\mathcal{O}_{N,\epsilon})$:*

$$\mathcal{E}_h(E(u)) \leq C_0\big(\mathcal{E}_{h,M}(u) + h^2\|u\|^2_{L^2}\big). \tag{4.63}$$

Proof Thanks to Lemma 2.2 we have

$$\begin{aligned}\mathcal{E}_h(E(u)) \leq C_0\bigg(\int_{\mathcal{O}_{N,\epsilon}\times\mathcal{O}_{N,\epsilon}} &(u(x) - u(y))^2 c_0 h^{-Nd} \\ &\varphi_{Nd}\left(\frac{x-y}{c_1 h}\right) dy\, dx + h^2\|u\|_{L^2(\mathcal{O}_{N,\epsilon})}\bigg).\end{aligned} \tag{4.64}$$

Combined with (4.32), this shows that

$$\begin{aligned}\mathcal{E}_h(E(u)) \leq C_0\bigg(\int_{\mathcal{O}_{N,\epsilon}\times\mathcal{O}_{N,\epsilon}} &(u(x) - u(y))^2 T_h^M(x, dy)\, dx \\ &+ h^2\|u\|_{L^2(\mathcal{O}_{N,\epsilon})}\bigg),\end{aligned} \tag{4.65}$$

and the proof is complete. □

Lemma 4.8 *For any $0 \leq \lambda \leq \delta_0/h^2$, the number of eigenvalues of T_h in $[1 - h^2\lambda, 1]$ (with multiplicity) is bounded by $C_1(1 + \lambda)^{Nd/2}$. Moreover, any eigenfunction $T_h(u) = \lambda u$ with $\lambda \in]1 - \delta_0, 1]$ satisfies the bound*

$$\|u\|_{L^\infty} \leq C_2 h^{-Nd/2}\|u\|_{L^2}. \tag{4.66}$$

Proof Suppose that $T_h(u) = \lambda u$ with $\lambda \in [1 - \delta_0, 1]$, then $T_h^M u = \lambda^M u$ and thanks to (4.32), we get

$$\|(\mu_h - \lambda^M)u\|_{L^\infty} = O(h^{-Nd/2}). \tag{4.67}$$

The estimate (4.66) follows from (4.57). Let $\zeta_k(\lambda, h)$ be the number of eigenvalues of T_h^k in the interval $[1 - h^2\lambda, 1]$ for $h^2\lambda < \delta_0$. Thanks to Lemma 4.7, we can mimick the proof of Lemma 2.3 to get

$$\zeta_M(\lambda, h) \leq C(1+\lambda)^{Nd/2}. \tag{4.68}$$

Then from (4.59), one has

$$\zeta_1(\lambda, h) = \zeta_k\left(\frac{1-(1-h^2\lambda)^k}{h^2}, h\right). \tag{4.69}$$

Combining (4.68) and (4.69), we easily obtain the announced estimate. The proof of Lemma 4.8 is complete. □

The rest of the proof of Theorem 4.6 follows the strategy of Sects. 2 and 3. Using the spectral decomposition (2.45), (2.46) we get easily the estimates (2.52) and (2.54), and it remains to estimate $T_{1,h}^n$. Following the proof of Lemma 2.4, we can find $\alpha > 0$ small enough and $C > 0$ such that the following Nash inequality holds with $1/D = 2 - 4/p > 0$:

$$\|u\|_{L^2}^{2+1/D} \leq Ch^{-2}\big(\mathcal{E}_{h,M}(u) + h^2\|u\|_{L^2}^2\big)\|u\|_{L^1}^{1/D}, \quad \forall u \in E_\alpha. \tag{4.70}$$

From this inequality, we deduce that for $k \geq h^{-2}$,

$$\|T_{1,h}^{kM}\|_{L^\infty, L^\infty} \leq Ce^{-kMg(h)}, \tag{4.71}$$

and this implies for $k \geq h^{-2}$, since the contributions of $T_{2,h}^{kM}, T_{3,h}^{kM}$ are negligible,

$$\|T_h^{kM}\|_{L^\infty, L^\infty} \leq C'e^{-kMg(h)}. \tag{4.72}$$

As T_h is bounded by 1 on L^∞ we can replace kM by $n \geq h^{-2}$ in (4.72) and (4.56) is proved. Assertion (4.55) is an obvious consequence of (4.54). The proof of (4.54) is the same as the one of Theorem 1.2. Thus, the following lemma will end the proof of Theorem 4.6.

Lemma 4.9 *Let* $\theta \in C^\infty(\overline{\mathcal{O}}_{N,\epsilon})$ *be such that* $\mathrm{supp}(\theta) \cap \Gamma_{\mathrm{sing}} = \emptyset$ *and* $\partial_n\theta|_{\Gamma_{\mathrm{reg}}} = 0$. *Then*

$$(1-T_h)\theta = h^2|\Delta|_N\theta + r, \quad \|r\|_{L^2} = O(h^{5/2}). \tag{4.73}$$

Proof Let $\theta \in C^\infty(\overline{\mathcal{O}}_{N,\epsilon})$ be such that $\mathrm{supp}(\theta) \cap \Gamma_{\mathrm{sing}} = \emptyset$ and $\partial_n\theta|_{\Gamma_{\mathrm{reg}}} = 0$ and denote $Q_h = 1 - T_h$. Then $Q_h = \frac{1}{N}\sum_{j=1}^N Q_{j,h}$ with

$$Q_{j,h}\theta(x) = \frac{h^{-d}}{\mathrm{vol}(B_1)}\int_\Omega 1_{|x_j-y|<h}\prod_{k\neq j}1_{|x_k-y|>\epsilon}(\theta(x) - \theta(\pi_j(x) + \sigma_j(y)))\,dy. \tag{4.74}$$

Let $\chi_0(x) = 1_{\mathrm{dist}(x,\partial\mathcal{O}_{N,\epsilon})<2h}$. The same proof as in Sect. 3 shows that

$$(1-\chi_0)Q_{j,h}\theta(x) = -\frac{\alpha_d}{2}h^2\partial_j^2\theta(x) + O_{L^\infty}(h^3), \tag{4.75}$$

so that

$$(1-\chi_0)Q_h\theta(x) = h^2|\Delta|_N\theta(x) + O_{L^2}(h^3). \tag{4.76}$$

We study $\chi_0 Q_h\theta$. As $\|\chi_0\|_{L^2} = O(h^{1/2})$ it suffices to show that $\|\chi_0 Q_h\theta\|_{L^\infty} = O(h^2)$. On the other hand, by Taylor expansion we have

$$\chi_0 Q_{j,h}\theta(x) = -\frac{h\chi_0(x)}{\mathrm{vol}(B_1)}\int_{|z|<1}\prod_{k\neq j} 1_{|x_j+hz-x_k|>\epsilon}1_{x_j+hz\in\Omega} z.\partial_j\theta(x)\,dz$$
$$+ O_{L^\infty}(h^2). \tag{4.77}$$

Hence, it suffices to show that

$$v(x) = \chi_0(x)\sum_{j=1}^N\int_{|z|<1}\prod_{k\neq j} 1_{|x_j+hz-x_k|>\epsilon}1_{x_j+hz\in\Omega} z.\partial_j\theta(x)\,dz \tag{4.78}$$

satisfies $\|v\|_{L^\infty} = O(h)$. Since $\mathrm{dist}(\mathrm{supp}\,\varphi_{Nd}(\theta), \Gamma_{\mathrm{sing}}) > 0$, there exists disjoint compact sets $F_l \subset \{s(x) = 0, R(x) = l\}$, and $F_{i,j} \subset \{r(x) = 0, S(x) = (i,j)\}$ such that

$$\mathrm{supp}(\chi_0\theta) \subset \bigcup_l \{x, \mathrm{dist}(x, F_l) \le 4h\} \bigcup_{i,j} \{x, \mathrm{dist}(x, F_{i,j}) \le 4h\}.$$

If $x \in \mathrm{supp}(\chi_0\theta)$ is in $\{x, \mathrm{dist}(x, F_1) \le 4h\}$, then the same parity arguments as in Sect. 3 show that

$$v(x) = \chi_0(x)\int_{|z|<1, x_1+hz\in\Omega} z.\partial_1\theta(x)\,dz = O(h). \tag{4.79}$$

If $x \in \mathrm{supp}(\chi_0\theta)$ is in $\{x, \mathrm{dist}(x, F_{1,2}) \le 4h\}$, then

$$v(x) = \chi_0(x)\int_{|z|<1} z.(\partial_1\theta(x)1_{|x_1+hz-x_2|>\epsilon} + \partial_2\theta(x)1_{|x_2+hz-x_1|>\epsilon})\,dz \tag{4.80}$$

and the result follows from $(x_1 - x_2).(\partial_1\theta - \partial_2\theta)(x) = 0(h)$ for $\{x, \mathrm{dist}(x, F_{1,2}) \le 4h\}$, since $\partial_n\theta$ vanishes on the boundary $|x_1 - x_2| = \epsilon$. The proof of Lemma 4.9 is complete. □

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