HEAT TRACE ASYMPTOTICS AND BOUNDEDNESS IN H^2 OF ISOSPECTRAL POTENTIALS FOR THE DIRICHLET LAPLACIAN

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Abstract. Let Ω be a C^∞-smooth bounded domain of $\mathbb{R}^n$, $n \geq 1$, and let the matrix $\mathbf{a} \in C^\infty(\overline{\Omega}; \mathbb{R}^{n^2})$ be symmetric and uniformly elliptic. We consider the $L^2(\Omega)$-realization A of the operator $-\mathrm{div}(\mathbf{a}\nabla\cdot)$ with Dirichlet boundary conditions. We perturb A by some real valued potential $V \in C_0^\infty(\Omega)$ and note $A_V = A + V$. We compute the asymptotic expansion of $\mathrm{tr}\left(e^{-tA_V} - e^{-tA}\right)$ as $t \downarrow 0$ for any matrix $\mathbf{a}$ with constant coefficients. In the particular case where A is the Dirichlet Laplacian in Ω, that is when $\mathbf{a}$ is the identity of $\mathbb{R}^{n^2}$, we make the four main terms appearing in the asymptotic expansion formula explicit and prove that L^∞-bounded sets of isospectral potentials of A are bounded in $H^2(\Omega)$.

Key words : Heat trace asymptotics, isospectral potentials.

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Contents

1. Introduction

In the present paper we investigate the compactness issue for isospectral potentials sets of the Dirichlet Laplacian by means of heat kernels asymptotics.

1.1. Second order strongly elliptic operator.

Let $\mathbf{a} = (a_{ij})_{1 \leq i,j \leq n} n \geq 1$, be a symmetric matrix, with coefficients in $C^\infty(\mathbb{R}^n)$. We assume that $\mathbf{a}$ is uniformly elliptic, in the sense that there is a constant $\mu \geq 1$ such that the estimate

$$\mu^{-1} \leq \mathbf{a}(x) \leq \mu, \tag{1.1}$$

holds for all $x \in \mathbb{R}^n$ in the sense of quadratic forms on $\mathbb{R}^n$.

We consider a bounded domain $\Omega \subset \mathbb{R}^n$, with C^∞ boundary $\partial\Omega$ and introduce the self-adjoint operator A generated in $L^2(\Omega)$ by the closed quadratic form

$$\mathfrak{a}[u] = \int_\Omega \mathbf{a}(x)\nabla u(x) \cdot \nabla u(x) dx,\ u \in D(\mathfrak{a}) = H_0^1(\Omega), \tag{1.2}$$

where $H_0^1(\Omega)$ is the closure of $C_0^\infty(\Omega)$ in the topology of the standard first-order Sobolev space $H^1(\Omega)$. Here ∇ stands for the gradient operator on $\mathbb{R}^n$. By straightforward computations we find out that A acts on its domain $D(A) = H^2(\Omega) \cap H_0^1(\Omega)$, as

$$A = -\mathrm{div}(\mathbf{a}(x)\nabla\,\cdot\,) = -\sum_{i,j=1}^n \partial_j(a_{ij}(x)\partial_i\,\cdot\,). \tag{1.3}$$

Let $V \in C_0^\infty(\mathbb{R}^n)$ be real-valued. We define the perturbed operator $A_V = A + V$ as a sum in the sense of quadratic forms. Then we have $D(A_V) = D(A)$ by [RS2, Theorem X.12, page 162].

1.2. **Main results.** Put

$$Z_\Omega^V(t) = \mathrm{tr}\left(e^{-tA_V} - e^{-tA}\right),\ t > 0. \tag{1.4}$$

Much of the technical work developed in this paper is devoted to proving the existence of real coefficients $c_k(V)$, $k \geq 1$, depending only on V, such that following symptotic expansion

$$Z_\Omega^V(t) = t^{-n/2}\left(tc_1(V) + t^2c_2(V) + \ldots + t^pc_p(V) + O\left(t^{p+1}\right)\right),\ t \downarrow 0, \tag{1.5}$$

holds for $\mathbf{a}$ constant. Moreover we shall see that (1.4)-(1.5) remain valid upon replacing Ω by $\mathbb{R}^n$ in the definition of A (and subsequently $H_0^1(\Omega)$ by $H^1(\mathbb{R}^n)$ in (1.2)).

Since Ω is bounded then the injection $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ is compact. Thus the resolvent of A_V is a compact operator and A_V has a pure point spectrum. Let $\{\lambda_j^V,\ j \in \mathbb{N}^*\}$ be the non-decreasing sequence of the eigenvalues of A_V, repeated according to their multiplicities. We define the isospectral set associated with the potential $V \in C_0^\infty(\Omega)$ by

$$\mathrm{Is}(V) = \{W \in C_0^\infty(\Omega);\ \lambda_k^V = \lambda_k^W,\ k \in \mathbb{N}^*\}.$$

The computation carried out in section 5.2 of the coefficients $c_j(V)$ appearing in (1.5), for $j = 1, 2, 3, 4$, leads to the following result.

Theorem 1.1. *Let* $\mathbf{a}$ *be the identity of* $\mathbb{R}^{n^2}$. *Then for all* $V \in C_0^\infty(\Omega)$ *and any bounded subset* $\mathcal{B} \subset L^\infty(\Omega)$, *the set* $Is(V) \cap \mathcal{B}$ *is bounded in* $H^2(\Omega)$.

Since $H^2(\Omega)$ is compactly embedded in $H^s(\Omega)$, for any $s < 2$, Theorem 1.1 entails the:

Corollary 1.1. *Under the conditions of Theorem 1.1, the set* $Is(V) \cap \mathcal{B}$ *is compact in* $H^s(\Omega)$ *for each* $s \in (-\infty, 2)$.

It is worth mentioning that the method developed to calculate the first coefficients of the expansion formula (1.5) when $\mathbf{a}$ is the identity of $\mathbb{R}^{n^2}$ may be generalized to the case of a constant matrix $\mathbf{a}$ at the expense of heavier computations. Nevertheless, for the sake of computational simplicity, this specific part of the analysis was restricted to the case of the Laplace operator.

1.3. **What is known so far.** It turns out that the famous problem addressed by M. Kac in [Ka], as whether one can hear the shape of drum, is closely related to the following asymptotic expansion formula for the trace of $e^{t\Delta_g}$ on a compact Riemannian manifold (M, g):

$$\mathrm{tr}\left(e^{t\Delta_g}\right) = t^{-n/2}\left(e_0 + te_1 + t^2e_2 + \ldots + t^ke_k + O\left(t^{k+1}\right)\right). \tag{1.6}$$

Here Δ_g is the Laplace-Beltrami operator associated with the metric g and the coefficients e_k, $k \geq 0$, are Riemannian invariants depending on the curvature tensor and its covariant derivatives. There is a wide mathematical literature about (1.6), with many authors focusing more specifically on the explicit calculation of e_k, $k \geq 0$. This is due to the fact that these coefficients actually provide useful information on g and consequently on the geometry of the manifold M. The key point in the proof of (1.6) is the construction of a parametrix for the heat equation $\partial_t - \Delta_g$, which was initiated by S. Minakshisudaram and Å. Pleijel in [MP].

A survey on isospectral manifolds can be found in [GPS]. This problem is still at the center of the attention of geometers. As a matter of fact Dryden, Gordon, Greenwald and Webb recently calculated the asymptotic expansion of the heat kernel for orbifolds in [DGGW]. In the same spirit, the heat trace asymptotics for general connections has been expressed by Beneventano, Gilkey, Kirsten and Santangelo in [BGKS].

Since the present work is not directly related to the analysis of the asymptotic expansion formula (1.6), we shall not go into that matter further and we refer to [BGM, Ch, Gi2, Ka, MS] for more details.

The asymptotic expansion formula (1.5), for the Laplacian in the whole space, was proved by Y. Colin de Verdière in [Co] by adapting (1.6). An alternative proof, based on the Fourier transform, was given in [BB] by R. Bañuelos and A. Sá Barreto. The approach developed in this text is rather different in the sense that (1.5) is obtained by linking the heat kernel of e^{-tA_V} to the one of e^{-tA} through Duhamel's formula. The asymptotic expansion formulae (1.5) and (1.6) are nevertheless quite similar, but, here, the coefficients c_k, $k \geq 1$, are given as integrals over Ω of polynomial functions in V and its derivatives. This situation is reminiscent of [BB, Theorem 2.1, page 2154] where the same coefficients are expressed in terms of the tensor products $\widehat{V} \otimes \ldots \otimes \widehat{V}$, where $\widehat{V}$ is the Fourier transform of the potential V. Let us finally mention that Colin de Verdière obtained a semi-classical trace formula for heat kernels of magnetic Schrödinger operators in [Co2]

As will appear in section 5, the proof of the compactness Theorem 1.1 boils down to the calculation of the four main terms in the asymptotic expansion formula (1.5). This follows from the basic identity

$$\sum_{k \geq 1} e^{-\lambda_k^V t} = \operatorname{tr}\left(e^{-tA_V}\right) = \operatorname{tr}\left(e^{-tA}\right) + Z_\Omega^V(t),$$

linking the isospectral sets of A_V to the heat trace of A. Compactness results for isospectral potentials associated with the operator $\Delta_g + V$ were already obtained by Brüning in [Br, Theorem 3, page 696] for a compact Riemannian manifold with dimension no greater than 3, and further improved by Donnelly in [Don]. Their approach is based on trace asymptotics borrowed to [Gi1, Theorem 4.3, page 230]. Our strategy is rather similar but the heat kernels asymptotics needed in this text are explicitly computed in the first part of the article.

1.4. **Outline.** Section 2 gathers several definitions and auxiliary results on heat kernels and trace asymptotics needed in the remaining part of the article. The asymptotic formula (1.5) is established in Section 3. Finally section 5 contains the proof of Theorem 1.1.

2. Preliminaries

In this section we introduce some notations used throughout this text and derive auxiliary results needed in the remaining part of this paper.

2.1. **Heat kernels and trace asymptotics.** With reference to the definitions and notations introduced in section 1 we first recall from [Ou, Chapter 4, page 102] that the operator $-A_V$, where $V \in C_0^\infty(\Omega)$, generates an analytic semi-group e^{-tA_V} on $L^2(\Omega)$. We denote K^V the heat kernel associated with e^{-tA_V}, in such a way that the identity

$$\left(e^{-tA_V} f\right)(x) = \int_\Omega K^V(t,x,y) f(y) dy,\ t > 0,\ x \in \Omega, \tag{2.1}$$

holds for every $f \in L^2(\Omega)$. Let M_V be the multiplication operator induced by V. Then we have

$$e^{-tA_V} = e^{-tA} - \int_0^t e^{-(t-s)A} M_V e^{-sA_V} ds,\ t > 0,$$

from Duhamel's formula. From this and (2.1) then follows that

$$K^V(t,x,y)=K(t,x,y)-\int_0^t\int_\Omega K(t-s,x,z)V(z)K^V(s,z,y)dzds,\ t>0,\ x,y\in\Omega, \tag{2.2}$$

where K denotes the heat kernel of e^{-tA}. Upon solving the integral equation (2.2) with the unknown function K^V by the successive approximation method, we obtain that

$$K^V(t,x,y)=\sum_{j\geq 0}K_j^V(t,x,y),\ t>0,\ x,y\in\Omega, \tag{2.3}$$

with

$$K_0^V(t,x,y)=K(t,x,y) \text{ and } K_{j+1}^V(t,x,y)=-\int_0^t\int_\Omega K(t-s,x,z)V(z)K_j^V(s,z,y)dsdz \text{ for all } j\in\mathbb{N}. \tag{2.4}$$

Thus, for each $t>0$ and $x,y\in\Omega$, we get by induction on $j\in\mathbb{N}^*$ that

$$K_j^V(t,x,y)=(-1)^j\int_{\Omega^n}\int_0^t\int_0^{t_1}\dots\int_0^{t_{j-1}}\left[\prod_{i=1}^j K(t_{i-1}-t_i,z_{i-1},z_i)V(z_i)\right]K(t_j,z_j,y)dz^jdt^j,$$

where $t_0=t$, $z_0=x$, and $du^j=du_1\dots du_j$ for $u=z,t$. From this, the following reproducing property

$$\int_\Omega K(t-s,x,z)K(s,z,y)dz=K(t,x,y),\ t>0,\ s\in(0,t),\ x,y\in\Omega, \tag{2.5}$$

and the estimate $K\geq 0$, arising from [Fr], then follows that

$$|K_j^V(t,x,y)|\leq\frac{\|V\|_\infty^j t^j}{j!}K(t,x,y),\ t>0,\ x,y\in\Omega,\ j\in\mathbb{N}. \tag{2.6}$$

Therefore, for any fixed $x,y\in\Omega$, the series in the right hand side of (2.3) converges uniformly in $t>0$.

Having said that we consider the fundamental solution Γ to the equation

$$\partial_t-\operatorname{div}(\mathbf{a}(x)\nabla\cdot)=\partial_t-\sum_{i,j=1}^n\partial_j(a_{ij}(x)\partial_i\ ,\cdot)=0 \text{ in } \mathbb{R}^n.$$

Then there is a constant $c>0$, depending only on n and μ, such that we have

$$\Gamma(t,x,y)\leq(ct)^{-n/2}e^{-c|x-y|^2/t},\ t>0,\ x,y\in\mathbb{R}^n, \tag{2.7}$$

according to [FS]. Further, arguing as in the proof of Lemma 2.1 below, it follows from the maximum principle that

$$0\leq K(t,x,y)\leq\Gamma(t,x,y),\ t>0,\ x,y\in\Omega. \tag{2.8}$$

Thus, by (2.6)-(2.7), for all fixed $t>0$, the series in the right hand side of (2.3) converges uniformly with respect to x and y in Ω, and we have

$$\int_\Omega K^V(t,x,x)dx=\sum_{j\geq 0}A_j^V(t) \text{ where } A_j^V(t)=\int_\Omega K_j^V(t,x,x)dx,\ j\in\mathbb{N}. \tag{2.9}$$

As λ_k^V scales like $k^{2/n}$ by [Kav, Lemma 3.1, page 229] then we have $\sum_{k=1}^\infty e^{-t\lambda_k^V}<\infty$, hence e^{-tA_V} is trace class since $\sigma(e^{-tA_V})\setminus\{0\}=\{e^{-t\lambda_k^V},\ k\geq 1\}$ from the spectral theorem (see e.g. [EnNa1, Corollary 3.2, page 289] or [EnNa2, Corollary 2.10, page 183]). On the other hand, e^{-tA_V} being an integral operator with smooth kernel (see e.g. [Da]), we have

$$\operatorname{tr}\left(e^{-tA_V}\right)=\int_\Omega K^V(t,x,x)dx=\sum_{k\geq 1}e^{-t\lambda_k^V},\ t>0. \tag{2.10}$$

Notice that the right identity in (2.10) is a direct consequence of Mercer's theorem (see e.g. [Ho]), entailing

$$K^V(t,x,y)=\sum_{k\geq 1}e^{-t\lambda_k^V}\phi_k^V(x)\times\phi_k^V(y),\ t>0,\ x,y\in\Omega,$$

where $\{\phi_k^V,\ k \in \mathbb{N}^*\}$ is an orthonormal basis of eigenfunctions ϕ_k^V of A_V, associated with the eigenvalue λ_k^V. Finally, putting (1.4) and (2.9)-(2.10) together, we find out that

$$Z_\Omega^V(t) = \sum_{j \geq 1} A_j^V(t),\ t > 0. \tag{2.11}$$

2.2. **Estimation of Green functions.** We start with the following useful comparison result:

Lemma 2.1. *For $\delta > 0$ put $\Omega_\delta = \{x \in \Omega;\ \mathrm{dist}(x, \partial\Omega) > \delta\}$. Then we have*

$$0 \leq \Gamma(t,x,y) - K(t,x,y) \leq (ct)^{-n/2} e^{-c\delta^2/t},\ 0 < t \leq \frac{2c\delta^2}{n},\ x \in \Omega,\ y \in \Omega_\delta,$$

where c is the constant appearing in the right hand side of (2.7).

Proof. Fix $y \in \Omega_\delta$. Then $u_y(t,x) = \Gamma(t,x,y) - K(t,x,y)$ being the solution to the following initial boundary value problem

$$\begin{cases} \partial_t u_y(t,x) - \sum_{i,j=1}^n \partial_j (a_{ij} \partial_i u_y(t,x)) = 0, & t > 0,\ x \in \Omega, \\ u_y(0,x) = 0, & x \in \Omega, \\ u_y(t,x) = \Gamma(t,x,y), & t > 0,\ x \in \partial\Omega, \end{cases}$$

we get from the parabolic maximum principle (see e.g. [Fr]) that $u_y(t,x) \leq \max_{\substack{z \in \partial\Omega \\ 0 < s \leq t}} \Gamma(s,z,y)$. Therefore we have

$$u_y(t,x) \leq \max_{\substack{z \in \partial\Omega \\ 0 < s \leq t}} (cs)^{-n/2} e^{-c|z-y|^2/s} \leq \max_{0 < s \leq t} (cs)^{-n/2} e^{-c\delta^2/s},\ t > 0,\ x \in \Omega,$$

by (2.7). Now the desired result follows readily from this and (2.8) upon noticing that $s \mapsto (cs)^{-n/2} e^{-c\delta^2/s}$ is non-decreasing on $(0, 2c\delta^2/n)$. $\square$

Remark 2.1. a) The functions $K(t,\cdot,\cdot)$ and $\Gamma(t,\cdot,\cdot)$ being symmetric for all $t > 0$, the statement of Lemma 2.1 remains valid for $x \in \Omega_\delta$ and $y \in \Omega$ as well.
b) A result similar to Lemma 2.1 can be found in [Mi] for the Dirichlet Laplacian, which corresponds to the operator A in the particular case where $\mathbf{a}$ is the identity matrix. This claim, which was actually first proved by H. Weyl in [We], is a cornerstone in the derivation of the classical Weyl's asymptotic formula for the eigenvalues counting function (see e.g. [Dod]).
c) We refer to [Co] for an alternative proof of Lemma 2.1 that is based on the classical Feynman-Kac formula (see e.g. [SV]) instead of the maximum principle.

Let us extend $V \in C_0^\infty(\Omega)$ to $\mathbb{R}^n$ by setting $V(x) = 0$ for all $x \in \mathbb{R}^n \setminus \Omega$, and, with reference to (2.3)-(2.4), put

$$\Gamma_0^V(t,x,y) = \Gamma(t,x,y) \text{ and } \Gamma_{j+1}^V(t,x,y) = -\int_0^t \int_{\mathbb{R}^n} \Gamma(t-s,x,z) V(z) \Gamma_j^V(s,z,y) ds dz, j \in \mathbb{N}, \tag{2.12}$$

for all $t > 0$ and $x, y \in \mathbb{R}^n$. Armed with Lemma 2.1 we may now relate the asymptotic behavior of $A_j^V(t)$ as $t \downarrow 0$ to the one of

$$B_j^V(t) = \int_\Omega \Gamma_j^V(t,x,x) dx,\ t > 0,\ j \in \mathbb{N}. \tag{2.13}$$

Proposition 2.1. *Let $j \in \mathbb{N}^*$. Then for each $k \in \mathbb{N}$ we have $A_j^V(t) = B_j^V(t) + O(t^k)$ as $t \downarrow 0$.*

Proof. Choose $\delta > 0$ so small that $\mathrm{supp}(V) \subset \Omega_\delta$, where Ω_δ is the same as in Lemma 2.1, and pick $t \in (0, 2c\delta^2/n)$. Then, for all $x, y \in \Omega$, we have

$$\begin{aligned} |\Gamma_1^V(t,x,y) - K_1^V(t,x,y)| &\leq \int_0^t \int_{\Omega_\delta} \Gamma(t-s,x,z) |V(z)| [\Gamma(s,z,y) - K(s,z,y)] dz ds \\ &+ \int_0^t \int_{\Omega_\delta} [\Gamma(t-s,x,z) - K(t-s,x,z)] |V(z)| K(s,z,y) dz ds, \end{aligned}$$

by (2.4) and (2.12). This, together with Lemma 2.1 and part a) in Remark 2.1, yields

$$|\Gamma_1^V(t,x,y)-K_1^V(t,x,y)| \leq \|V\|_\infty (ct)^{-n/2}e^{-c\delta^2/t}\left(\int_0^t\int_{\mathbb{R}^n}\Gamma(s,x,z)dzds+\int_0^t\int_{\mathbb{R}^n}\Gamma(s,z,y)dzds\right), \tag{2.14}$$

for all $t>0$ and a.e. $x,y\in\Omega$. Here we used the estimate $0\leq K\leq\Gamma$ and the fact that the function $s\mapsto(cs)^{-n/2}e^{-c\delta^2/s}$ is non-decreasing on $(-\infty,2c\delta^2/n]$. Further, due to (2.7), there is a positive constant C, independent of t, such that

$$\int_0^t\int_{\mathbb{R}^n}\Gamma(s,x,z)dzds+\int_0^t\int_{\mathbb{R}^n}\Gamma(s,z,y)dzds\leq Ct,\ t>0,x,y\in\Omega,$$

so we obtain

$$|\Gamma_1^V(t,x,y)-K_1^V(t,x,y)|\leq C\|V\|_\infty t(ct)^{-n/2}e^{-c\delta^2/t},\ t>0,\ x,y\in\Omega,$$

by (2.14). Similarly, using (2.6) and arguing as above, we get

$$|\Gamma_j^V(t,x,y)-K_j^V(t,x,y)|\leq (C\|V\|_\infty)^j\frac{t^j}{j!}(ct)^{-n/2}e^{-c\delta^2/t},\ t>0,\ x,y\in\Omega,$$

by induction on $j\in\mathbb{N}^*$. Now the result follows from this, (2.9) and (2.13). □

2.3. **The case of a constant metric.** We now express the function $(t,x)\in\mathbb{R}_+^*\times\mathbb{R}^n\mapsto\Gamma_j^V(t,x,x)$, $j\in\mathbb{N}^*$, defined by (2.12), in terms of the heat kernel Γ and the perturbation V, in the particular case where $\mathbf{a}$ is constant. Since $\mathbf{a}$ is regular (i.e. invertible) by (1.1) then $\Gamma(t,x,y)$ is explicitly known and coincides with the following Gaussian kernel

$$G(t,x-y)=(4\pi t)^{-n/2}\left(\det\mathbf{a}^{-1}\right)^{-1/2}e^{-\mathbf{a}^{-1}(x-y)\cdot(x-y)/(4t)},\ t>0,\ x,y\in\mathbb{R}^n, \tag{2.15}$$

where $\mathbf{a}^{-1}$ is the inverse matrix of $\mathbf{a}$. The result is as follows.

Lemma 2.2. *Assume that* $\mathbf{a}$ *is constant and fix* $j\in\mathbb{N}^*$*. Then we have*

$$\begin{aligned}\Gamma_j^V(t,x,x) &= (-1)^j t^{j-n/2}\int_{(\mathbb{R}^n)^j}\int_0^1\int_0^{s_1}\ldots\int_0^{s_{j-1}}\left[\prod_{i=1}^j G(s_{i-1}-s_i,w_{i-1}-w_i)V(x+\sqrt{t}w_i)\right]\\ &\qquad\times G(s_j,w_j)ds^jdw^j,\end{aligned}$$

for all $t>0$ *and* $x\in\mathbb{R}^n$*, where* G *is defined by* (2.15)*. Here we have set* $s_0=1$*,* $w_0=0$ *and* $du^j=du_1\ldots du_j$ *for* $u=s,w$*.*

Proof. The main benefit of dealing with a constant matrix $\mathbf{a}$ is the following property:

$$\Gamma(ts,x,y)=t^{-n/2}\Gamma\left(s,\frac{x}{\sqrt{t}},\frac{y}{\sqrt{t}}\right),\ t,s>0,\ x,y\in\mathbb{R}^n.$$

From this and the following identity arising from (2.12) for all $t>0$ and $x,y\in\mathbb{R}^n$,

$$\Gamma_j^V(t,x,y) = (-1)^j t^j\int_{(\mathbb{R}^n)^j}\int_0^1\int_0^{s_1}\ldots\int_0^{s_{j-1}}\left[\prod_{i=1}^j\Gamma(t(s_{i-1}-s_i),z_{i-1},z_i)V(z_i)\right]\Gamma(ts_j,z_j,y)ds^jdz^j,$$

with $z_0=x$, then follows that

$$\begin{aligned}&\Gamma_j^V(t,x,y)\\ &= (-1)^jt^{j-(j+1)n/2}\int_{(\mathbb{R}^n)^j}\int_0^1\int_0^{s_1}\ldots\int_0^{s_{j-1}}\left[\prod_{i=1}^j\Gamma\left(s_{i-1}-s_i,\frac{z_{i-1}}{\sqrt{t}},\frac{z_i}{\sqrt{t}}\right)V(z_i)\right]\Gamma\left(s_j,\frac{z_j}{\sqrt{t}},\frac{y}{\sqrt{t}}\right)ds^jdz^j.\end{aligned}$$

Thus, by performing the change of variables $(z_1, \dots z_j) = \sqrt{t}(w_1, \dots w_j) + (x, \dots, x)$ in the above integral, we find out that

$$\Gamma_j^V(t,x,y) = (-1)^j t^{j-n/2} \int_{(\mathbb{R}^n)^j} \int_0^1 \int_0^{s_1} \dots \int_0^{s_{j-1}} \left[\prod_{i=1}^j \Gamma\left(s_{i-1} - s_i, \frac{x}{\sqrt{t}} + w_{i-1}, \frac{x}{\sqrt{t}} + w_i \right) V\left(x + \sqrt{t} w_i \right) \right] \times \Gamma\left(s_j, \frac{x}{\sqrt{t}} + w_j, \frac{y}{\sqrt{t}} \right) ds^j dw^j.$$

Finally, we obtain the desired result upon taking $y = x$ in the above identity and recalling that Γ verifies

$$\Gamma\left(t, \frac{x}{\sqrt{t}} + z, \frac{x}{\sqrt{t}} + w \right) = \Gamma(t,z,w) = G(t, z-w),$$

for all $t > 0$ and x, z, w in $\mathbb{R}^n$. □

3. Asymptotic expansion formulae

In this section we establish the asymptotic expansion formula (1.5). The strategy of the proof is, first, to establish (1.5) where

$$Z^V(t) = \mathrm{tr}(e^{-tH_V} - e^{-tH}),\ t > 0, \tag{3.1}$$

is substituted for $Z_\Omega^V(t)$, and, second, to relate the asymptotics of $Z_\Omega^V(t)$ as $t \downarrow 0$ to the one of $Z^V(t)$.

Here H is the self-adjoint operator generated in $L^2(\mathbb{R}^n)$ by the closed quadratic form

$$\mathfrak{h}[u] = \int_{\mathbb{R}^n} \mathbf{a}(x) \nabla u(x) \cdot \nabla u(x) dx,\ u \in D(\mathfrak{h}) = H^1(\mathbb{R}^n),$$

and $H_V = H + V$ as a sum in the sense of quadratic forms. It is easy to check that H acts on its domain $D(H) = H^2(\mathbb{R}^n)$, the second-order Sobolev space on $\mathbb{R}^n$, as the right hand side of (1.3). Moreover we have $D(H_V) = D(H)$ since $V \in L^\infty(\mathbb{R}^n)$. In other words H (resp., H_V) may be seen as the extension of the operator A (resp., A_V) acting in $L^2(\mathbb{R}^n)$, and, due to (2.12) and (3.1), we have

$$Z^V(t) = \sum_{j \geq 1} H_j^V(t),\ t > 0,\ \text{where } H_j^V(t) = \int_{\mathbb{R}^n} \Gamma_j^V(t,x,x) dx,\ j \in \mathbb{N}. \tag{3.2}$$

In light of this and Lemma 2.2, we apply Taylor's formula to $V \in C_0^\infty(\Omega)$, getting for all $j \geq 1$ and $p \geq 1$,

$$\prod_{k=1}^j V(x + tw_k) = \sum_{\ell=0}^{p-1} t^\ell \left[\sum_{|\alpha_1| + \dots |\alpha_j| = \ell} \frac{1}{\alpha_1! \dots \alpha_j!} \prod_{k=1}^j \partial^{\alpha_k} V(x) w_k^{\alpha_k} \right] + t^p R_j^p(t, x, w_1 \dots, w_j), \tag{3.3}$$

where

$$R_j^p(t,x,w_1 \dots, w_j) = \sum_{|\alpha_1| + \dots |\alpha_j| = p} \frac{p}{\alpha_1! \dots \alpha_j!} \int_0^1 (1-s)^{p-1} \prod_{k=1}^j \partial^{\alpha_k} V(x + stw_k) w_k^{\alpha_k} ds. \tag{3.4}$$

For the sake of notational simplicity we note

$$\alpha^j = (\alpha_1^j, \dots, \alpha_j^j) \in (\mathbb{N}^n)^j,\ \alpha^j! = \prod_{k=1}^j \alpha_k^j! \text{ and } W_j^{\alpha^j} = \prod_{k=1}^j w_k^{\alpha_k^j}, \tag{3.5}$$

so that (3.3)-(3.4) may be reformulated as

$$\prod_{k=1}^j V(x + tw_k) = \sum_{\ell=0}^{p-1} t^\ell \left[\sum_{|\alpha^j| = \ell} \frac{W_j^{\alpha^j}}{\alpha^j!} \prod_{k=1}^j \partial^{\alpha_k^j} V(x) \right] + t^p R_j^p(t,x,w_1 \dots, w_j), \tag{3.6}$$

with

$$R_j^p(t,x,w_1 \dots, w_j) = \sum_{|\alpha^j| = p} \frac{p W_j^{\alpha^j}}{\alpha^j!} \int_0^1 (1-s)^{p-1} \prod_{k=1}^j \partial^{\alpha_k} V(x + stw_k) ds,\ j, p \in \mathbb{N}^*. \tag{3.7}$$

Next, with reference to (3.5) we define for further use

$$c_{\alpha^j}=\frac{1}{\alpha^j!}\int_{(\mathbb{R}^n)^j}\int_0^1\int_0^{s_1}\dots\int_0^{s_{j-1}}W_j^{\alpha^j}\left[\prod_{i=1}^j G(s_{i-1}-s_i,w_{i-1}-w_i)\right]G(s_j,w_j)ds^jdw^j, \tag{3.8}$$

where, as usual, $s_0=1$, $w_0=0$, and du^j stands for $du_1\dots du_j$ with $u=s,w$. Putting

$$P_{\alpha^j}(V)=\int_\Omega\prod_{k=1}^j\partial^{\alpha_k^j}V(x)dx,\ j\in\mathbb{N}^*, \tag{3.9}$$

we may now state the main result of this section.

Proposition 3.1. *For any $p\in\mathbb{N}^*$, the asymptotics of $Z^V(t)$ and $Z_\Omega^V(t)$ as $t\downarrow 0$ have the expression*

$$\sum_{\ell=1}^p t^\ell\mathcal{P}_{2\ell}(V)+O(t^{p+1}),$$

where

$$\mathcal{P}_\ell(V)=\sum_{1\le j\le \ell/2}(-1)^j\sum_{|\alpha^j|=\ell-2j}c_{\alpha^j}P_{\alpha^j}(V), \tag{3.10}$$

the coefficients c_{α^j} and $P_{\alpha^j}(V)$ being defined by (3.8)-(3.9).

Proof. In view of (2.13), Lemma 2.2 and (3.9) we have

$$t^nB_j^V(t^2)=(-1)^j\sum_{\ell=0}^{p-1}t^{\ell+2j}\sum_{|\alpha^j|=\ell}c_{\alpha^j}P_{\alpha^j}(V)+O(t^{p+2j}),\ t>0,\ j\in\mathbb{N}^*,$$

and hence

$$t^nB_j^V(t^2)=(-1)^j\sum_{\ell=2j}^{p-1}t^{\ell}\sum_{|\alpha^j|=\ell-2j}c_{\alpha^j}P_{\alpha^j}(V)+O(t^{p}),\ t>0,\ j\in\mathbb{N}^*.$$

Summing up the above identity over all integers j between 1 and $(p-1)/2$, we find that

$$t^n\sum_{1\le j\le (p-1)/2}B_j^V(t^2)=\sum_{1\le j\le (p-1)/2}(-1)^j\sum_{\ell=2j}^{p-1}t^\ell\sum_{|\alpha^j|=\ell-2j}c_{\alpha^j}P_{\alpha^j}(V)+O(t^p)$$

and hence

$$t^n\sum_{1\le j\le (p-1)/2}B_j^V(t^2)=\sum_{\ell=2}^{p-1}t^\ell\sum_{1\le j\le \ell/2}(-1)^j\sum_{|\alpha^j|=\ell-2j}c_{\alpha^j}P_{\alpha^j}(V)+O(t^p).$$

As a consequence we have $t^n\sum_{1\le j\le (p-1)/2}B_j^V(t^2)=\sum_{\ell=2}^{p-1}t^\ell\mathcal{P}_\ell(V)+O(t^p)$, hence

$$t^n\sum_{j\ge 1}B_j^V(t^2)=\sum_{\ell=2}^{p-1}t^\ell\mathcal{P}_\ell(V)+O(t^p). \tag{3.11}$$

Now, upon performing the change of variables $(w_1,\dots,w_j)\longrightarrow(-w_1,\dots,-w_j)$ in the right hand side of (3.8) we get that $c_{\alpha^j}=(-1)^{|\alpha^j|}c_{\alpha^j}$. Therefore $c_{\alpha^j}=0$ for $|\alpha^j|$ odd. As a consequence we have

$$\mathcal{P}_{2\ell+1}(V)=\sum_{1\le j\le \ell}(-1)^j\sum_{|\alpha^j|=2(\ell-j)+1}c_{\alpha^j}P_{\alpha_j}(V)=0.$$

Thus, applying (3.11) where $2(p+1)$ is substituted for p, we find out that

$$t^n\sum_{j\ge 1}B_j^V(t^2)=\sum_{\ell=2}^{2p+1}t^\ell\mathcal{P}_\ell(V)+O(t^{2(p+1)})=\sum_{\ell=1}^{p}t^{2\ell}\mathcal{P}_{2\ell}(V)+O(t^{2(p+1)}),$$

which, in turn, yields

$$t^{n/2}\sum_{j\geq 1}B_j^V(t)=\sum_{\ell=1}^{p}t^{\ell}\mathcal{P}_{2\ell}(V)+O(t^{p+1}). \tag{3.12}$$

Next, bearing in mind that V is supported in Ω, we see that $P_{\alpha^j}(V)=\int_{\mathbb{R}^n}\prod_{k=1}^{j}\partial^{\alpha_k^j}V(x)dx$ for all $j\in\mathbb{N}^*$. This entails

$$t^{n/2}\sum_{j\geq 1}H_j^V(t)=\sum_{\ell=1}^{p}t^{\ell}\mathcal{P}_{2\ell}(V)+O(t^{p+1}). \tag{3.13}$$

upon substituting (3.2) for (2.13) in the above reasoning. Finally, putting (2.11), (3.12) and Proposition 2.1 (resp. (3.2) and (3.13)) together we obtain the result for Z_Ω^V (resp. Z^V). □

Proposition 3.1 immediately entails the:

Corollary 3.1. *Let $V_0\in C_0^\infty(\Omega)$. Then, under the conditions of Proposition 3.1, each $V\in Is(V_0)$ verifies*

$$\mathcal{P}_\ell(V)=\mathcal{P}_\ell(V_0),\ \ \ell\geq 2.$$

Remark 3.1. It is clear that the asymptotic formula stated in Proposition 3.1 for Z^V remains valid if V is taken in the Schwartz class $\mathscr{S}(\mathbb{R}^n)$.

4. Two parameter integrals

In this section we collect useful properties of two parameter integrals appearing in the proof of Theorem 1.1, presented in section 5. As a preamble we consider the integral

$$I_n(f)=\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_0^1\int_0^{s_1}f(w_1,w_2)G(1-s_1,w_1)G(s_1-s_2,w_1-w_2)G(s_2,w_2)dw_1dw_2ds_1ds_2, \tag{4.1}$$

where $f\in C^\infty(\mathbb{R}^n\times\mathbb{R}^n)$ and G is defined by (2.15). For all $\sigma\in\sigma_n$, the set of permutations of $\{1,\dots,n\}$, and all $z=(z_1,\dots,z_n)\in\mathbb{R}^n$, we write $\sigma z=(z_{\sigma(1)},\dots,z_{\sigma(n)})$. Similarly, for every $w_1,w_2\in\mathbb{R}^n$, we note $\sigma(w_1,w_2)=(\sigma w_1,\sigma w_2)$ and $f\circ\sigma(w_1,w_2)=f(\sigma(w_1,w_2))$. The following result gathers several properties of I_n that are required in the remaining part of this section.

Lemma 4.1. *Let $f\in C^\infty(\mathbb{R}^n\times\mathbb{R}^n)$. Then it holds true that:*

i) $I_n(f)=I_n(Sf)$, where S denotes the "mirror symmetry" operator acting as $Sf(w_1,w_2)=f(w_2,w_1)$;
ii) $I_n(f)=I_n(f\circ\sigma)$ for all $\sigma\in\sigma_n$;
iii) If there are $f_k\in C^\infty(\mathbb{R}\times\mathbb{R})$, $k=1,\dots,n$, such that

$$f(w_1,w_2)=\prod_{k=1}^{n}f_k(w_1^k,w_2^k),\ \ w_i=(w_i^1,\dots,w_i^n),i=1,2,$$

and if any of the f_k is an odd function of (w_1^k,w_2^k), then we have $I_n(f)=0$.

Proof. i) Upon performing successively the two changes of variables $\tau_1=1-s_1$ and $\tau_2=1-s_2$ in the right hand side of (4.1), we get that

$$\begin{aligned}I_n(f)&=\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_0^1\int_{\tau_1}^1 f(w_1,w_2)G(\tau_1,w_1)G(\tau_2-\tau_1,w_1-w_2)G(1-\tau_2,w_2)dw_1dw_2d\tau_2d\tau_1\\&=\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_0^1\int_0^{\tau_2} f(w_1,w_2)G(\tau_1,w_1)G(\tau_2-\tau_1,w_1-w_2)G(1-\tau_2,w_2)dw_1dw_2d\tau_1d\tau_2,\end{aligned}$$

so the result follows by relabelling (w_1,w_2) as (w_2,w_1).
ii) In light of (2.15) we have $G(t,w)=G(t,\sigma^{-1}w)$ for all $t>0$, $w\in\mathbb{R}^n$ and $\sigma\in\sigma_n$, hence $I_n(f)$ is equal to

$$\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_0^1\int_0^{s_1}f(w_1,w_2)G(1-s_1,\sigma^{-1}w_1)G(s_1-s_2,\sigma^{-1}w_1-\sigma^{-1}w_2)G(s_2,\sigma^{-1}w_2)dw_1dw_2ds_1ds_2,$$

according to (4.1). The result follows readily from this upon performing the change of variable $(\widetilde{w}_1,\widetilde{w}_2)=\sigma^{-1}(w_1,w_2)$.
iii) This point is a direct consequence of the obvious identity $I_n(f)=\prod_{k=1}^n I_1(f_k)$, arising from (2.15) and (4.1). $\square$

We turn now to evaluating integrals of the form

$$I_{\alpha,\beta}=I_{\alpha,\beta}(s_1,s_2)=\int_{\mathbb{R}}\int_{\mathbb{R}} x^\alpha y^\beta g(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy,\ \alpha,\beta\in\mathbb{N},\ s_1,s_2\in\mathbb{R}, \tag{4.2}$$

where g denotes the one-dimensional Gaussian kernel defined by (2.15) in the particular case where $n=1$. This can be achieved upon using the following result.

Lemma 4.2. *Let $\alpha,\beta\in\mathbb{N}$. If $\alpha+\beta$ is odd we have $I_{\alpha,\beta}=0$ and if $\alpha+\beta$ is even, it holds true for all $s_1,s_2\in\mathbb{R}$ that*

i) $I_{1,1}(s_1,s_2)=2(4\pi)^{-1/2}(1-s_1)s_2$;
ii) $I_{\alpha,\beta}(s_1,s_2)=2(1-s_1)s_2\left[2(\alpha-1)(\beta-1)(s_1-s_2)I_{\alpha-2,\beta-2}(s_1,s_2)+(\alpha+\beta-1)I_{\alpha-1,\beta-1}(s_1,s_2)\right]$;
iii) $I_{\alpha,\beta}(s_1,s_2)=2(1-s_1)\left[(\alpha-1)s_1I_{\alpha-2,\beta}(s_1,s_2)+\beta s_2I_{\alpha-1,\beta-1}(s_1,s_2)\right]$;
iv) $I_{\alpha,\beta}(s_1,s_2)=2(1-s_1)\left[(\alpha+\beta-1)s_1I_{\alpha-2,\beta}(s_1,s_2)-2\beta(\beta-1)s_2(s_1-s_2)I_{\alpha-2,\beta-2}(s_1,s_2)\right]$;
v) $I_{2\alpha,0}(s_1,s_2)=(4\pi)^{-1/2}(2\alpha)!/(\alpha!)s_1^\alpha(1-s_1)^\alpha$;
vi) $I_{0,2\alpha}(s_1,s_2)=(4\pi)^{-1/2}(2\alpha)!/(\alpha!)s_2^\alpha(1-s_2)^\alpha$.

Proof. a) In light of the basic identity

$$zg(t,z)=-2t\partial_z g(t,z),\ t>0,\ z\in\mathbb{R}, \tag{4.3}$$

we have

$$\begin{aligned}
&\int_{\mathbb{R}}\int_{\mathbb{R}} xyg(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy\\
=\ &-2(1-s_1)\int_{\mathbb{R}}\int_{\mathbb{R}} y\partial_x g(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy\\
=\ &2(1-s_1)\int_{\mathbb{R}}\int_{\mathbb{R}} yg(1-s_1,x)\partial_x g(s_1-s_2,x-y)g(s_2,y)dxdy,
\end{aligned}$$

by integrating by parts. Thus, applying (4.3) once more, we obtain that

$$\begin{aligned}
&\int_{\mathbb{R}}\int_{\mathbb{R}} xyg(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy\\
=\ &-2(1-s_1)\int_{\mathbb{R}}\int_{\mathbb{R}} yg(1-s_1,x)\partial_y g(s_1-s_2,x-y)g(s_2,y)dxdy\\
=\ &2(1-s_1)\int_{\mathbb{R}}\int_{\mathbb{R}} yg(1-s_1,x)g(s_1-s_2,x-y)\partial_y g(s_2,y)dxdy+2(1-s_1)(4\pi)^{-1/2}\\
=\ &2(1-s_1)\int_{\mathbb{R}} yg(1-s_2,y)\partial_y g(s_2,y)dy+2(1-s_1)(4\pi)^{-1/2}, \qquad (4.4)
\end{aligned}$$

with the help of the reproducing property. On the other hand, an integration by parts gives

$$\begin{aligned}
\int_{\mathbb{R}} yg(1-s_2,y)\partial_y g(s_2,y)dy &= -\int_{\mathbb{R}} g(1-s_2,y)g(s_2,y)dy-\int_{\mathbb{R}} y\partial_y g(1-s_2,y)g(s_2,y)dy\\
&= -(4\pi)^{-1/2}-\frac{s_2}{1-s_2}\int_{\mathbb{R}} yg(1-s_2,y)\partial_y g(s_2,y)dy,
\end{aligned}$$

and we get that $\int_{\mathbb{R}} yg(1-s_2,y)\partial_y g(s_2,y)dy = -(4\pi)^{-1/2}(1-s_2)$. Thus Part i) follows from this and (4.4).
b) Applying (4.3) with $z=x$ and $t=1-s_1$ we find that

$$\begin{aligned} I_{\alpha,\beta}(s_1,s_2) &= -2(1-s_1)\int_{\mathbb{R}}\int_{\mathbb{R}} x^{\alpha-1}y^{\beta}\partial_x g(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy \\ &= 2(\alpha-1)(1-s_1)\int_{\mathbb{R}}\int_{\mathbb{R}} x^{\alpha-2}y^{\beta} g(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy \\ &\quad -\frac{2(1-s_1)}{2(s_1-s_2)}\int_{\mathbb{R}}\int_{\mathbb{R}} x^{\alpha-1}y^{\beta}(x-y) g(1-s_1,x)g(s_1-s_2,x-y)g(s_2,y)dxdy, \end{aligned}$$

by integrating by parts wrt x, so we get

$$(1-s_2)I_{\alpha,\beta}(s_1,s_2) = 2(\alpha-1)(1-s_1)(s_1-s_2)I_{\alpha-2,\beta}(s_1,s_2) + (1-s_1)I_{\alpha-1,\beta+1}(s_1,s_2). \tag{4.5}$$

Doing the same with $z=y$ and $t=s_2$ we obtain that

$$s_1 I_{\alpha,\beta}(s_1,s_2) = 2(\beta-1)(s_1-s_2)s_2 I_{\alpha,\beta-2}(s_1,s_2) + s_2 I_{\alpha+1,\beta-1}(s_1,s_2). \tag{4.6}$$

Thus, upon successively substituting $(\alpha-1,\beta+1)$ and $(\alpha-2,\beta)$ for (α,β) in (4.6), we find that

$$s_1 I_{\alpha-1,\beta+1}(s_1,s_2) = 2\beta s_2(s_1-s_2)I_{\alpha-1,\beta-1}(s_1,s_2) + s_2 I_{\alpha,\beta}(s_1,s_2) \tag{4.7}$$

and

$$s_1 I_{\alpha-2,\beta}(s_1,s_2) = 2(\beta-1)(s_1-s_2)I_{\alpha-2,\beta-2}(s_1,s_2) + s_2 I_{\alpha-1,\beta-1}(s_1,s_2). \tag{4.8}$$

Plugging (4.7)-(4.8) in (4.5) we end up getting part ii). Further we obtain part iii) by following the same lines as in the derivation of part ii), and part iv) is a direct consequence of parts ii) and iii).
c) Arguing as in the derivation of part i) in a), we establish for any $\alpha \geq 2$ that

$$I_{\alpha,0}(s_1,s_2) = 2(\alpha-1)s_1(1-s_1)I_{\alpha-2,0}(s_1,s_2).$$

This and the obvious identity $I_{0,0}(s_1,s_2) = (4\pi)^{-1/2}$ yields part v) upon proceeding by induction on α. Finally, part vi) follows from part v) upon noticing from (4.2) that $I_{0,\alpha}(s_1,s_2) = I_{\alpha,0}(1-s_2,1-s_1)$. □

Further, for all $\alpha = (\alpha_k)_{1\leq k\leq n}$ and $\beta = (\beta_k)_{1\leq k\leq n}$ in $\mathbb{N}^n$, we put

$$\mathscr{I}(\alpha,\beta) = \int_0^1\int_0^{s_1}\left(\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} x^{\alpha}y^{\beta}G(1-s_1,x)G(s_1-s_2,x-y)G(s_2,y)dxdy\right)ds_1 ds_2, \tag{4.9}$$

and establish the:

Lemma 4.3. *For each $\alpha = (\alpha_k)_{1\leq k\leq n}$ and $\beta = (\beta_k)_{1\leq k\leq n}$ in $\mathbb{N}^n$ we have:*

i) $\mathscr{I}(\alpha,\beta) = \int_0^1\int_0^{s_1}\prod_{k=1}^n I_{\alpha_k,\beta_k}(s_1,s_2)ds_1 ds_2$.
ii) $\mathscr{J}(\alpha,\beta) = \mathscr{J}(\beta,\alpha)$.
iii) $\mathscr{J}(\alpha,\beta) = 0$ *if any of the sums* $\alpha_k+\beta_k$ *for* $1\leq k\leq n$*, is odd.*

Proof. Part i) follows readily from the identity $G(s,z) = \prod_{k=1}^n g(s,z_k)$ arising from (2.15) for all $s\in\mathbb{R}^*$ and all $z=(z_k)_{1\leq k\leq n}\in\mathbb{R}^n$, and from the very definitions (4.2) and (4.9). Next, part ii) is a direct consequence of the first assertion of Lemma 4.1, while part iii) follows from the third point of Lemma 4.1. □

5. Proof of Theorem 1.1

We start by establishing two identities which are useful for the proof of Theorem 1.1.

5.1. **Two useful identities.** They are collected in the following:

Proposition 5.1. *Let $V \in C_0^\infty(\Omega)$ be real-valued and assume that $\mathbf{a} = \mathbf{I}$. Then, with reference to the definitions* (3.9)-(3.10), *we have*

$$(4\pi)^{n/2} \sum_{|\alpha^2|=2} c_{\alpha^2} P_{\alpha^2}(V) = -\frac{1}{12} \int_\Omega |\nabla V|^2 dx \tag{5.1}$$

and

$$(4\pi)^{n/2} \sum_{|\alpha^2|=4} c_{\alpha^2} P_{\alpha^2}(V) = \frac{1}{120} \sum_k \int_\Omega \left(\partial_{kk}^2 V\right)^2 dx + \frac{13}{360} \sum_{k\neq\ell} \int_\Omega \left(\partial_{k\ell}^2 V\right)^2 dx. \tag{5.2}$$

Proof. Since

$$c_{\alpha^2} = \frac{\mathscr{I}(\alpha_1^2, \alpha_2^2)}{\alpha^2!},\ \alpha^2 = (\alpha_1^2, \alpha_2^2), \tag{5.3}$$

by (3.8) and (4.9), we know from the two last points in Lemma 4.3 that

$$c_{\alpha^2} = 0 \text{ if the sum } (\alpha_1^2)_k + (\alpha_2^2)_k \text{ is odd for any } k \in \{1, \ldots, n\}, \tag{5.4}$$

and

$$c_{\alpha^2} = c_{\widetilde{\alpha}^2} \text{ for } \widetilde{\alpha}^2 = (\alpha_2^2, \alpha_1^2). \tag{5.5}$$

We first compute $\sum_{|\alpha^2|=4} c_{\alpha^2} P_{\alpha^2}(V)$. In what follows we note $(0, \ldots, \underset{k}{\beta}, \ldots, 0)$, $1 \leq k \leq n$, $\beta \in \mathbb{R}$, the vector $(\beta_j)_{1\leq j\leq n} \in \mathbb{R}^n$ such that $\beta_j = 0$ for all $1 \leq j \neq k \leq n$ and $\beta_k = \beta$. In view of (5.3) we apply the first point in Lemma 4.3 for $\alpha^2 = ((0, \ldots \underset{k}{2}, \ldots 0), (0, \ldots, 0))$, $1 \leq k \leq n$, getting

$$c_{\alpha^2} = \int_0^1 \int_0^{s_1} I_{0,0}(s_1, s_2)^{n-1} I_{2,0}(s_1, s_2) ds_1 ds_2 = \frac{(4\pi)^{-(n-1)/2}}{2} \int_0^1 \int_0^{s_1} I_{2,0}(s_1, s_2) ds_1 ds_2 = \frac{(4\pi)^{-n/2}}{12}, \tag{5.6}$$

with the aid of part v) in Lemma 4.2. Similarly, for $\alpha^2 = ((0, \ldots, \underset{k}{1}, \ldots, 0), (0, \ldots, \underset{k}{1}, \ldots, 0))$, $1 \leq k \leq n$, we use the first part of Lemma 4.2 and obtain that

$$c_{\alpha^2} = (4\pi)^{-(n-1)/2} \int_0^1 \int_0^{s_1} I_{1,1}(s_1, s_2) ds_1 ds_2 = \frac{(4\pi)^{-n/2}}{12}. \tag{5.7}$$

In light of (5.4)-(5.5) we deduce from (5.6)-(5.7) that

$$\sum_{|\alpha^2|=2} c_{\alpha^2} P_{\alpha^2}(V) = \frac{1}{6} (4\pi)^{-n/2} \int_\Omega \Delta V V dx + \frac{1}{12} (4\pi)^{-n/2} \int_\Omega |\nabla V|^2 dx.$$

Taking into account that $\int_\Omega \Delta V V dx = -\int_\Omega |\nabla V|^2 dx$, we obtain (5.1) from the above line.

We now compute $\sum_{|\alpha^2|=4} c_{\alpha^2} P_{\alpha^2}(V)$. As a preamble we first invoke Lemma 4.2 and get simultaneously

$$I_{2,2}(s_1, s_2) = 2(1 - s_1)[s_1 I_{0,2}(s_1, s_2) + 2s_2 I_{1,1}(s_1, s_2)] = 4(4\pi)^{-1/2}(1 - s_1)s_2[s_1(1 - s_2) + 2(1 - s_1)s_2], \tag{5.8}$$

and

$$I_{3,1}(s_1, s_2) = 2(1 - s_1)[2s_1 I_{1,1}(s_1, s_2) + s_2 I_{2,0}(s_1, s_2)] = 12(4\pi)^{-1/2}(1 - s_1)^2 s_1 s_2, \tag{5.9}$$

from part iii), and

$$I_{4,0}(s_1, s_2) = 12(4\pi)^{-1/2} s_1^2 (1 - s_1)^2, \tag{5.10}$$

from part v). Thus, for all $k \in \{1, \ldots, n\}$ it follows from the first part of Lemma 4.3 and (5.10) upon taking $\alpha^2 = ((0, \ldots, \underset{k}{4}, \ldots, 0), (0, \ldots, 0))$ in (5.3) that

$$c_{\alpha^2} = \frac{(4\pi)^{-(n-1)/2}}{4!} \int_0^1 \int_0^{s_1} I_{4,0}(s_1, s_2) ds_1 ds_2 = \frac{1}{120} (4\pi)^{-n/2}. \tag{5.11}$$

Further, choosing $\alpha^2=((0,\dots,\underset{k}{3},\dots,0),(0,\dots,\underset{k}{1},\dots,0))$ we deduce in the same way from (5.9) that,

$$c_{\alpha^2}=\frac{(4\pi)^{-(n-1)/2}}{3!}\int_0^1\int_0^{s_1}I_{3,1}(s_1,s_2)ds_1ds_2=\frac{1}{60}(4\pi)^{-n/2}, \tag{5.12}$$

and with $\alpha^2=((0,\dots,\underset{k}{2},\dots,0),(0,\dots,\underset{k}{2},\dots,0))$, we get from (5.8) that

$$c_{\alpha^2}=\frac{(4\pi)^{-(n-1)/2}}{2!2!}\int_0^1\int_0^{s_1}I_{2,2}(s_1,s_2)ds_1ds_2=\frac{1}{40}(4\pi)^{-n/2}. \tag{5.13}$$

Finally, upon taking $\alpha^2=((0,\dots,\underset{k}{2},\dots,0),(0,\dots,\underset{\ell}{2},\dots,0))$ in (5.3), for $1\le k\neq \ell\le n$, we derive from the two last parts of Lemma 4.2 that

$$c_{\alpha^2}=\frac{(4\pi)^{-(n-2)/2}}{2!2!}\int_0^1\int_0^{s_1}I_{2,0}(s_1,s_2)I_{0,2}(s_1,s_2)ds_1ds_2=\frac{1}{72}(4\pi)^{-n/2}, \tag{5.14}$$

while the choice $\alpha^2=((0,\dots,\underset{k}{1},\dots,\underset{\ell}{1},\dots 0),(0,\dots,\underset{k}{1},\dots,\underset{\ell}{1},\dots,0))$ leads to

$$c_{\alpha^2}=(4\pi)^{-(n-2)/2}\int_0^1\int_0^{s_1}I_{1,1}(s_1,s_2)^2ds_1ds_2=\frac{1}{45}(4\pi)^{-n/2}, \tag{5.15}$$

with the aid of the first part. Putting (5.11)–(5.15) together and recalling (5.4)-(5.5) we end up getting (5.2). $\square$

Armed with Proposition 5.1 we are now in position to prove Theorem 1.1.

5.2. **Completion of the proof.** By applying the reproducing property (2.5) to the kernel G, defined in (2.15), we derive from (3.8) for all $j\ge 1$ that

$$c_{\alpha^j=0}=\int_{(\mathbb{R}^n)^n}\int_0^1\int_0^{s_1}\dots\int_0^{s_{j-1}}G(1-s_1,w_1)\prod_{k=1}^{j}G(s_k-s_{k+1},w_k-w_{k+1})dw^jds^j=\frac{(4\pi)^{-n/2}}{j!}, \tag{5.16}$$

where $s_{j+1}=w_{j+1}=0$. In light of (3.10), (5.16) then yields that

$$\mathcal{P}_2(V)=-c_{\alpha^1=0}P_{\alpha^1=0}(V)=-(4\pi)^{-n/2}\int_\Omega V\,dx. \tag{5.17}$$

Next, bearing in mind that the potential V is compactly supported in Ω, we notice from (3.9) that

$$P_{\alpha^1}(V)=\int_\Omega \partial^{\alpha^1}V(x)dx=0,\ |\alpha^1|\ge 1. \tag{5.18}$$

As a consequence we have

$$\mathcal{P}_4(V)=c_{\alpha^2=0}P_{\alpha^2=0}(V)-\sum_{|\alpha^1|=2}c_{\alpha^1}P_{\alpha^1}(V)=\frac{(4\pi)^{-n/2}}{2}\int_\Omega V(x)^2dx. \tag{5.19}$$

Further, as $\mathcal{P}_6=-c_{\alpha^3=0}P_{\alpha^3=0}(V)+\sum_{|\alpha^2|=2}c_{\alpha^2}P_{\alpha^2}(V)-\sum_{|\alpha^1|=4}c_{\alpha^1}P_{\alpha^1}(V)$, it follows from (5.1) and (5.16) that

$$\mathcal{P}_6(V)=-\frac{(4\pi)^{-n/2}}{6}\left(\frac{1}{2}\int_\Omega|\nabla V(x)|^2dx+\int_\Omega V(x)^2dx\right). \tag{5.20}$$

Finally, since $\int_\Omega \partial_{km}^2V(x)V(x)^2dx=-2\int_\Omega\partial_kV(x)\partial_mV(x)V(x)dx$ for all natural numbers $1\le k,m\le n$, by integrating by parts, we see that there is a constant C_n depending only on n such that we have

$$\left|\sum_{|\alpha^3|=2}c_{\alpha^3}P_{\alpha^3}(V)\right|\le C_n\|V\|_\infty\int_\Omega|\nabla V(x)|^2dx,$$

according to (3.9). This, together with the identity

$$\mathcal{P}_8(V) = c_{\alpha^4=0}P_{\alpha^4=0}(V) - \sum_{|\alpha^3|=2} c_{\alpha^3}P_{\alpha^3}(V) + \sum_{|\alpha^2|=4} c_{\alpha^2}P_{\alpha^2}(V) - \sum_{|\alpha^1|=6} c_{\alpha^1}P_{\alpha^1}(V),$$

arising from (3.10), and (5.2), (5.16), (5.18), then yield

$$\sum_{|\gamma|=2}\int_\Omega |\partial^\gamma V(x)|^2dx + \int_\Omega V(x)^4dx \le C_n'\left(|\mathcal{P}_8(V)| + \|V\|_\infty \int_\Omega |\nabla V(x)|^2dx.\right), \tag{5.21}$$

for some constant $C_n' > 0$ depending only on n. In light of (5.20)-(5.21) the set $\mathrm{Is}(V_0)\cap\mathcal{B}$ is thus bounded in $H^2(\Omega)$ from Corollary 3.1.

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