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HEAT TRACES AND EXISTENCE OF SCATTERING RESONANCES FOR BOUNDED POTENTIALS

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Abstract. We show that, in odd dimensions, any real valued, bounded potential of compact support has at least one scattering resonance. In dimensions 3 and greater this was previously known only for sufficiently smooth potentials. The proof is based on an inverse result, which shows that the regularized trace of the associated heat kernel admits a full asymptotic expansion if and only if the potential is smooth.

1. Introduction and statements of results

Let $V \in L^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R})$ be a bounded, compactly supported, real valued potential and let $n \geqslant 3$ be odd. We consider the Schrödinger operator,

$$P_V = -\Delta + V(x), \tag{1.1}$$

and ask the question whether P_V always (for $V \neq 0$) has infinitely many scattering resonances. Scattering resonances are defined as poles of the meromorphic continuation of the resolvent

$$R_V(\lambda) := (-\Delta + V - \lambda^2)^{-1}, \quad n \text{ odd}, \tag{1.2}$$

from $\Im\lambda \gg 1$ to $\lambda \in \mathbb{C}$. In particular, we count eigenvalues as resonances. The multiplicity of a resonance at $\lambda \neq 0$ is defined as

$$m_V(\lambda) = \operatorname{rank} \oint_\lambda R_V(\zeta) d\zeta, \tag{1.3}$$

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where the integral is over a circle around λ enclosing no other singularities of R_V than (possibly) λ – see [14, §3.2]. We set $m_V(\lambda) = 0$ if λ is not a resonance. At $\lambda = 0$ we put

$$m_V(0) = \frac{1}{2}\operatorname{rank}\oint_0 R_V(\zeta)d\zeta + \operatorname{rank}\oint_0 R_V(\zeta)2\zeta d\zeta. \tag{1.4}$$

If $m_V(0) = m \in \mathbb{N}$, then P_V has an eigenvalue of multiplicity m at 0. If $m_V(0) = m + \frac{1}{2}$, $m \in \mathbb{N}$, then in addition P_V has a zero resonance – see [14, §3.3], [18] and [19].

These poles have many interesting interpretations and in particular appear in expansions of solutions to the wave equation – see §2 and references given there. For n even the situation is more complicated as the meromorphic continuation has a logarithmic branch singularity at $\lambda = 0$ – see [10] and references given there. Here we prove that

Theorem 1.1. — *Suppose that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$ and that n is odd. Then the meromorphic continuation of the resolvent* (1.2),

$$R_V(\lambda) : L^2_{\mathrm{c}}(\mathbb{R}^n) \to L^2_{\mathrm{loc}}(\mathbb{R}^n), \quad \lambda \in \mathbb{C},$$

has at least one pole. If $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R}) \cap H^{\frac{n-3}{2}}(\mathbb{R}^n)$ then R_V has infinitely many poles.

For $V \in C^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$ existence of infinitely many resonances was proved by Melrose [22] for $n = 3$ and by Sá Barreto–Zworski [24] for all odd n. Soon afterwards quantitative statements about the counting function, $N(r)$, of resonances in $\{|\lambda| \leqslant r\}$ were obtained by Christiansen [5] and Sá Barreto [23]:

$$\limsup_{r\to\infty} \frac{N(r)}{r} > 0.$$

For potentials generic in $C^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{F})$ or $L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{F})$, $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$, Christiansen and Hislop [6],[9] proved a stronger statement

$$\limsup_{r\to\infty} \frac{\log N(r)}{\log r} = n. \tag{1.5}$$

This means that the upper bound $N(r) \leqslant Cr^n$ from [29] is optimal for generic complex or real valued potentials. The only case in which asymptotics $\sim r^n$ for *non-radial* potentials are known was provided by Dinh and Vu [12] who proved that a large class of L^∞ potentials supported in $B(0,1)$ has resonances satisfying a Weyl law.

A corollary of our argument is the following result, which was pointed out to us by Christiansen:

Theorem 1.2. — *Suppose that $V_j \in L^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R})$, $j = 1,2$ and n is odd. If, in the notation of* (1.3) *and* (1.4),

$$m_{V_1}(\lambda) = m_{V_2}(\lambda) \qquad \forall\, \lambda \in \mathbb{C}, \tag{1.6}$$

then for any $m \in \mathbb{N}$,

$$V_1 \in H^m(\mathbb{R}^n) \iff V_2 \in H^m(\mathbb{R}^n).$$

This is interesting because of the dearth of results on resonance inverse problems. It is known that resonances alone may not determine the potential uniquely – see Korotyav [20], [31] and also Autin [1], [8] where references to more general "isopolar" problems can be found. In the positive direction Datchev–Hezari [11] showed that in the semiclassical setting certain radial potentials are determined by the asymptotic behaviour of resonances. That paper contains further references to inverse problems for resonances.

To prove Theorem 1.1 we proceed by contradiction, as in [2], [22] and [24], and assume that there are no resonances. By a direct argument (Proposition 2.1) this implies that the scattering phase is a polynomial. This in turn implies (Proposition 2.2) that the heat trace has an asymptotic expansion. The main result of this note, Theorem 1.3 below, shows that this implies that $V \in C^\infty_{\rm c}(\mathbb{R}^n)$, and since it is real valued we obtain a contradiction by [22] and [24]. (We provide a direct argument of the contradiction in §2.) See §2.4 for why our arguments do not yield a contradiction for a finite number of resonances if $n \geqslant 5$ and $V \in L^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R})$.

Although we expect (1.5), or possible even $N(r) > r^n/C$ when $r \gg 1$, to be true for all non-zero real valued potentials, Christiansen [7] gave classes of examples of non-zero $V \in C^\infty_{\rm c}(\mathbb{R}^n;\mathbb{C})$ which have no resonances.

Our argument outlined above depends on the following, which is the principal new result of this paper.

Theorem 1.3. — *Suppose that P_V is given by* (1.1), *and $V \in L^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R})$, where $n \geqslant 1$ may be even or odd. If*

$$t^{\frac{n}{2}} \operatorname{tr}\left(e^{-tP_V} - e^{-tP_0}\right) \in C^\infty([0,\infty)) \tag{1.7}$$

then $V \in C^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R})$.

Theorem 1.3 is a direct consequence of a more precise result presented in Theorem 3.1 in §3. The study of heat expansions has a very long tradition going back to Kac, Berger and McKean–Singer – see [28],[15],[17] for more recent accounts and references. Theorem 1.3, although not surprising, seems to be new. However, closely related inverse results are well known. They concern recovering Sobolev norms from the coefficients of expansion of smooth potentials, and using those a priori bounds to prove compactness of sets of isospectral potentials – see Brüning [4] and Donnelly [13], and for the origins of that approach, McKean–van Moerbeke [21].

The paper is organized as follows. In §2 we review the scattering theory needed for the proofs of Theorems 1.1 and 1.2. For detailed arguments we refer to the original papers and to the on-line notes [14]. The section on the heat trace §3 is by contrast completely self-contained. Some aspects of the approach in §3 appear to be new, in particular the use of Gagliardo–Nirenberg inequalities in a bootstrap regularity scheme.

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2. Review of scattering theory

Here we recall various facts in scattering theory and show how Theorem 1.1 follows from Theorem 1.3.

2.1. The scattering matrix

The continued resolvent, $R_V(\lambda)$, given in (1.2) does not have any poles on $\mathbb{R}\setminus\{0\}$ – that is a well known consequence of the Rellich uniqueness theorem – see [14, §3.6]. This implies that, for $\lambda\in\mathbb{R}\setminus\{0\}$ and $\omega\in\mathbb{S}^{n-1}$, there exist (unique) solutions to

$$
\begin{gathered}
(P_V-\lambda^2)w(x,\lambda,\omega)=0, \quad w(x,\lambda,\omega)=e^{-i\lambda\langle x,\omega\rangle}+u(x,\lambda,\omega),\\
u(x,\lambda,\omega)=|x|^{-\frac{n-1}{2}}e^{i\lambda|x|}\left(b(\lambda,x/|x|,\omega)+\mathcal{O}(|x|^{-1})\right), \quad |x|\to\infty.
\end{gathered}
\tag{2.1}
$$

The *radiation pattern* $b(\lambda,\theta,\omega)$, is the observed field in a scattering experiment. The *scattering matrix*, $S_V(\lambda)$, can be defined using $b(\lambda,\theta,\omega)$. This definition is not the most intuitive, and we refer to [14, §3.7] for motivation. Here we define $S_V(\lambda): L^2(\mathbb{S}^{n-1})\to L^2(\mathbb{S}^{n-1})$ as

$$
\begin{gathered}
S_V(\lambda)f(\theta)=f(\theta)+\int_{\mathbb{S}^{n-1}}a(\lambda,\theta,\omega)f(\omega)d\omega,\\
a(\lambda,\theta,\omega):=(2\pi)^{-\frac{n-1}{2}}e^{\frac{\pi}{4}(n-1)i}\lambda^{\frac{n-1}{2}}b(\lambda,\theta,-\omega).
\end{gathered}
\tag{2.2}
$$

We also have the following useful representations of $a(\lambda,\theta,\omega)$:

(2.3)
$$\begin{aligned} a(\lambda,\theta,\omega) &= a_n\lambda^{n-2}\int_{\mathbb{R}^n} e^{-i\lambda\langle x,\theta\rangle}V(x)w(x,\lambda,-\omega)dx \\ &= a_n\lambda^{n-2}\int_{\mathbb{R}^n} e^{-i\lambda\langle x,\omega-\theta\rangle}V(x)(1-e^{-i\lambda\langle x,\omega\rangle})R_V(\lambda)(e^{\lambda\langle\bullet,\omega\rangle}V)(x)dx, \end{aligned}$$

where $a_n = (2\pi)^{-n+1}/2i$.

The scattering matrix is unitary for λ real, and from (2.3) we see that it continues meromorphically to all of $\mathbb{C}$. Hence we have

$$S_V(\lambda)^{-1} = S_V(\bar\lambda)^*, \quad \lambda\in\mathbb{C}. \tag{2.4}$$

Another symmetry comes from changing λ to $-\lambda$:

$$S_V(\lambda)^{-1} = JS_V(-\lambda)J, \quad Jf(\theta) := f(-\theta). \tag{2.5}$$

The operator $S_V(\lambda)-I$ is of trace class, and hence $\det S_V(\lambda)$ is well defined. The following result, see [14, §3.9] or [30], is important for the investigation of scattering resonances:

Proposition 2.1. — *Suppose that $V\in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$, where n is odd. Then $\det S_V(\lambda)$ is a meromorphic function of order n. More precisely,*

$$\det S_V(\lambda) = (-1)^m\left(\prod_{k=1}^K \frac{i\mu_k+\lambda}{i\mu_k-\lambda}\right)\frac{P(-\lambda)}{P(\lambda)}, \tag{2.6}$$

where $\mu_k\geqslant 0$, $-\mu_1^2 < -\mu_2^2 \leqslant \cdots \leqslant -\mu_K^2 \leqslant 0$ are the eigenvalues of P_V, included according to multiplicity, $P(\lambda)$ is entire and non-zero for $\Im\lambda\geqslant 0$, and

$$|P(\lambda)| \leqslant C_\varepsilon e^{C_\varepsilon r^{n+\varepsilon}}, \qquad \text{for any } \varepsilon>0. \tag{2.7}$$

The power m in (2.6) is the multiplicity of the zero resonance, $m=0$ or 1 for $n=1,3$ and $m=0$ for for $n\geqslant 5$; see [14, §3.3] and [19].

We make the following observation based on the second representation in (2.3):

$$\lambda \text{ is a pole of } \det S_V \implies \lambda \text{ is a pole of } S_V \implies \lambda \text{ is a pole of } R_V.$$

A more precise statement is possible (see [14, Theorem 3.42]) but we do not need it for Theorem 1.1. To show existence of poles of R_V we only need to show existence of poles of $\det S_V$.

2.2. A trace formula

The tool connecting the scattering matrix to the heat trace is the Birman–Krein trace formula. In §3 we will recall the argument showing that the operator $e^{-tP_V} - e^{-tP_0}$ is of trace class.

Proposition 2.2. — *Suppose that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$. Then, in the notation of Proposition 2.1,*

$$\operatorname{tr}(e^{-tP_V}-e^{-tP_0}) = \frac{1}{2\pi i}\int_0^\infty \operatorname{tr}\left(S_V(\lambda)^{-1}\partial_\lambda S_V(\lambda)\right)e^{-t\lambda^2}d\lambda + \sum_{k=1}^K e^{t\mu_k^2} + \tfrac{1}{2}m. \tag{2.8}$$

If $V \in C^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$, this is proved for $n = 3$ in [27], and for $n \geqslant 5$ in [16] and references given there. The proofs for $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$ can be found in [14, §3.8, §4.6].

Since $|\det S_V(\lambda)| = 1$ for $\lambda \in \mathbb{R}$ (which follows from (2.4), the unitarity of the scattering matrix) we can define the winding number of the scattering phase:

$$\sigma(\lambda) := \frac{1}{2\pi i}\log\det S_V(\lambda), \qquad \sigma'(\lambda) = \frac{1}{2\pi i}\operatorname{tr}\left(S_V(\lambda)^{-1}\partial_\lambda S_V(\lambda)\right), \quad \lambda \in \mathbb{R}.$$

In the case of $V \in C^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$, n odd, $\sigma(\lambda)$ admits a full asymptotic expansion for $\lambda \to \infty$, with only odd powers of λ except for the constant term. For proofs see [27], [16], [14, §3.7], and for less regular potentials but fewer expansion terms [18].

2.3. Proof of Theorem 1.1

If V has no resonances then Proposition 2.1 shows that

$$\det S_V(\lambda) = \frac{P(-\lambda)}{P(\lambda)},$$

where $P(\lambda)$ is an entire function with no zeros and of order n. This implies that $P(\lambda) = e^{G(\lambda)}$ where $G(\lambda)$ is a polynomial of degree at most n; see for instance [26, 8.24]. We then obtain the following, where we define the odd polynomial $g(\lambda) = (G(-\lambda) - G(\lambda))/(2\pi i)$,

$$\det S_V(\lambda) = e^{2\pi i g(\lambda)}, \qquad \sigma'(\lambda) = g'(\lambda).$$

The unitarity of $S_V(\lambda)$ for λ real shows that $g(\lambda)$ has real coefficients, $g(\lambda) = a_0\lambda^n + a_1\lambda^{n-2} + \cdots + a_{\frac{n-1}{2}}\lambda$. Hence,

$$\int_0^\infty \sigma'(\lambda)\,e^{-t\lambda^2}d\lambda = t^{-\frac{n}{2}}\sum_{j=0}^{\frac{n-1}{2}} a_j' t^j, \tag{2.9}$$

where $a_j' := a_j\Gamma(n/2 - j + 1)$.

We combine (2.9) with (2.8) to see that $t^{n/2}\operatorname{tr}(e^{-tP_V} - e^{-tP_0})$ has a full asymptotic expansion $\sum_{j=0}^{\infty} c_j t^j$ as $t \to 0+$. That means that the assumption of Theorem 1.3 is satisfied, and hence $V \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$. But the result of [24] (see also [14, §3.7]) then contradicts our assumption that V has no resonances: every nonzero potential in $C_c^\infty(\mathbb{R}^n;\mathbb{R})$ has to have infinitely many resonances.

Christiansen's argument [5] that there must be at least one resonance for nonzero $V \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$ is simple and elegant, and we reproduce it here. As above, absence of resonances would give $\sigma'(\lambda) = a_0'\lambda^{n-1} + a_1'\lambda^{n-3} + \cdots a_n'$. Comparison with the heat expansion shows that $a_2' = c_n \int V^2 \neq 0$. That immediately provides a contradiction in the case of $n = 3$. If $n \geqslant 5$ we use the representation (2.3):

$$\begin{aligned}\sigma'(\lambda) &= \operatorname{tr} S_V(\lambda)^* \partial_\lambda S_V(\lambda)\\ &= \int_{\mathbb{S}^{n-1}} \partial_\lambda a(\lambda,\theta,\theta)d\theta + \int_{\mathbb{S}^{n-1}}\int_{\mathbb{S}^{n-1}} \overline{a(\lambda,\omega,\theta)}\,\partial_\lambda a(\lambda,\omega,\theta)d\omega d\theta.\end{aligned}$$

Under the assumption that R_V is holomorphic, i.e. that it has no poles, (2.3) then shows that $\sigma'(\lambda) = \mathcal{O}(\lambda^{n-3})$ as $\lambda \to 0$. But this contradicts $a_2' \neq 0$, since that would imply a lower order of vanishing at $\lambda = 0$.

We now use Theorem 3.1 to show that if $V \in L_c^\infty(\mathbb{R}^n;\mathbb{R}) \cap H^{\frac{n-3}{2}}(\mathbb{R}^n)$, $V \neq 0$, then R_V has infinitely many poles. This is again seen by contradiction, by assuming that $\det S_V(\lambda)$ has only finitely many resonances. In that case, let $-\mu_1^2 < -\mu_2^2 \leqslant \cdots \leqslant -\mu_{K'}^2 < 0$, $\mu_k > 0$, denote the negative eigenvalues of P_V, and let $i\rho_j$, $\rho_j < 0$, $j = 1,\ldots,J_1$, $\lambda_j \neq -\bar\lambda_j$, $j = 1,\ldots,J_2$ the remaining finite set of resonances. Proposition 2.1 gives

$$\det S_V(\lambda) = (-1)^m e^{2\pi i g(\lambda)} \prod_{k=1}^{K'} \frac{i\mu_k + \lambda}{i\mu_k - \lambda} \prod_{j=1}^{J_1} \frac{i\rho_j + \lambda}{i\rho_j - \lambda} \prod_{j=1}^{J_2} \frac{\lambda_j + \lambda}{\lambda_j - \lambda}\frac{\bar\lambda_j - \lambda}{\bar\lambda_j + \lambda}.$$

Hence for $\lambda \in \mathbb{R}$,

$$\begin{aligned}\sigma'(\lambda) - g'(\lambda) = &-\frac{1}{\pi}\sum_{k=1}^{K'} \frac{\mu_k}{\lambda^2 + \mu_k^2} - \frac{1}{\pi}\sum_{j=1}^{J_1} \frac{\rho_j}{\lambda^2 + \rho_j^2}\\ &-\frac{1}{\pi}\sum_{j=1}^{J_2}\left(\frac{\Im\lambda_j}{|\lambda - \lambda_j|^2} + \frac{\Im\lambda_j}{|\lambda + \lambda_j|^2}\right),\end{aligned} \tag{2.10}$$

This yields the equality

$$\int_0^\infty (\sigma'(\lambda) - g'(\lambda))\,d\lambda = -\tfrac{1}{2}K' + \tfrac{1}{2}J_1 + J_2. \tag{2.11}$$

where $K' \leqslant K$ is the number of strictly negative eigenvalues. We compare this with Proposition 2.2 and the expansion given in Theorem 3.1: if $V \in L^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R}) \cap H^{\frac{n-3}{2}}(\mathbb{R}^n)$, then (3.1) shows that

$$\operatorname{tr}(e^{-tP_V} - e^{-tP_0}) = \sum_{k=1}^{\frac{n-1}{2}} c_k' \, t^{-\frac{n}{2}+k} + \mathcal{O}(t^{\frac12}).$$

In particular,

$$\operatorname{tr}(e^{-tP_V} - e^{-tP_0}) - \sum_{k=1}^{\frac{n-1}{2}} c_k' \, t^{-\frac{n}{2}+k} \to 0, \qquad t \to 0+\,. \tag{2.12}$$

Since the terms on the right hand side of (2.10) make bounded contributions, comparison with (2.8) shows that

$$\sum_{k=1}^{\frac{n-1}{2}} c_k' \, t^{-\frac{n}{2}+k} = \int_0^\infty g'(\lambda) e^{-t\lambda^2} dt.$$

Using (2.8) and (2.11) we obtain

$$\begin{aligned}\operatorname{tr}(e^{-tP_V} - e^{-tP_0}) - \sum_{k=1}^{\frac{n-1}{2}} c_k' \, t^{-\frac{n}{2}+k} &= \operatorname{tr}(e^{-tP_V} - e^{-tP_0}) - \int_0^\infty g'(\lambda) e^{-t\lambda^2} d\lambda \\ &= \int_0^\infty (\sigma'(\lambda) - g'(\lambda)) e^{-t\lambda^2} d\lambda + \sum_{k=1}^{K} e^{t\mu_k^2} + \tfrac12 m\,.\end{aligned}$$

Taking the limit as $t \to 0+$ we obtain

$$\int_0^\infty (\sigma'(\lambda) - g'(\lambda))\, d\lambda + K + \tfrac12 m \;=\; K - \tfrac12 K' + \tfrac12 m + \tfrac12 J_1 + J_2 > 0\,,$$

since there must be at least one pole. But this contradicts (2.12).

2.4. Why not infinitely many?

A frustrating aspect of the argument in §2.3 is that for $V \in L^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R})$, $n \geqslant 5$, it only shows existence of *one* resonance. The reason for that is the strong assumption in Theorem 1.3. If we allowed, for example, a unique (non-zero) resonance $\lambda_0 = i\rho_0$ (it has to be purely imaginary, as the symmetry $\lambda \mapsto -\bar\lambda$ would otherwise imply that there are two) then the factorization argument above would imply

$$\det S_V(\lambda) = e^{2\pi i g(\lambda)} \frac{i\rho_0 + \lambda}{i\rho_0 - \lambda}\,, \qquad \sigma'(\lambda) = g'(\lambda) - \frac{1}{\pi} \frac{\rho_0}{\lambda^2 + \rho_0^2}\,.$$

We now note that

$$\frac{1}{\pi}\int_0^\infty \frac{e^{-sr^2}}{1+r^2}\,dr \sim \tfrac{1}{2}e^s + s^{\frac{1}{2}}\sum_{j=0}^\infty b_j s^j, \quad s\to 0+\,. \tag{2.13}$$

To see (2.13), let $I(s) := (1/\pi)\int_0^\infty e^{-s(1+r^2)}/(1+r^2)dr$. Then the right hand side of (2.13) is $e^s I(s)$, while $\partial_s I(s) = -(1/\pi)\int_0^\infty e^{-s(1+r^2)}dr = \alpha e^{-s}/s^{\frac{1}{2}}$, $\alpha = 1/2\sqrt{\pi}$. Hence $I(s) = I(0) + \alpha\int_0^s e^{-s_1}s_1^{-\frac{1}{2}} \sim \frac{1}{2} + s^{\frac{1}{2}}\sum_{j=0}^\infty b_j' s^j$. Multiplying by e^s gives (2.13).

Inserting (2.13) into the trace formula (2.8), and noting that if $\rho_0 > 0$ we have an eigenvalue, gives

$$\operatorname{tr}(e^{-tP_V} - e^{-tP_0}) = t^{-n/2}\sum_{j=1}^\infty a_j t + \tfrac{1}{2}e^{t\rho_0^2},$$

and we *cannot* use Theorem 1.3 to conclude that V is smooth. The same problem arises if we assume there are two (or more) resonances, λ_0, $-\bar{\lambda}_0$.

The following simple example does not fit into our hypotheses, but it suggests a possible complication. Consider $n=1$ and $V=\delta_0$. Then there is only one resonance, at $\lambda = -2i$, and the heat trace has an expansion with both integers and half-integers.

2.5. Proof of Theorem 1.2

We again use the Birman–Krein formula (2.8) to see that, under the assumption that the eigenvalue and zero resonance contributions cancel,

$$\operatorname{tr}\left(e^{-tP_{V_1}} - e^{-tP_{V_2}}\right) = \frac{1}{2\pi i}\int_0^\infty \partial_\lambda \det\left(S_{V_2}(\lambda)^{-1}S_{V_1}(\lambda)\right)e^{-t\lambda^2}d\lambda.$$

The assumption (1.6) and [14, Theorem 3.42] show that $\det S_{V_j}(\lambda)$, $j=1,2$, have the same poles and zeros (with the same multiplicities). Arguing as in §2.3 we then see that

$$\det\left(S_{V_2}(\lambda)^{-1}S_{V_1}(\lambda)\right) = e^{2\pi i h(\lambda)}, \quad h(\lambda) = b_0\lambda^n + b_1\lambda^{n-2} + \cdots b_{\frac{n-1}{2}}\lambda.$$

Then as in (2.9) we see that

$$\operatorname{tr}\left(e^{-tP_{V_1}} - e^{-tP_{V_2}}\right) = t^{-n/2}\sum_{j=0}^{\frac{n-1}{2}} b_j' t^j, \quad b_j' = \frac{b_j}{\Gamma(n/2-j+1)}.$$

That means that (3.1) holds for V_1 if and only if it holds for V_2, and Theorem 1.2 follows from Theorem 3.1.

3. Heat trace expansions

For P_V as in (1.1) with $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{C})$, the operator $e^{-tP_V} - e^{-tP_0}$ is trace class for $t > 0$, and if $V \in C^\infty_{\mathrm{c}}(\mathbb{R}^n)$ then $\operatorname{tr}\big(e^{-tP_V} - e^{-tP_0}\big)$ admits a full asymptotic expansion as $t \to 0^+$; see for instance [3] and references given there.

Theorem 1.3 is a consequence of a converse result which gives a sharp relation between existence of a finite expansion for the trace, and a given finite order of Sobolev regularity for V, assuming that V is real-valued.

Theorem 3.1. — *Suppose that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$, and that for some $m \in \mathbb{N}$ one can write*

$$\operatorname{tr}\Big(e^{-tP_V} - e^{-tP_0}\Big) = (4\pi t)^{-\frac{n}{2}}\Big(c_1 t + c_2 t^2 + \cdots + c_{m+1}t^{m+1} + r_{m+2}(t)t^{m+2}\Big)\,, \tag{3.1}$$

where $|r_{m+2}(t)| \leqslant C$ for $0 < t \leqslant 1$. Then $V \in H^m(\mathbb{R}^n)$. Conversely, if $V \in H^m(\mathbb{R}^n)$ then (3.1) holds with such an $r_{m+2}(t)$, and $\lim_{t\to 0^+} r_{m+2}(t) = c_{m+2}$ exists.

The proof of Therem 3.1 begins by using iteration to expand the heat kernel for $P_V = -\Delta + V$. The formula is

$$e^{-tP_V} - e^{-tP_0} = \sum_{k=1}^{\infty} W_k(t)\,,$$

where

$$W_k(t) = \int_{0<s_1<\cdots<s_k<t} e^{-(t-s_k)P_0}\, V\, e^{-(s_k-s_{k-1})P_0}\, V\, \cdots \\ \times\, V\, e^{-(s_2-s_1)P_0}\, V\, e^{-s_1P_0} ds_1\cdots ds_k\,.$$

Convergence of the expansion in the L^2 operator norm follows from the bound $\|W_k(t)\|_{L^2\to L^2} \leqslant \|V\|^k_{L^\infty} t^k/k!$, which holds since for all s_j and t the integrand is L^2 bounded by $\|V\|^k_{L^\infty}$, and the volume of integration is $t^k/k!$.

We also have a bound on the trace class norm:

$$\|W_k(t)\|_{\mathcal{L}^1} \leqslant C^k\, k^{\frac{n}{2}}\, t^{k-\frac{n}{2}}/k!, \tag{3.2}$$

where n is the dimension. For this we use that the trace class is an ideal, so it suffices to show that one pair of successive terms in the product has $\mathcal{L}^1$ bound less than $C\, k^{\frac{n}{2}}\, t^{-\frac{n}{2}}$. We then observe that at least one of $t - s_k$, $s_{j+1}-s_j$ or s_1 is greater than t/k, and for that term we use the trace bound

$$\|e^{-sP_0}\chi\|_{\mathcal{L}^1} \leqslant C\, s^{-n/2}, \tag{3.3}$$

where $\chi \in C_c^\infty(\mathbb{R}^n)$ is chosen to be 1 on the support of V. To prove (3.3) we choose $\chi_1 \in C_c^\infty(\mathbb{R}^n)$ equal to 1 on $\operatorname{supp}\chi$. Then the explicit Schwartz kernel, $K_1(x,y)$ of $(1-\chi_1)e^{-sP_0}\chi$ satisfies $|\partial^\alpha K_1| \leqslant C_{\alpha,N} s^N(1+|x|+|y|)^{-N}$, for any α and N. Hence $\|(1-\chi_1)e^{sP_0}\chi\|_{\mathcal{L}^1} = \mathcal{O}(s^\infty)$. On the other hand, if $K_2(x,y)$ is the Schwartz kernel of $e^{-sP_0/2}\chi_1$ then $\iint |K_2(x,y)|^2 dxdy \leqslant Cs^{-n/2}$ which provides an estimate $\mathcal{O}(s^{-n/4})$ on the Hilbert–Schmidt norm. These two bounds give (3.3):

$$\begin{aligned}\|e^{-sP_0}\chi\|_{\mathcal{L}^1} &\leqslant C\|\chi_1 e^{-sP_0}\chi_1\|_{\mathcal{L}^1} + \|(1-\chi_1)e^{-sP_0}\chi\|_{\mathcal{L}^1} \\ &\leqslant C\|\chi_1 e^{-sP_0/2}\|^2_{\mathcal{L}^2} + C_N s^N \leqslant C\, s^{-n/2}.\end{aligned}$$

Using (3.2), we see that $e^{-tP_V} - e^{-tP_0}$ is of trace class for $t > 0$. The trace can be brought into the sum, and we write

$$\operatorname{tr}\Big(e^{-tP_V} - e^{-tP_0}\Big) = \sum_{k=1}^{\infty} \operatorname{tr}\big(W_k(t)\big)\,.$$

It is well known, and we include the proof, that

$$\operatorname{tr}\big(W_1(t)\big) = (4\pi t)^{-\frac{n}{2}}\, t \int V(y)\, dy\,,$$

which shows that $c_1 = \int V$, and the expansion (3.1) is equivalent to

$$\sum_{k=2}^{\infty} \operatorname{tr}\big(W_k(t)\big) = (4\pi t)^{-\frac{n}{2}} \Big(c_2 t^2 + \cdots + c_{m+1} t^{m+1} + r_{m+2}(t)\Big)\,.$$

Theorem 3.1 will then follow as a result of the following two propositions that concern the asymptotics of the individual terms $\operatorname{tr}\big(W_k(t)\big)$.

Proposition 3.2. — *If $V \in L_c^\infty(\mathbb{R}^n;\mathbb{R}) \cap H^m(\mathbb{R}^n)$, then one can write*

$$\operatorname{tr}\big(W_2(t)\big) = (4\pi t)^{-\frac{n}{2}} \Big(c_{2,2} t^2 + \cdots + c_{2,2+m} t^{2+m} + \varepsilon(t) t^{2+m}\Big)\,, \tag{3.4}$$

with $\lim_{t\to 0^+} \varepsilon(t) = 0$ and $c_{2,2+j} = a_j \||D|^j V\|_{L^2}$ for $0 \leqslant j \leqslant m$, for constants $a_j \neq 0$.

Conversely, assuming $V \in L_c^\infty(\mathbb{R}^n;\mathbb{R}) \cap H^{m-1}(\mathbb{R}^n)$, if one can write

$$\operatorname{tr}\big(W_2(t)\big) = (4\pi t)^{-\frac{n}{2}} \Big(c_{2,2} t^2 + \cdots + c_{2,1+m} t^{1+m} + r_{2,2+m}(t) t^{2+m}\Big)\,, \tag{3.5}$$

where $|r_{2,2+m}(t)| \leqslant C$ for $0 < t \leqslant 1$, then $V \in H^m(\mathbb{R}^n)$, and hence (3.4) holds.

Proposition 3.3. — *If $V \in L_c^\infty(\mathbb{R}^n;\mathbb{R}) \cap H^m(\mathbb{R}^n)$, then for $k \geqslant 3$ one can write*

$$\operatorname{tr}\big(W_k(t)\big) = (4\pi t)^{-\frac{n}{2}} \Big(c_{k,k} t^k + \cdots + c_{k,k+m-1} t^{k+m-1} + r_{k,k+m}(t) t^{k+m}\Big)\,, \tag{3.6}$$

where, for a constant C depending on k and m, for $0 \leqslant j \leqslant m$,

$$|c_{k,k+j}| \leqslant C \,\|V\|_{L^\infty}^{k-2} \|V\|_{H^j}^2 \,, \qquad \sup_{0<t<1} |r_{k,k+m}(t)| \leqslant C \,\|V\|_{L^\infty}^{k-2} \|V\|_{H^m}^2 \,.$$

The fact that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R}) \cap H^m(\mathbb{R}^n)$ implies existence of the asymptotic expansion (3.1) of order $m+2$ is an easy consequence of the above propositions. By the bound $\|W_k(t)\|_{\mathcal{L}^1} \leqslant C^k\, k^{\frac{n}{2}}\, t^{k-\frac{n}{2}}/k!$ we have that

$$\operatorname{tr} \sum_{k=m+3}^{\infty} W_k(t) \leqslant C\, t^{m+3-\frac{n}{2}} \,, \qquad 0 < t \leqslant 1 \,. \tag{3.7}$$

On the other hand, Propositions 3.2 and 3.3 show that

$$\operatorname{tr} \sum_{k=1}^{m+2} W_k(t) = (4\pi t)^{-\frac{n}{2}} \Big(c_1 t + c_2 t^2 + \cdots + c_{m+1} t^{m+1} + c_{m+2} t^{m+2} + \varepsilon(t) t^{m+2} \Big) \,,$$

where for $j \geqslant 2$ we have $c_j = \sum_{k=2}^{j} c_{k,j}$.

The other direction of Theorem 3.1, that existence of an asymptotic expansion implies regularity, is carried out by induction. Assume $m \geqslant 1$ and $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R}) \cap H^{m-1}(\mathbb{R}^n)$, which trivially holds when $m = 1$ since $L^\infty_{\mathrm{c}}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$. Assume (3.1) holds. By (3.7) this implies

$$\operatorname{tr} \sum_{k=2}^{m+2} W_k(t) = (4\pi t)^{-\frac{n}{2}} \Big(c_1 t + c_2 t^2 + \cdots + c_{m+1} t^{m+1} + r_{m+2}(t) t^{m+2} \Big) \,,$$

where $|r_{m+2}(t)| \leqslant C$.

By Proposition 3.3, since $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R}) \cap H^{m-1}(\mathbb{R}^n)$ the same relation holds for $\operatorname{tr} \sum_{k=3}^{m+2} W_k(t)$, with different coefficients which can be bounded in terms of L^∞ and H^j norm bounds for V with $j \leqslant m-1$. Hence the relation (3.5) holds, and we conclude $V \in H^m(\mathbb{R}^n)$.

3.1. The trace of $W_1(t)$.

We calculate the trace of $W_1(t)$ by integrating over the diagonal

$$\operatorname{tr}\big(W_1(t)\big) = (4\pi)^{-n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_0^t (t-s)^{-\frac{n}{2}} s^{-\frac{n}{2}} e^{-\frac{|x-y|^2}{4(t-s)}}\, V(y)\, e^{-\frac{|y-x|^2}{4s}}\, ds\, dx\, dy \,.$$

The integral dx is carried out

$$\int_{\mathbb{R}^n} e^{-\frac{|x-y|^2}{4} \frac{t}{(t-s)s}}\, dx = (4\pi)^{\frac{n}{2}} t^{-\frac{n}{2}} (t-s)^{\frac{n}{2}} s^{\frac{n}{2}}$$

leading to

$$\operatorname{tr}\big(W_1(t)\big) = (4\pi t)^{-\frac{n}{2}}\, t \int V(y)\, dy \,.$$

(From now on the integrals without integration limits will denote integrals over $\mathbb{R}^n$.)

3.2. The trace of $W_2(t)$.

Again we integrate over the diagonal to write $\operatorname{tr}\big(W_2(t)\big)$ as

$$(4\pi)^{-\frac{3n}{2}} \int_{0<r<s<t} (t-s)^{-\frac{n}{2}} (s-r)^{-\frac{n}{2}} r^{-\frac{n}{2}} e^{-\frac{|x-y|^2}{4(t-s)} - \frac{|y-z|^2}{4(s-r)} - \frac{|z-x|^2}{4r}} \times V(y)\, V(z)\, dr\, ds\, dx\, dy\, dz\,.$$

We let $u = t - s$ and $x_0 = \left(\frac{r}{r+u}\right) y + \left(\frac{u}{r+u}\right) z$ and carry out the integral over x by writing

$$\frac{|x-y|^2}{u} + \frac{|z-x|^2}{r} = \frac{r+u}{ru} |x - x_0|^2 + \frac{1}{r+u} |y-z|^2 \tag{3.8}$$

which expresses $\operatorname{tr}\big(W_2(t)\big)$ as

$$(4\pi)^{-n} \int_{\substack{r+u<t \\ 0<r,u}} (t-u-r)^{-\frac{n}{2}} (u+r)^{-\frac{n}{2}} e^{-\frac{|y-z|^2}{4}\left(\frac{1}{t-u-r} + \frac{1}{u+r}\right)} \times V(y)\, V(z)\, dr\, du\, dy\, dz\,.$$

Let $r = tv - u$, so $dr\, du = t\, dv\, du$, the integrand is then independent of u, the new limits are $0 < u < tv$, $0 < v < 1$, and we get

$$t^2 (4\pi t)^{-n} \int\int\int_0^1 (1-v)^{-\frac{n}{2}} v^{-\frac{n}{2}+1} e^{-\frac{|y-z|^2}{4t} \frac{1}{v(1-v)}} V(y)\, V(z)\, dv\, dy\, dz\,.$$

Since V is real, we can use the Plancherel theorem to write this as

$$t^2 (4\pi t)^{-\frac{n}{2}} \int_0^1 v \left((2\pi)^{-n} \int e^{-t(1-v)v|\xi|^2} \big|\widehat{V}(\xi)\big|^2 d\xi \right) dv\,.$$

By symmetry under $v \to 1 - v$ we can also write this as

$$\frac{1}{2} t^2 (4\pi t)^{-\frac{n}{2}} \int_0^1 \left((2\pi)^{-n} \int e^{-t(1-v)v|\xi|^2} \big|\widehat{V}(\xi)\big|^2 d\xi \right) dv\,.$$

The term in parentheses is continuous in t, and at $t = 0$ equals $\|V\|^2_{L^2}$, so

$$\operatorname{tr}\big(W_2(t)\big) = \frac{1}{2} t^2 (4\pi t)^{-\frac{n}{2}} \left(\|V\|^2_{L^2} + \varepsilon(t) \right), \qquad \lim_{t\to 0^+} \varepsilon(t) = 0\,. \tag{3.9}$$

This settles the case $m = 0$ of Theorem 3.1 which, since $L^\infty_{\rm c}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$, is nontrivial only for the existence of the expansion (3.1) for $m = 0$. It also shows that we can recover $\|V\|_{L^2}$ from $\lim_{t\to 0^+} r_2(t)$.

3.3. Proof of Proposition 3.2

First consider the case $m = 1$, and suppose that we have an expansion

$$\operatorname{tr}\big(W_2(t)\big) = (4\pi t)^{-\frac{n}{2}}\left(c_2\, t^2 + \mathcal{O}(t^3)\right), \quad t \leqslant 1\,.$$

From (3.9) we must have $c_2 = \frac{1}{2}\|V\|_{L^2}^2$. This leads to the estimate

$$\int_0^1 \int \left(\frac{1 - e^{-t(1-v)v|\xi|^2}}{t}\right) \big|\widehat{V}(\xi)\big|^2\, d\xi\, dv \leqslant C\,, \qquad 0 < t \leqslant 1\,.$$

The integrand is positive, so by Fatou's lemma we get

$$\left(\int_0^1 (1-v)v\, dv\right) \int |\xi|^2 \big|\widehat{V}(\xi)\big|^2\, d\xi \leqslant C\,,$$

implying that $V \in H^1(\mathbb{R}^n)$. Conversely, if $V \in H^1(\mathbb{R}^n) \cap L^\infty_{\mathrm{c}}(\mathbb{R}^n;\mathbb{R})$ we would get such an expansion by dominated convergence.

To consider higher values of m, write

$$e^{-s} \;=\; \sum_{j=0}^{m-1} \frac{(-1)^j}{j!}\, s^j \;+\; r_m(s)\, \frac{(-1)^m}{m!}\, s^m\,, \tag{3.10}$$

where $r_m(s)$ is a smooth function, and by the Lagrange form for the remainder,

$$0 \leqslant r_m(s) \leqslant 1 \quad \text{if} \quad s \geqslant 0\,, \qquad r_m(0) = 1\,, \qquad \partial_s r_m(0) = \frac{-1}{m+1}\,. \tag{3.11}$$

Now suppose that $V \in H^m(\mathbb{R}^n)$ for some $m \geqslant 1$. Then we can expand

$$\begin{aligned} &\int_0^1 \left(\int e^{-t(1-v)v|\xi|^2}\, \big|\widehat{V}(\xi)\big|^2\, d\xi\right) dv \\ &\qquad = \sum_{j=0}^{m-1} \left(\frac{1}{j!}\int_0^1 (1-v)^j v^j\, dv\right)\left(\int |\xi|^{2j}\, \big|\widehat{V}(\xi)\big|^2\, d\xi\right) t^j \\ &\quad + \frac{(-1)^m}{m!}\left(\int_0^1 \int r_m\big(t(1-v)v|\xi|^2\big)(1-v)^m v^m\, |\xi|^{2m}\big|\widehat{V}(\xi)\big|^2\, d\xi\, dv\right) t^m\,. \end{aligned}$$

The coefficient of t^m is continuous in t, and converges to $a_m\, \||D|^m V\|_{L^2}^2$ as $t \to 0$, where $a_m \neq 0$. Thus, if we can write

$$\operatorname{tr}\big(W_2(t)\big) = (4\pi t)^{-\frac{n}{2}}\left(\sum_{j=0}^{m} c_j\, t^j + \mathcal{O}\big(t^{m+1}\big)\right), \quad t \leqslant 1\,,$$

then $c_j = a_j \||D|^j V\|_{L^2}^2$ for $0 \leqslant j \leqslant m$, and in addition we have uniform bounds for $0 < t \leqslant 1$

$$\int_0^1 \int \left(\frac{1 - r_m\big(t(1-v)v|\xi|^2\big)}{t}\right)(1-v)^m v^m |\xi|^{2m}\big|\widehat{V}(\xi)\big|^2\, d\xi\, dv \leqslant C\,.$$

Then by Fatou's lemma and (3.11) we get

$$\frac{1}{m+1}\left(\int_0^1 (1-v)^{m+1}v^{m+1}\,dv\right)\left(\int |\xi|^{2(m+1)}\big|\widehat{V}(\xi)\big|^2\,d\xi\right) \leqslant C\,,$$

so necessarily $V \in H^{m+1}(\mathbb{R}^n)$, completing the proof of Proposition 3.2.

3.4. The trace of $W_k(t)$ for $k \geqslant 3$.

To estimate products of derivatives, we will use the following particular case of the Gagliardo–Nirenberg inequalities.

LEMMA 3.4. — *Suppose $\{\alpha_j\}_{j=1}^k$ are multi-indices, with $|\alpha_j| \leqslant m$, and $\sum_j |\alpha_j| = 2m$. If $u \in L^\infty(\mathbb{R}^n) \cap H^m(\mathbb{R}^n)$, then for a constant C depending only on n and m,*

$$\Big\|\prod_{j=1}^k (\partial^{\alpha_j} u_j)\Big\|_{L^1} \leqslant C\left(\sum_{j=1}^k \|u_j\|_{L^\infty}\right)^{k-2}\left(\sum_{j=1}^k \|D^m u_j\|_{L^2}\right)^2.$$

Proof. — We use the following bound [25, (3.17) in §13.3]. Assuming $u \in L^\infty(\mathbb{R}^n) \cap H^m(\mathbb{R}^n)$,

$$\|\partial^{\alpha_j} u_j\|_{L^{\frac{2m}{|\alpha_j|}}} \leqslant C\, \|u_j\|_{L^\infty}^{1-\frac{|\alpha_j|}{m}}\, \|D^m u_j\|_{L^2}^{\frac{|\alpha_j|}{m}}\,.$$

The desired estimate then follows from Hölder's inequality. □

We now write $\mathrm{tr}\big(W_k(t)\big)$ for $t > 0$ as an integral

$$\int_{0<s_1<\cdots<s_k<t} \frac{e^{-\frac{|x-y_k|^2}{4(t-s_k)}-\frac{|y_k-y_{k-1}|^2}{4(s_k-s_{k-1})}\cdots-\frac{|y_1-x|^2}{4s_1}}\, V(y_k)\cdots V(y_1)}{(4\pi)^{\frac{n}{2}(k+1)}(t-s_k)^{\frac{n}{2}}\cdots(s_2-s_1)^{\frac{n}{2}}(s_1)^{\frac{n}{2}}} \times dy_1\cdots dy_k\, ds_1\cdots ds_k\, dx\,.$$

After integrating over x, and letting $s_j = tr_j$, then letting $\Sigma \subset \mathbb{R}^k$ denote the set $\{r \in \mathbb{R}^k \,:\, 0 < r_1 < \cdots < r_k < 1\}$, we obtain

$$t^k \int_\Sigma \int_{(\mathbb{R}^n)^k} \frac{e^{-\frac{|y_k-y_{k-1}|^2}{4t(r_k-r_{k-1})}\cdots-\frac{|y_2-y_1|^2}{4t(r_2-r_1)}-\frac{|y_1-y_k|^2}{4t(1+r_1-r_k)}}\, V(y_k)\cdots V(y_1)}{(4\pi t)^{\frac{n}{2}k}(r_k-r_{k-1})^{\frac{n}{2}}\cdots(r_2-r_1)^{\frac{n}{2}}(1+r_1-r_k)^{\frac{n}{2}}}\, dy\, dr\,.$$

To analyse this, we introduce variables $u_1 = y_1$, and $u_j = y_j - y_1$ for $2 \leqslant j \leqslant k$. Then $du_1 \wedge \cdots \wedge du_k = dy_1 \wedge \cdots \wedge dy_k$, so the formula for $\mathrm{tr}\big(W_k(t)\big)$ becomes

$$\frac{t^k}{(4\pi t)^{\frac{n}{2}}} \int_\Sigma \int_{(\mathbb{R}^n)^k} G_{r,t}(u')\; V(u_1+u_k)\cdots V(u_1+u_2)V(u_1)\, du\, dr\,, \tag{3.12}$$

where $G_{r,t}(u')$ is the Gaussian function of $u' = (u_2, \dots, u_k) \in (\mathbb{R}^n)^{k-1}$

$$G_{r,t}(u_2, \dots, u_k) = \frac{e^{-\frac{1}{4t}\left(\frac{|u_k|^2}{1+r_1-r_k} + \frac{|u_k-u_{k-1}|^2}{r_k-r_{k-1}} \cdots + \frac{|u_3-u_2|^2}{r_3-r_2} + \frac{|u_2|^2}{r_2-r_1}\right)}}{(4\pi t)^{\frac{n}{2}(k-1)}(1+r_1-r_k)^{\frac{n}{2}}(r_k-r_{k-1})^{\frac{n}{2}} \cdots (r_2-r_1)^{\frac{n}{2}}}\,.$$

Applying successively the following equality, which is a special case of (3.8),

$$\begin{aligned} &\frac{|u_{j+1}-u_j|^2}{r_{j+1}-r_j} + \frac{|u_j|^2}{r_j - r_1} \\ &\quad = \frac{r_{j+1}-r_1}{(r_{j+1}-r_j)(r_j-r_1)} \left| u_j - \frac{r_j - r_1}{r_{j+1}-r_1}\, u_{j+1} \right|^2 + \frac{1}{r_{j+1}-r_1}\, |u_{j+1}|^2 \end{aligned}$$

we can write the quadratic term in the exponent of $G_{r,t}$ as

$$\frac{|u_k|^2}{(1+r_1-r_k)(r_k-r_1)} + \sum_{j=2}^{k-1} \frac{(r_{j+1}-r_1)}{(r_{j+1}-r_j)(r_j-r_1)} \left| u_j - \frac{r_j-r_1}{r_{j+1}-r_1}\, u_{j+1} \right|^2 \tag{3.13}$$

In particular we see that, for all $t > 0$ and $r \in \Sigma$,

$$\int_{(\mathbb{R}^n)^{k-1}} G_{r,t}(u')\, du' = 1\,.$$

For $t > 0$ consider the k-linear form

$$B_t(V_1, \dots, V_k) = \int_\Sigma \int_{(\mathbb{R}^n)^k} G_{r,t}(u')\; V_k(u_1+u_k) \cdots V_2(u_1+u_2) V_1(u_1)\, du\, dr\,.$$

By Hölder's inequality applied to the integral over u_1, we have

$$|B_t(V_1, \dots, V_k)| \leqslant \prod_{j=1}^{k} \|V_j\|_{L^k(\mathbb{R}^n)}\,,$$

and thus B_t is uniformly continuous on bounded sets in $L^k(\mathbb{R}^n)^k$. The quadratic form (3.13) is bounded below by $c\,|u'|^2$, for $c > 0$ independent of $r \in \Sigma$. An approximation to the identity argument then shows that B_t is continuous over $t \in [0, \infty)$, for fixed elements of $L^k(\mathbb{R}^n)^k$, where we set

$$B_0(V_1, \dots, V_k) = \frac{1}{k!} \int_{\mathbb{R}^n} V_k(u_1) \cdots V_1(u_1)\, du_1\,.$$

Consequently, we can write $\operatorname{tr}\big(W_k(t)\big) = (4\pi t)^{-\frac{n}{2}}\, t^k\, B_t(V)$, where

$$B_t(V) \in C\big([0,\infty)\big)\,, \quad B_0(V) = \frac{1}{k!} \int V(y)^k\, dy\,.$$

Here we set $B_t(V) = B_t(V, \dots, V)$, which, by the above, is for each t a continuous function of $V \in L^k(\mathbb{R}^n)$.

We start by demonstrating an m-th order expansion of $B_t(V)$ when $V \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$, after which we show it applies to $V \in L_c^\infty(\mathbb{R}^n;\mathbb{R}) \cap H^m(\mathbb{R}^n)$ by taking limits.

For $2 \leqslant j \leqslant k$ we write

$$V(u_j + u_1) = (2\pi)^{-n} \int e^{i\eta_j\cdot(u_1+u_j)} \widehat{V}(\eta_j)$$

and plug this into (3.12) to express

$$B_t(V) = (2\pi)^{-n(k-1)} \int_\Sigma \int_{(\mathbb{R}^n)^{k-1}} e^{-tQ_r(\eta')} \widehat{V}(\eta_k) \cdots \widehat{V}(\eta_2) \\ \times \overline{\widehat{V}(\eta_2 + \cdots + \eta_k)}\, d\eta_2 \cdots d\eta_k\, dr\,.$$

where $Q_r(\eta')$ is the quadratic form inverse to (3.13), and where $\widehat{V}(-\zeta) = \overline{\widehat{V}(\zeta)}$ since V is real valued.

We expand $\exp\big(-tQ_r(\eta')\big)$ as in (3.10). The first $m-1$ terms give contributions to $B_t(V)$ of the form

$$(2\pi)^{-n(k-1)} \sum_{j=0}^{m-1} \frac{(-1)^j}{j!}\, t^j \int Q(\eta')^j\, \widehat{V}(\eta_k) \cdots \widehat{V}(\eta_2) \\ \times \overline{\widehat{V}(\eta_2 + \cdots + \eta_k)}\, d\eta_2 \cdots d\eta_k\,,$$

where $Q(\eta')$ is the quadratic form obtained by integrating $Q_r(\eta')$ over r. The key observation we need is that we can write

$$Q(\eta')^j = \sum C_{\alpha_k,\ldots,\alpha_1}\, \eta_k^{\alpha_k} \cdots \eta_2^{\alpha_2} (\eta_2 + \cdots + \eta_k)^{\alpha_1}$$

where $\sum_{i=1}^k |\alpha_i| = 2j$, and $|\alpha_i| \leqslant j$ for every i.

Thus, the coefficient of t^j is such a linear combination of terms of the form

$$(2\pi)^{-n(k-1)} \int (\widehat{\partial^{\alpha_k} V})(\eta_k) \cdots (\widehat{\partial^{\alpha_2} V})(\eta_2)\, \overline{(\widehat{\partial^{\alpha_1} V})(\eta_2 + \cdots + \eta_k)}\, d\eta_2 \cdots d\eta_k\,,$$

This integral is equal to

$$\int (\partial^{\alpha_k} V)(y) \cdots (\partial^{\alpha_2} V)(y)\, (\partial^{\alpha_1} V)(y)\, dy\,,$$

which by Lemma 3.4 is bounded by $C\, \|V\|_{L^\infty}^{k-2} \|D^j V\|_{L^2}^2$. This establishes the bounds of Proposition 3.3 on the coefficients $c_{k,j+k}$ when $V \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$.

The m-th order remainder is a constant times

$$t^m \int_0^1 (1-s)^{m-1} \int_\Sigma \int_{(\mathbb{R}^n)^{k-1}} e^{-stQ_r(\eta')} Q_r(\eta')^m \times \widehat{V}(\eta_k)\cdots\widehat{V}(\eta_2)\,\overline{\widehat{V}(\eta_2+\cdots+\eta_k)}\,d\eta'\,dr\,ds\,,$$

which by a similar argument can be written as an integral over r and s of various polynomials in r, s times

$$t^m \int e^{-stQ_r(\eta')} (\widehat{\partial^{\alpha_k} V})(\eta_k)\cdots(\widehat{\partial^{\alpha_2} V})(\eta_2)\,\overline{(\widehat{\partial^{\alpha_1} V})(\eta_2+\cdots+\eta_k)}\,d\eta_2\cdots d\eta_k\,,$$

with $|\alpha_i| \leqslant m$, and $\sum_i |\alpha_i| = 2m$. We now show that, uniformly over $r \in \Sigma$, and $t > 0$,

$$\frac{1}{(2\pi)^{n(k-1)}}\left|\int e^{-tQ_r(\eta')}\widehat{v_k}(\eta_k)\cdots\widehat{v_2}(\eta_2)\,\overline{\widehat{v_1}(\eta_2+\cdots+\eta_k)}\,d\eta'\right| \leqslant \prod_{j=1}^k \|v_j\|_{L^{p_j}}\,, \tag{3.14}$$

whenever $2 \leqslant p_j \leqslant \infty$ and $\sum_j p_j^{-1} = 1$. Here we note that the proof of Lemma 3.4 bounds the right hand side, with $p_j = 2m/|\alpha_j|$ and $v_j = \partial^{\alpha_j} V$, by $\|V\|_{L^\infty}^{k-2}\|V\|_{H^m}^2$. The bounds on $r_{k,k+m}(t)$ in Proposition 3.3 will follow for $V \in C_c^\infty(\mathbb{R}^n)$.

The left hand side of (3.14) equals

$$\left|\int G_{r,t}(y_2-x,\ldots,y_k-x)\,v_k(y_k)\cdots v_2(y_2)\,v_1(x)\,dx\,dy_2\cdots dy_k\right|.$$

The kernel $G_{r,t}$ is positive and has total integral 1, so for proving the bound we may assume each v_j is nonnegative. By interpolation, we may restrict to the case that two of the p_j's are equal to 2, and the rest equal ∞. There are then two distinct cases to consider: $p_1 = p_2 = 2$, or $p_2 = p_3 = 2$. In the first case, we dominate the integral by

$$\|v_k\|_{L^\infty}\cdots\|v_3\|_{L^\infty}\int K(y_2-x)\,v_2(y_2)\,v_1(x)\,dy_2\,dx \tag{3.15}$$

where

$$K(z) = \int G_{r,t}(z,y_3,\ldots,y_k)\,dy_3\cdots dy_k\,.$$

Since $\int K = 1$, by Young's inequality the integral in (3.15) is bounded by $\|v_2\|_{L^2}\|v_1\|_{L^2}$.

In case $p_2 = p_3 = 2$, we bound the integral by

(3.16)
$$\|v_k\|_{L^\infty} \cdots \|v_4\|_{L^\infty} \|v_1\|_{L^\infty} \int K(y_2, y_3)\, v_3(y_3 - x)\, v_2(y_2 - x)\, dy_2\, dy_3\, dx\,,$$

where now

$$K(y_2, y_3) = \int G_{r,t}(y_2, y_3, y_4, \ldots, y_k)\, dy_4 \cdots dy_k\,.$$

Thus $\widehat{K}(\eta_2, \eta_3) = e^{-tQ_r(\eta_2,\eta_3,0,\ldots,0)}$. Writing v_2 and v_3 in terms of their Fourier transforms, and integrating out y_2 and y_3, expresses the integral in (3.16) as

$$(2\pi)^{-2n} \int e^{-ix(\eta_2+\eta_3)} e^{-tQ_r(-\eta_2,-\eta_3,0,\ldots,0)}\, \widehat{v_3}(\eta_3)\, \widehat{v_2}(\eta_2)\, d\eta_2\, d\eta_3\, dx$$
$$= (2\pi)^{-n} \int e^{-tQ_r(-\eta_2,\eta_2,0,\ldots,0)} \widehat{v_3}(-\eta_2) \widehat{v_2}(\eta_2)\, d\eta_2\,,$$

which is bounded by $\|v_3\|_{L^2} \|v_2\|_{L^2}$ by the Schwarz inequality, as $Q_r \geqslant 0$.

It remains to show the expansion holds for general $V \in L^\infty(\mathbb{R}^n; \mathbb{R}) \cap H^m(\mathbb{R}^n)$. We set $\phi_\varepsilon * V = V_\varepsilon \in C^\infty_{\mathrm{c}}(\mathbb{R}^n)$, where $\phi_\varepsilon = \varepsilon^{-n}\phi(\varepsilon^{-1}\cdot)$ is a family of smooth compactly supported mollifiers.

Recall that $\operatorname{tr}\big(W_k(t)\big) = (4\pi t)^{-n/2} t^k B_t(V)$. Since for each t, $B_t(V)$ is continuous in V in the $L^k(\mathbb{R}^n)$ topology, then $B_t(V) = \lim_{\varepsilon \to 0} B_t(V_\varepsilon)$. Furthermore, since $\|V_\varepsilon\|_{L^\infty} \leqslant \|V\|_{L^\infty}$, $\|V_\varepsilon\|_{H^m} \leqslant \|V\|_{H^m}$, we have the following bounds, uniform for $t > 0$ and $\varepsilon > 0$,

$$\|r_{k,k+m}(t, V_\varepsilon)\| \leqslant C\, \|V\|_{L^\infty}^{k-2} \|V\|_{H^m}^2\,.$$

It thus remains to show that $\lim_{\varepsilon\to 0} c_{k,k+j}(V_\varepsilon) = c_{k,k+j}(V)$ if $j \leqslant m-1$, for appropriately defined $c_{k,k+j}(V)$ satisfying the bounds of Proposition 3.3.

Recall that $c_{k,k+j}(V_\varepsilon)$ can be written as a linear combination of terms of the form

(3.17)
$$\int (\partial^{\alpha_k} V_\varepsilon)(y) \cdots (\partial^{\alpha_1} V_\varepsilon)(y)\, dy\,,$$

where $|\alpha_i| \leqslant j$ for all i, and $\sum_{i=1}^k |\alpha_i| = 2j$. We define $c_{k,k+j}(V)$ by the same formula, which by Lemma 3.4 is well defined, and absolutely dominated by $\|V\|_{L^\infty}^{k-2} \|D^j V\|_{L^2}^2$. To see that (3.17) converges, as $\varepsilon \to 0$, to the same expression with V_ε replaced by V, we note that, by the proof of Lemma 3.4, $\partial^{\alpha_i} V \in L^{\frac{2m}{|\alpha_i|}}(\mathbb{R}^n)$, so for $|\alpha_i| > 0$,

$$\lim_{\varepsilon \to 0} \|\partial^{\alpha_i} V_\varepsilon - \partial^{\alpha_i} V\|_{L^{\frac{2m}{|\alpha_i|}}} = 0\,.$$

Thus, the product over the terms in (3.17) with $|\alpha_i| \neq 0$ converges in $L^{\frac{m}{j}}(\mathbb{R}^n)$ to the same product with V_ε replace by V. Since $\frac{m}{j} > 1$, the integral in (3.17) converges as $\varepsilon \to 0$ by the fact that $V_\varepsilon \to V$ in $L^p(\mathbb{R}^n)$ for all $p < \infty$.

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