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ON THE TRACE OF THE WAVE GROUP AND REGULARITY OF POTENTIALS

by Hart F. SMITH

ABSTRACT. — We consider the wave equation with a compactly supported, real-valued bounded potential, and show that the relative trace of the associated evolution group admits an asymptotic expansion to order $m+2$ if and only if the potential belongs to the Sobolev space of order m.

RÉSUMÉ. — Nous considérons l'équation des ondes avec un potentiel borné, à support compact et à valeurs réelles, et montrons que la trace régularisée de l'opérateur d'évolution associé admet un développement asymptotique à l'ordre $m+2$ si et seulement si le potentiel appartient à l'espace de Sobolev d'ordre m.

1. Introduction and statement of results

Suppose that V is a real valued, bounded measurable function of compact support on $\mathbb{R}^d$. Define the wave group U_V by $U_V(f,g)=(u,\partial_t u)$, where u is the solution to the initial value problem for the following wave equation

$$\big(\partial_t^2-\Delta+V\big)u(t,x)=0\,,\quad (u,\partial_t u)\big|_{t=0}=(f,g)\in H^1\times L^2(\mathbb{R}^d).$$

Let $U_V(s)$ denote the map $(f,g)\to(u,\partial_t u)|_{t=s}$.

If $V\in C_{\mathrm{c}}^\infty(\mathbb{R}^d)$, it is well known that for $\phi\in C_{\mathrm{c}}^\infty(\mathbb{R})$ the operator

$$\langle\phi,U_V-U_0\rangle=\int\phi(t)\big(U_V(t)-U_0(t)\big)\,\mathrm{d}t$$

is trace class; see e.g. [6, 11, 12, 13]. The map $\phi\to\mathrm{Tr}\langle\phi,U_V-U_0\rangle$ defines an even distribution on $\mathbb{R}$, denoted by $\mathrm{Tr}(U_V-U_0)$. For $V\in C_{\mathrm{c}}^\infty(\mathbb{R}^d)$ this

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distribution is smooth on $\mathbb{R}\backslash\{0\}$, and admits an asymptotic expansion in t for t near 0. If d is odd, the expansion takes the form

$$\operatorname{Tr}(U_V - U_0) = \sum_{j=1}^{(d-1)/2} w_j(V) D^{d-1-2j}\delta(t) + \sum_{j=(d+1)/2}^{\infty} w_j(V)\,|t|^{2j-d},$$

and if d is even it takes the form

$$\operatorname{Tr}(U_V - U_0) = \sum_{j=1}^{(d-2)/2} w_j(V) D^{d-1-2j}\mathrm{p.v.}(1/t) + \sum_{j=d/2}^{\infty} w_j(V)\, t^{2j-d}.$$

The expansion holds in the sense that the difference between the left side and the finite sum to $j = m$ is a continuous function on $\mathbb{R}$ that is $\mathcal{O}(|t|^{2m+2-d})$ for t near 0, provided $m \geqslant d/2$.

In this paper we consider the existence of similar expansions to finite order when V is of limited regularity, and show that for real valued, compactly supported potentials V, existence of such an expansion to order $j = m + 2$ is equivalent to the Sobolev regularity condition $V \in H^m(\mathbb{R}^d)$. Our proof shows that $\langle \phi, U_V - U_0\rangle$ is of trace-class for $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$, but if $d \geqslant 4$ then the proof of the expansion in t for the trace relies on L^1 bounds on the Fourier transform $\widehat{V}$ of V, and thus for $d \geqslant 4$ we need to place the stronger a priori assumption that $\widehat{V} \in L^1(\mathbb{R}^d)$ when proving bounds on various remainder terms.

We define the space $\widehat{L}^1(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$ with norm

$$\|V\|_{\widehat{L}^1} = (2\pi)^{-d} \int |\widehat{V}(\xi)|\,\mathrm{d}\xi,$$

and let $\widehat{L}^1_{\mathrm{c}} \subset L^\infty_{\mathrm{c}}$ denote the space of $V \in \widehat{L}^1$ with compact support.

We define the space X_d according to whether $d \leqslant 3$ or not,

$$X_d = \begin{cases} L^\infty_{\mathrm{c}}(\mathbb{R}^d), & d \leqslant 3,\\ \widehat{L}^1_{\mathrm{c}}(\mathbb{R}^d), & d \geqslant 4. \end{cases}$$

Finally, let

$$\|V\|_{X_d \cap H^m} = \|V\|_{X_d} + \|V\|_{H^m},$$

and note that $H^s_{\mathrm{c}}(\mathbb{R}^d) \subset X_d$ if $s > d/2$.

Theorem 1.1. — *Assume that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$. If $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R})$, then the operator on $H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$ defined by*

$$(f,g) \to \int \phi(t)\big(U_V(t)(f,g) - U_0(t)(f,g)\big)\,\mathrm{d}t$$

is trace-class, and its trace defines an even distribution acting on ϕ, which we denote by $\mathrm{Tr}\langle\phi, U_V - U_0\rangle$*.*

If $V \in X_d$, and $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R})$ is an even function, there are distributions ν_d and $\mu_{d,V}$ on $\mathbb{R}$ such that

$$\mathrm{Tr}\langle\phi, U_V - U_0\rangle = \nu_d(\phi)\int V(x)\,\mathrm{d}x + \mu_{d,V}(\phi)$$

where $\mu_{d,V}$ has the following form, with $\alpha_V(t) \in C(\overline{\mathbb{R}_+})$,

$$\mu_{d,V}(\phi) = \begin{cases} \displaystyle\int_0^\infty t^{4-d}\alpha_V(t)\,\phi(t)\,\mathrm{d}t, & 1 \leqslant d \leqslant 4,\\ \displaystyle\int_0^\infty \alpha_V(t)\,\partial_t(t^{-1}\partial_t)^{\frac{d-5}{2}}\phi(t)\,\mathrm{d}t, & d \geqslant 5 \text{ odd},\\ \displaystyle\int_0^\infty \alpha_V(t)\,(t^{-1}\partial_t)^{\frac{d-4}{2}}\phi(t)\,\mathrm{d}t, & d \geqslant 6 \text{ even}. \end{cases}$$

If $V \in X_d \cap H^m(\mathbb{R}^d)$, m an integer, then $\alpha_V(t) \in C^{2m}(\overline{\mathbb{R}_+})$, and its Taylor expansion at 0 is of the form

$$\alpha_V(t) = \sum_{j=0}^{m} a_{j+2}(V)t^{2j} + o(t^{2m})\,, \tag{1.1}$$

where $a_{j+2}(V)$ is a dimension dependent multiple of the Schrödinger heat invariant $c_{j+2}(V)$.

Conversely, if $V \in X_d$ is real valued, and there are constants $b_j \in \mathbb{C}$ and $C < \infty$ so that

$$\left|\alpha_V(t) - \sum_{j=0}^{m-1} b_j t^{2j}\right| \leqslant C\,t^{2m} \quad \text{for} \quad 0 \leqslant t \leqslant 1, \tag{1.2}$$

then $V \in H^m(\mathbb{R}^d)$, and hence (1.1) holds.

We note that the $a_j(V)$ in (1.1) differ by a constant from the $w_j(V)$ in the expansion presented for smooth potentials. The form of ν_d is given in Theorem 2.2, and agrees with the term $j = 1$ in the expansion for smooth V above. It can also be written in a form similar to that for $\mu_{d,V}$.

The proof of Theorem 1.1 establishes pointwise bounds on α_V and its derivatives. In particular the following holds,

$$|\alpha_V(t)| \leqslant C_d\,\|V\|^2_{L^2}\cosh\Big(t\|V\|^{1/2}_{X_d}\Big).$$

An analogous result for the heat kernel of $-\Delta + V$ on Euclidean space was established by the author and Zworski in [15]. There it was proven for

$V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$ in all dimensions d. The same result was subsequently established by the author in [14] for the heat kernel on complete Riemannian manifolds under mild geometric assumptions. The study of heat traces has an extensive history, going back to Kac, Berger and McKean–Singer. For detailed discussions of the heat trace for Schrödinger operators we refer to Bañuelos–Sà Baretto [2], Colin de Verdière [17], Hitrik–Polterovich [10], and Gilkey [8]. The coefficients $c_j(V)$ in the expansion of the relative heat trace, known as heat invariants, are a key tool in the proof of compactness of isospectral families of potentials; see Brüning [3] and Donnelly [5].

There appears to be far fewer treatments of the trace of the wave kernel for $-\Delta + V$, even though it is a more fundamental operator in the sense that the trace expansion for the heat kernel follows easily from that for the wave kernel, but not vice versa; see Remark 2.6 below. The wave invariants $w_j(V)$ are dimension dependent multiples of the heat invariants $c_j(V)$, as noted by Sà Baretto–Zworski [13], thus on a compact manifold they do not give new spectral invariants. In Euclidean space of odd dimension, on the other hand, the wave-trace restricted to $t \neq 0$ is related to the resonances of $-\Delta + V$ by the trace formula of Melrose; see [6, Theorem 3.53]. As a consequence, if V_1 and V_2 are bounded real potentials with the same set of resonances and eigenvalues, counted with the appropriate multiplicity, then

$$t^d \operatorname{Tr}(U_{V_1} - U_0) = t^d \operatorname{Tr}(U_{V_2} - U_0).$$

As observed by Hislop–Wolf [9], in odd dimensions this shows that if the V_j are smooth potentials, then V_j have the same heat coefficients, $c_k(V_1) = c_k(V_2)$, if $k \geqslant (d+1)/2$. This in turn is used in [9] to establish a compactness theorem for iso-resonant families of C^∞_{c} potentials with support in a common ball, when $d = 1$ or 3.

A different proof of this result was given by Christiansen, who proved equality of $c_k(V_j)$ for $k \geqslant (d+1)/2$ by using the Birman–Krein formula to relate the trace of the heat kernel to the poles of the scattering phase. See [15, Theorem 1.2] for a discussion of her proof in odd dimensions. This method was extended by Christiansen in [4] to prove iso-resonant compactness and related results for C^∞_{c} potentials in even dimensions.

One of the motivations for this paper was a remark by the authors of [9] that existence of the expansion of Theorem 1.1 would extend certain results of [9] to potentials of Sobolev regularity. Precisely, if d is odd then Theorem 1.1 can be combined with the Melrose trace formula to prove equality of the heat coefficients $c_k(V)$ for $(d+1)/2 \leqslant k \leqslant m+2$, assuming $V \in X_d \cap H^m(\mathbb{R}^d)$ is real and $m \geqslant (d-3)/2$. Christiansen's method combined with the heat trace expansion of [15] also implies this result. In dimensions $d = 1, 3$, this implies $\|V_1\|_{L^2} = \|V_2\|_{L^2}$, and one can bootstrap to obtain the following inverse result.

Theorem 1.2. — *Suppose that $d = 1, 3$ and that $V_1, V_2 \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$ are iso-resonant. If $V_1 \in H^m(\mathbb{R}^d)$, where $m \geqslant 0$ is an integer, then $V_2 \in H^m(\mathbb{R}^d)$, and there is a polynomial bounded function F_m such that*

$$\|V_2\|_{H^m(\mathbb{R}^d)} \leqslant F_m\big(\|V_1\|_{H^m(\mathbb{R}^d)}\big). \tag{1.3}$$

Given equality of the heat coefficients for V_1 and V_2, the bound (1.3) follows from the papers [3] and [5], where it was shown that for $1 \leqslant d \leqslant 3$, one can bound

$$\|V\|_{H^m} \leqslant P_{m,d}\big(c_2(V), \dots, c_{m+2}(V)\big),$$

for a dimension dependent polynomial $P_{m,d}$. This is obtained by induction from a bound of the form

$$\||D|^m V\|_{L^2} \leqslant C_{m,d}\, c_{m+2}(V) + P_{m,d}\big(\|V\|_{H^{m-1}}\big).$$

The papers [3] and [5] work on compact manifolds, but the estimates hold globally on $\mathbb{R}^d$.

Consequently, the family of L^∞_{c} real potentials that are iso-resonant to a given potential in $H^m(\mathbb{R}^d)$ forms a bounded subset of $H^m(\mathbb{R}^d)$, if $d = 1, 3$. That this family is closed is shown in [9]. If one restricts attention to potentials with support in fixed ball of finite radius, then by Rellich's Lemma such potentials are a compact subset of $H^s(\mathbb{R}^d)$ if $s < m$.

2. Preliminary reductions

We prove Theorem 1.1 using the iterative construction of U_V. Define

$$\mathbf{C}(t) = \cos\big(t|D|\big), \qquad \mathbf{S}(t) = \frac{\sin\big(t|D|\big)}{|D|}.$$

Then the free wave group is given by

$$U_0(t) = \begin{bmatrix} \mathbf{C}(t) & \mathbf{S}(t) \\ \Delta\mathbf{S}(t) & \mathbf{C}(t) \end{bmatrix}.$$

Let $\mathbf{\Lambda}$ denote the following operator on $C([-T,T]; H^1 \times L^2)$, $T < \infty$,

$$\mathbf{\Lambda}(F,G)(t,\cdot) = \int_0^t U_0(t-s)(F,G)(s,\cdot)\,\mathrm{d}s.$$

Then

$$U_V - U_0 = \sum_{k=1}^{\infty} (-\mathbf{\Lambda}\mathbf{V})^k U_0, \qquad \mathbf{V} = \begin{bmatrix} 0 & 0 \\ V & 0 \end{bmatrix},$$

where the sum converges absolutely in the $H^1 \times L^2 \to C(H^1 \times L^2)$ operator norm, for each $T < \infty$.

We recall some basic properties of trace-class operators. For a compact operator A on a Hilbert space with principal values $\sigma_j(A)$, one defines the Schatten-p norms of A for $1 \leqslant p \leqslant \infty$ by

$$\|A\|_{\mathcal{L}^p} = \left(\sum_{j=1}^{\infty} \sigma_j(A)^p \right)^{1/p}.$$

The $\mathcal{L}^\infty$ norm is the operator norm, and $\mathcal{L}^1$ is the trace-class norm. As a corollary of [7, Theorem 1] of Ky Fan, we note the following Hölder type estimate,

$$\|A_1 A_2 \cdots A_n\|_{\mathcal{L}^1} \leqslant \prod_{j=1}^{n} \|A_j\|_{\mathcal{L}^{p_j}} \quad \text{if} \quad \sum_{j=1}^{n} p_j^{-1} = 1, \;\; 1 \leqslant p_j \leqslant \infty. \tag{2.1}$$

When $p_j = \infty$ we may replace the $\mathcal{L}^\infty$ norm by the operator norm, and assume only that A_j is a bounded operator, not necessarily compact. This holds since [7, Theorem 1] follows from uniform estimates over finite rank operators.

Lemma 2.1. — *If $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$, then for $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R})$ the sum*

$$\sum_{k=1}^{\infty} (-1)^k \int_{-\infty}^{\infty} \phi(t) \big((\mathbf{\Lambda V})^k U_0 \big)(t)\, \mathrm{d}t \equiv \sum_{k=1}^{\infty} (-1)^k \langle \phi, W_{k,V} \rangle \tag{2.2}$$

converges absolutely to $\langle \phi, U_V - U_0 \rangle$ in the trace-class norm on $H^1 \times L^2(\mathbb{R}^d)$.

Proof. — Let $R = 1 + \mathrm{diam}(\mathrm{supp}(V))$, and given $t > 0$ let K be a cube of sidelength $\ell(K) = 2(R+t)$ that contains all points within distance t of $\mathrm{supp}(V)$. Then for $|s| < t$ the Schwartz kernel of $V\mathbf{S}(s)$ is supported entirely within $K \times K$, so the Schatten-p norm of $V\mathbf{S}(s)$ on $L^2(\mathbb{R}^d)$ is the same as that of its restriction to $L^2(K)$. We use the Fourier series basis for $L^2(K)$ with characters $\xi \in \Xi_K$,

$$e_\xi = |K|^{-1/2}\, \mathrm{e}^{\mathrm{i}\langle x, \xi \rangle}, \qquad \xi \in \Xi_K = 2\pi\, \ell(K)^{-1} \mathbb{Z}^d.$$

In this basis, we have

$$V\mathbf{S}(s) e_\xi = \frac{\sin(s|\xi|)}{|\xi|} V e_\xi.$$

Thus $V\mathbf{S}(s)$ factors into V times a diagonal operator, and we have

$$\begin{aligned}(2.3)\qquad \|V\mathbf{S}(s)\|_{\mathcal{L}^{d+1}} &\leqslant \|V\|_{L^\infty}\left(\sum_{\xi\in\Xi_K}\left|\frac{\sin(s|\xi|)}{|\xi|}\right|^{d+1}\right)^{1/(d+1)} \\ &\leqslant C_d\|V\|_{L^\infty}\big(t(R+t)^d\big)^{1/(d+1)}.\end{aligned}$$

Here we use the bound

$$(2.4)\qquad \left|\frac{\sin(s|\xi|)}{|\xi|}\right| \leqslant \frac{2s}{1+s|\xi|}\,,$$

and we use the fact that $\ell(K)^{-1}s \leqslant 1$ to estimate the sum by an integral.

We first show that the lower right corner $\langle\phi, W^{2,2}_{k,V}\rangle$ of the 2×2-block matrix in (2.2) converges in the trace class norm on L^2. All terms in the sum for this term are even in t, so we may assume that $\phi(t)$ is even in t. Let $\mathrm{d}^k s = \mathrm{d}s_1\cdots\mathrm{d}s_k$. Then $\langle\phi, W^{2,2}_{k,V}\rangle$ can be written as

$$\begin{aligned}&2\int_{\substack{s_1+\cdots s_k<t\\ s_1,\dots,s_k>0}}\phi(t)\mathbf{C}(t-(s_1+\cdots+s_k))V\mathbf{S}(s_k)V\cdots V\mathbf{S}(s_1)\,\mathrm{d}^k s\,\mathrm{d}t \\ &\qquad = 2\int_{\mathbb{R}^{k+1}_+}\phi(s_1+\cdots+s_{k+1})\mathbf{C}(s_{k+1})V\mathbf{S}(s_k)V\cdots V\mathbf{S}(s_1)\,\mathrm{d}^{k+1}s.\end{aligned}$$

First consider the case $k\geqslant d+1$. We use the bound

$$\|\mathbf{1}_{\mathrm{supp}(V)}\mathbf{S}(s)\mathbf{1}_{\mathrm{supp}(V)}\|_{L^2(K)\to L^2(K)} \leqslant C_d\, s\wedge \mathrm{diam}(\mathrm{supp}(V)).$$

This follows by scaling to the case that $\mathrm{diam}(\mathrm{supp}(V))=1$, in which case for $s\geqslant 2$ it follows from the fact that the kernel of $\mathbf{S}(s)$ is smooth and uniformly bounded on the set $|x|\leqslant 1$, and for $s\leqslant 2$ it follows by (2.4).

From (2.1) and (2.3), we conclude that, with $\mathcal{L}^1$ denoting the trace-class norm, and $R = 1+\mathrm{diam}(\mathrm{supp}(V))$ as above,

$$\begin{aligned}&\left\|\int_{\substack{s_1+\cdots s_k<t\\ s_1,\dots,s_k>0}}\mathbf{C}(t-(s_1+\cdots+s_k))V\mathbf{S}(s_k)V\cdots V\mathbf{S}(s_1)\,\mathrm{d}^k s\right\|_{\mathcal{L}^1} \\ &\qquad\qquad \leqslant \frac{C_d\|V\|^k_{L^\infty}(R+t)^d t^{k+1}\big((C_dR)^{k-d-1}\wedge t^{k-d-1}\big)}{k!}.\end{aligned}$$

Here we used that the volume of the domain of integration is $t^k/k!$. We conclude that if $k\geqslant d+1$ then $W^{2,2}_{k,V}$ is trace-class, with $\mathcal{L}^1$ norm given by a continuous function $\beta_{k,V}(t)$ satisfying

$$(2.5)\quad |\beta_{k,V}(t)| \leqslant \left(\frac{C_dR^dt^{2k-d}\|V\|^k_{L^\infty}}{k!}\right)\wedge\left(\left(\frac{t}{R}\right)^{d+1}\frac{\big(C_d\|V\|_{L^\infty}R\,t\big)^k}{k!}\right).$$

The sum of $W^{2,2}_{k,V}$ over $k \geqslant d+1$ thus converges absolutely in the trace class.

For later use we note that

$$\sum_{k=d+1}^{\infty} |\beta_{k,V}(t)| \leqslant \left(\frac{t}{R}\right)^{d+1} \mathrm{e}^{C_d R t \|V\|_{L^\infty}} . \tag{2.6}$$

It remains to show that $\langle \phi, W^{2,2}_{k,V}\rangle$ is trace class for $k \leqslant d$. Suppose that $\operatorname{supp}(\phi) \subset [-T,T]$, and let K be the cube of sidelength $2(T+R)$, which we identify with the torus by imposing periodic boundary conditions on Δ. In bounding the $\mathcal{L}^1$ norm of $\langle \phi, W^{2,2}_{k,V}\rangle$, we may then assume, by finite propagation velocity, that we are working with the wave equation on K.

We write

$$\mathbf{S}(s) = (1-\partial_s^2)\mathbf{S}(s)\,(1-\Delta)^{-1}.$$

Integration by parts in s_1 shows that $\frac{1}{2}\langle \phi, W^{2,2}_{k,V}\rangle$ equals the following,

$$\int_{\mathbb{R}_+^{k+1}} (\phi-\phi'')(s_1+\cdots+s_{k+1})\mathbf{C}(s_{k+1})V\mathbf{S}(s_k)\cdots V\mathbf{S}(s_1)\,\mathrm{d}^{k+1}s\cdot(1-\Delta)^{-1}$$
$$+\int_{\mathbb{R}_+^{k}} \phi(s_2+\cdots+s_{k+1})\mathbf{C}(s_{k+1})V\mathbf{S}(s_k)\cdots V\mathbf{S}(s_2)\,\mathrm{d}^{k}s\cdot V(1-\Delta)^{-1}.$$

We repeat this on each term, stopping if the total number of $\mathbf{S}(s_j)$ factors plus twice the number of $(1-\Delta)^{-1}$ factors in a term is at least $d+1$. Thus, we stop after at most $d+1-k$ steps. By a similar proof to that of (2.3), we note that

$$\|(1-\Delta)^{-1/2}\|_{\mathcal{L}^{d+1}} \leqslant C_d(R+T)^{d/(d+1)}.$$

If $2k \leqslant d+1$, there will arise terms of the form $\widehat{\phi^{(2m)}}\big(\sqrt{-\Delta}\big)Q$ with $2m \leqslant d+1-2k$, and Q consisting of a mixed product of k factors of V and $m+k$ factors of $(1-\Delta)^{-1}$, hence

$$\|Q\|_{\mathcal{L}^p} \leqslant C_d\|V\|^k_{L^\infty}\big(T+R\big)^{d/p}, \quad \text{if } p=(d+1)/(2m+2k).$$

For this value of p, we can bound

$$\|\widehat{\phi^{(2m)}}\big(\sqrt{-\Delta}\big)\|_{\mathcal{L}^{p'}} \leqslant C_d\big(T+R\big)^{d/p'}\big(\,\|\phi^{(2m)}\|_{L^1}+\|\phi^{(d+1-2k)}\|_{L^1}\big).$$

The terms that involve an integral over s_k are bounded as for $k \geqslant d+1$, and together we conclude that, if $\operatorname{supp}(\phi)\subset[-T,T]$, and $1\leqslant k\leqslant d$,

$$\big\|\langle\phi, W^{2,2}_{k,V}\rangle\big\|_{\mathcal{L}^1} \leqslant C_d\,(T+R)^{d+1}\,\|V\|^k_{L^\infty}\sum_{n=0}^{d+1-k}\int_{\mathbb{R}}|\phi^{(n)}(t)|\,\mathrm{d}t. \tag{2.7}$$

This concludes the proof of $\mathcal{L}^1$ summability over k of $\langle\phi, W^{2,2}_{k,V}\rangle$.

A similar proof shows that each of the following is absolutely summable over k in the trace class norm on $L^2(\mathbb{R}^d)$,

$$\langle D\rangle\langle\phi, W^{1,1}_{k,V}\rangle\langle D\rangle^{-1}, \qquad \langle D\rangle\langle\phi, W^{1,2}_{k,V}\rangle, \qquad \langle\phi, W^{2,1}_{k,V}\rangle\langle D\rangle^{-1},$$

with the same bound (2.5) on the $\mathcal{L}^1$ norm of $W^{i,j}_{k,V}$ if $k \geqslant d+1$. It follows that the sum of $\langle\phi, W_{k,V}\rangle$ converges absolutely in the trace class norm on $H^1 \times L^2$. □

The trace of $\langle\phi, W_{k,V}\rangle$ is thus well defined, and the sum in (2.2) converges in the trace class to $\langle\phi, U_V - U_0\rangle$. We next note that

$$\mathrm{Tr}_{H^1\times L^2}\langle\phi, W_{k,V}\rangle = \mathrm{Tr}_{H^1}\langle\phi, W^{1,1}_{k,V}\rangle + \mathrm{Tr}_{L^2}\langle\phi, W^{2,2}_{k,V}\rangle = 2\,\mathrm{Tr}_{L^2}\langle\phi, W^{1,1}_{k,V}\rangle.$$

The second inequality follows by noting that $W^{1,1}_{k,V}$ is the L^2 adjoint of $W^{2,2}_{k,V}$, and the trace of $W^{1,1}_{k,V}$ over $H^1(\mathbb{R}^d)$ is the same as the trace over $L^2(\mathbb{R}^d)$.

Since $W^{1,1}_{k,V}$ is even in t, we can assume that $\phi(t)$ is an even function of t when deriving a formula for $\mathrm{Tr}\langle\phi, W_{k,V}\rangle$. We will establish the other parts of Theorem 1.1 as a consequence of the following three results.

Theorem 2.2. — *Assume that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$ and $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R})$ is even. Then*

$$\mathrm{Tr}\langle\phi, W_{1,V}\rangle = \nu_d(\phi)\int V(x)\,\mathrm{d}x,$$

where, with $c_d = 2^{2-d}\pi^{1-\frac{d}{2}}/\Gamma(\frac{d}{2}-1)$, and $D = -i\partial_t$,

$$\nu_d(\phi) = \begin{cases} \displaystyle\int_0^\infty t\phi(t)\,\mathrm{d}t, & d=1,\\ \displaystyle\pi^{-1}\int_0^\infty \phi(t)\,\mathrm{d}t, & d=2,\\ c_d\big(D^{d-3}\phi\big)(0), & d\geqslant 3 \ \textit{odd},\\ c_d\big(|D|^{d-3}\phi\big)(0), & d\geqslant 4 \ \textit{even}. \end{cases}$$

For $d>1$ one also has the formulas,

$$\nu_d(\phi) = \begin{cases} \displaystyle(-2\pi)^{\frac{1-d}{2}}\int_0^\infty \partial_t(t^{-1}\partial_t)^{\frac{d-3}{2}}\phi(t)\,\mathrm{d}t, & d\geqslant 3 \ \textit{odd},\\ \displaystyle-2(-2\pi)^{-\frac{d}{2}}\int_0^\infty (t^{-1}\partial_t)^{\frac{d-2}{2}}\phi(t)\,\mathrm{d}t, & d\geqslant 2 \ \textit{even}. \end{cases}$$

THEOREM 2.3. — *Assume that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$. If $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R})$ is even, then one can write*

$$\mathrm{Tr}\langle \phi, W_{2,V}\rangle = \begin{cases} \displaystyle\int_0^\infty t^{4-d} a_{2,V}(t)\,\phi(t)\,\mathrm{d}t, & 1 \leqslant d \leqslant 4, \\ \displaystyle\int_0^\infty a_{2,V}(t)\,\partial_t (t^{-1}\partial_t)^{\frac{d-5}{2}}\phi(t)\,\mathrm{d}t, & d \geqslant 5 \text{ odd}, \\ \displaystyle\int_0^\infty a_{2,V}(t)\,(t^{-1}\partial_t)^{\frac{d-4}{2}}\phi(t)\,\mathrm{d}t, & d \geqslant 4 \text{ even}, \end{cases}$$

where $a_{2,V}(t) \in C\big(\overline{\mathbb{R}_+}\big)$, and $|a_{2,V}(t)| \leqslant (2\pi)^{-\lfloor \frac{d}{2}\rfloor}\|V\|^2_{L^2}$. If m is an integer and $V \in L^\infty_{\mathrm{c}} \cap H^m(\mathbb{R}^d)$, then $a_{2,V}(t) \in C^{2m}(\overline{\mathbb{R}_+})$, and

$$\|a_{2,V}\|_{C^{2m}(\mathbb{R})} \leqslant C_{m,d}\,\|V\|^2_{H^m}.$$

Additionally, for $0 \leqslant j \leqslant 2m$,

$$\partial_t^j a_{2,V}(0) = \begin{cases} 0, & j \text{ odd}, \\ c_{j,d}\,\||D|^j V\|^2_{L^2}, & j \text{ even}, \end{cases} \tag{2.8}$$

where $c_{j,d} \neq 0$.

Conversely, if $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$ is real valued, and there are constants $b_j \in \mathbb{C}$ and $C < \infty$ so that

$$\left| a_{2,V}(t) - \sum_{j=0}^{m-1} b_j t^{2j} \right| \leqslant C\,t^{2m} \quad \text{for} \quad 0 \leqslant t \leqslant 1, \tag{2.9}$$

then $V \in H^m(\mathbb{R}^d)$, and hence (2.8) holds.

THEOREM 2.4. — *Assume that $V \in X_d$, and $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R})$ is an even function. Then if $k \geqslant 3$ and $2k \geqslant d$, there exists $a_{k,V} \in C\big(\overline{\mathbb{R}_+}\big)$ such that*

$$\mathrm{Tr}\langle \phi, W_{k,V}\rangle = \int_0^\infty t^{2k-d} a_{k,V}(t)\,\phi(t)\,\mathrm{d}t.$$

If $k \geqslant 3$ and $2k < d$, there exists $a_{k,V} \in C\big(\overline{\mathbb{R}_+}\big)$ such that

$$\mathrm{Tr}\langle \phi, W_{k,V}\rangle = \begin{cases} \displaystyle\int_0^\infty a_{k,V}(t)\,\partial_t\big(t^{-1}\partial_t\big)^{\frac{d-2k-1}{2}}\phi(t)\,\mathrm{d}t, & d \geqslant 7 \text{ odd}, \\ \displaystyle\int_0^\infty a_{k,V}(t)\,\big(t^{-1}\partial_t\big)^{\frac{d-2k}{2}}\phi(t)\,\mathrm{d}t, & d \geqslant 6 \text{ even}. \end{cases} \tag{2.10}$$

In each of the above cases, if $m \geqslant 0$ is an integer and $V \in X_d \cap H^m(\mathbb{R}^d)$, then $a_{k,V} \in C^{2m}(\overline{\mathbb{R}_+})$, and $\partial_t^j a_{k,V}(0) = 0$ if $j < 2m$ is odd.

We show here how Theorem 1.1 follows from the above three theorems, together with bounds (8.3) and (9.5). It follows from Lemma 2.1 that the operator $\langle \phi, U_V - U_0\rangle$ is trace class, and the proof of Lemma 2.1 shows that its trace determines a distribution in ϕ, and that

$$\operatorname{Tr}\langle \phi, U_V - U_0\rangle = \sum_{k=1}^{\infty} (-1)^k \operatorname{Tr}\langle \phi, W_{k,V}\rangle.$$

If $d \leqslant 4$, then the expression for $\mu_{d,V}(\phi)$ holds with

$$\alpha_V(t) = \sum_{k=2}^{\infty} (-1)^k a_{k,V}(t) t^{2k-4}.$$

The bounds (8.3) and (9.5) show that the sum converges absolutely in C^{2m} when $V \in X_d \cap H^m$, and that

$$|\partial_t^j \alpha_V(t)| \leqslant C_d \, \|V\|^2_{H^{\lceil j/2\rceil}} p_j\big(t\|V\|^{1/2}_{X_d}\big) \cosh\big(t\|V\|^{1/2}_{X_d}\big), \tag{2.11}$$

where p_j is a polynomial of order at most $\max(0, j-2)$.

For $d \geqslant 5$ and $k \geqslant 3$, we need the following lemma.

Lemma 2.5. — *If $F \in C(\overline{\mathbb{R}_+})$, and $\phi(t)$ is an even Schwartz function, then for each $m \geqslant 1$ and $n \geqslant 0$ one can write*

$$\begin{aligned} \int_0^\infty t^n \, F(t)\, \phi(t)\, \mathrm{d}t &= \int_0^\infty t^{n+2m-1} F_{m,n}(t) \partial_t (t^{-1}\partial_t)^{m-1} \phi(t)\, \mathrm{d}t \\ &= \int_0^\infty t^{n+2m} F_{m,n}(t) (t^{-1}\partial_t)^m \phi(t)\, \mathrm{d}t, \end{aligned}$$

where $F_{m,n} \in C(\overline{\mathbb{R}_+})$. If $F \in C^j(\overline{\mathbb{R}_+})$ then so if $F_{m,n}$, and

$$\|\partial_t^j F_{m,n}\|_{L^\infty} \leqslant \frac{\Gamma(\frac{n+j+1}{2})}{2^m \Gamma(m + \frac{n+j+1}{2})} \, \|\partial_t^j F\|_{L^\infty}.$$

Proof. — The $F_{m,n}$ are obtained recursively by the formula

$$F_{m+1,n}(t) = -\int_0^1 s^{n+2m} F_{m,n}(st)\, \mathrm{d}s,$$

where $F_{0,n} = F$, and the lemma follows by induction. □

We observe that

$$\partial_t^j F_{m,n}(0) = \frac{(-1)^m \Gamma(\frac{n+j+1}{2})}{2^m \Gamma(m + \frac{n+j+1}{2})} \partial_t^j F(0). \tag{2.12}$$

For $d \geqslant 6$ even, define $\widetilde{a}_{k,V}$ as follows, where $F = a_{k,V}$ in each instance,

$$\widetilde{a}_{k,V}(t) = \begin{cases} F_{k-2,0}(t), & 3 \leqslant k < \frac{d}{2}, \\ F_{\frac{d-4}{2}, 2k-d}(t), & k \geqslant \frac{d}{2}. \end{cases} \tag{2.13}$$

For $d \geqslant 5$ odd, with $F = a_{k,V}$ we define

$$\widetilde{a}_{k,V}(t) = \begin{cases} F_{k-2,1}(t), & 3 \leqslant k < \frac{d}{2}, \\ F_{\frac{d-3}{2},2k-d}(t), & k > \frac{d}{2}. \end{cases} \tag{2.14}$$

Theorem 1.1 then holds with

$$\alpha_V(t) = a_{2,V}(t) + \sum_{k=3}^{\infty} (-1)^k t^{2(k-2)} \widetilde{a}_{k,V}(t).$$

The bounds (2.11) on $\partial_t^j \alpha_V(t)$ again follow from (8.3).

The fact that $\partial_t^{2j+1} \alpha_V(0) = 0$ for $0 \leqslant j < m$ follows from (2.8), Theorem 2.4, and (2.12). The particular form of the even order Taylor coefficients of $\alpha_V(t)$ at $t = 0$ is discussed in Remark 2.6 below.

For the final conclusion of Theorem 1.1, assume $V \in X_d$, and that the expansion (1.2) holds. By induction we may assume $V \in H^{m-1}(\mathbb{R}^d)$. It follows by the above steps that

$$\sum_{k=3}^{\infty} (-1)^k t^{2(k-3)} \widetilde{a}_{k,V}(t) \in C^{2(m-1)}(\overline{\mathbb{R}_+}),$$

and hence that we can write

$$\alpha_V(t) - a_{2,V}(t) = \sum_{j=0}^{m-1} \widetilde{b}_j t^{2j} + \mathcal{O}(t^{2m}).$$

We conclude that $a_{2,V}(t)$ admits an expansion of the form (2.9), and from Theorem 2.3 that $V \in H^m(\mathbb{R}^d)$.

Remark 2.6. — As observed in [13], one can use the Fourier transform of the Gaussian to express the relative trace of the heat kernel for $-\Delta + V$ in terms of the relative trace of the wave group. For $t > 0$, the following holds

$$\operatorname{Tr}\left(\mathrm{e}^{t(\Delta - V)} - \mathrm{e}^{t\Delta}\right) = \frac{1}{4\sqrt{\pi t}} \operatorname{Tr} \int_{\mathbb{R}} \mathrm{e}^{-\frac{s^2}{4t}} \left(U_V(s) - U_0(s)\right) \mathrm{d}s.$$

Although the Gaussian is not compactly supported, the estimates (2.6) and (2.7), combined with a partition of unity to decompose the integral over s, show that the right side converges in the trace-class norm if $t > 0$.

As noted in [13], if $V \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^d)$ this relates the coefficients $a_j(V)$ in (1.1) to the heat coefficients $c_j(V)$ for $-\Delta + V$. The relation also holds for finite order expansions under the assumptions in Theorem 1.1, using the fact that for $t > 0$,

$$\frac{1}{4\sqrt{\pi t}} \int_{-1}^{1} \mathrm{e}^{-\frac{s^2}{4t}}\ s^{2m}\, \epsilon(s)\, \mathrm{d}s = t^m \widetilde{\epsilon}(t),$$

where $\lim_{t\to 0^+}\widetilde{\epsilon}(t) = 0$ if $\lim_{s\to 0}\epsilon(s) = 0$. We remark that our proof expresses the $a_j(V)$ as multilinear integrals in $D^\alpha V$ with $|\alpha| \leqslant j-2$, just as for the $c_j(V)$ in [15].

In particular, Theorem 1.1 can be used to prove existence of finite order expansions of the relative trace for the heat kernel, but not vice versa. As mentioned above, the analogue of Theorem 1.1 for the heat kernel was established in [15], using only the a priori assumption $V \in L^\infty_{\mathrm{c}}$ in all dimensions, rather than $V \in \widehat{L}^1_{\mathrm{c}}$ if $d \geqslant 4$.

3. A formula for the trace of $W_{k,V}$

In this section we derive an integral formula for the trace of $\langle \phi, W_{k,V}\rangle$, which by the proof of Lemma 2.1 equals the trace of

$$4\int_{\mathbb{R}_+^{k+1}} \phi(s_1+\cdots+s_{k+1})\mathbf{C}(s_{k+1})V\mathbf{S}(s_k)V\cdots V\mathbf{S}(s_1)\,\mathrm{d}^{k+1}s.$$

Let ρ be a radial, compactly supported function on $\mathbb{R}^d$ such that $\rho(y)\geqslant 0$ and $\int\rho(y)\,\mathrm{d}y = 1$. By the proof of Lemma 2.1, we can write this as the limit as $\epsilon\to 0$ of the trace of the following operator,

$$4\int_{\mathbb{R}_+^{k+1}} \phi(s_1+\cdots+s_{k+1})\mathbf{C}(s_{k+1})V\mathbf{S}_\epsilon(s_k)V\cdots V\mathbf{S}_\epsilon(s_1)\,\mathrm{d}^{k+1}s,$$

where $\mathbf{S}_\epsilon(s_j) = \widehat{\rho}(\epsilon D)\mathbf{S}(s_j)$. For $\epsilon > 0$ the integrand is trace class for each value of s. Since the trace is cyclic, and the integral is invariant under $s_1 \leftrightarrow s_{k+1}$, we can equate this to the trace of

$$2\int_{\mathbb{R}_+^{k+1}} \phi(s_1+\cdots+s_{k+1})\mathbf{S}_\epsilon(s_k)V\cdots V\mathbf{S}_\epsilon(s_1+s_{k+1})V\,\mathrm{d}^{k+1}s,$$

which by a change of variables equals the trace of

$$2\int_{\mathbb{R}_+^{k}} s_1\phi(s_1+\cdots+s_{k})\mathbf{S}_\epsilon(s_k)V\cdots V\mathbf{S}_\epsilon(s_1)V\,\mathrm{d}^{k}s.$$

Introducing $\psi(s) = s\phi(s)$, the cyclic nature of the trace equates this with the trace of the following,

$$\frac{2}{k}\int_{\mathbb{R}_+^{k}} \psi(s_1+\cdots+s_{k})\mathbf{S}_\epsilon(s_k)V\cdots V\mathbf{S}_\epsilon(s_1)V\,\mathrm{d}^{k}s.$$

By the Plancherel formula, for $\epsilon > 0$ we can write its trace as

$$\frac{2}{k(2\pi)^{dk}}\int_{\mathbb{R}^{dk}}\int_{\mathbb{R}_+^{k}} \psi(s_1+\cdots+s_{k})\prod_{j=1}^{k}\widehat{\rho}(\epsilon\xi_j)\frac{\sin(s_j|\xi_j|)}{|\xi_j|}\,\widehat{V}(\xi_j-\xi_{j-1})\,\mathrm{d}^k s\,\mathrm{d}\xi,$$

where $\xi_0 \equiv \xi_k$. We show here that this converges, as $\epsilon \to 0$, to its value at $\epsilon = 0$, assuming $V \in L^\infty_{\mathrm{c}}$ if $k = 1, 2$, and $V \in \widehat{L}^1_{\mathrm{c}}$ if $k \geqslant 3$. The case of $V \in L^\infty_{\mathrm{c}}$ and $1 \leqslant d \leqslant 3$ will be handled in a later section.

By the proof of Lemma 2.1, the following function

$$\int_{\mathbb{R}^k_+} \psi(s_1 + \cdots + s_k) \prod_{j=1}^{k} \frac{\sin(s_j|\xi_j|)}{|\xi_j|} \, \mathrm{d}^k s$$

can be written as a sum of functions, each of which is dominated for some value of j by $(1+|\xi_j|)^{-d+1}$. Hence, it suffices by dominated convergence to show that

$$\sup_{\xi_1} \int \prod_{j=1}^{k} |\widehat{V}(\xi_j - \xi_{j-1})| \, \mathrm{d}\xi_2 \cdots \mathrm{d}\xi_k \leqslant C.$$

For $k = 1$ this holds since $V \in L^1$, and for $k = 2$ it holds since $V \in L^2$. For $k \geqslant 3$ it holds assuming $\widehat{V} \in L^1 \cap L^2$ by Young's inequality. We thus conclude the following.

Lemma 3.1. — *With $\psi(s) = s\phi(s)$, the trace of $\langle \phi, W_{k,V} \rangle$ is equal to*

$$\frac{2}{k(2\pi)^{dk}} \int_{\mathbb{R}^{dk}} \int_{\mathbb{R}^k_+} \psi(s_1 + \cdots + s_k) \prod_{j=1}^{k} \frac{\sin(s_j|\xi_j|)}{|\xi_j|} \, \widehat{V}(\xi_j - \xi_{j-1}) \, \mathrm{d}^k s \, \mathrm{d}\xi, \tag{3.1}$$

where we assume that $V \in \widehat{L}^1_{\mathrm{c}}(\mathbb{R}^d)$ if $k \geqslant 3$, and $V \in L^2_{\mathrm{c}}(\mathbb{R}^d)$ if $k = 1, 2$.

4. Proof of Theorem 2.2

For $k = 1$, we use (3.1) to write

$$\operatorname{Tr}\langle \phi, W_{1,V} \rangle = \frac{2}{(2\pi)^d} \int_{\mathbb{R}^d} \int_0^\infty \psi(s)|\xi|^{-1} \sin(s|\xi|) \widehat{V}(0) \, \mathrm{d}s \, \mathrm{d}\xi.$$

With $\psi(s) = s\phi(s)$ considered as a smooth, odd function on $\mathbb{R}$, this equals

$$\mathrm{i} \left(\int V(x) \, \mathrm{d}x \right) \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \widehat{\psi}(|\xi|)|\xi|^{-1} \, \mathrm{d}\xi$$
$$= \left(\int V(x) \, \mathrm{d}x \right) \frac{\omega_d}{(2\pi)^d} \int_0^\infty \mathrm{i} \, \tau^{d-2} \widehat{\psi}(\tau) \, \mathrm{d}\tau,$$

where $\omega_d = 2\pi^{\frac{d}{2}}/\Gamma(\frac{d}{2})$ is the area of the $d-1$ sphere.

If $d = 1$, then

$$\int_0^\infty \mathrm{i} \, \tau^{-1} \widehat{\psi}(\tau) \, \mathrm{d}\tau = \pi \int_0^\infty \psi(t) \, \mathrm{d}t = \pi \int_0^\infty t\phi(t) \, \mathrm{d}t,$$

and if $d \geqslant 3$ is odd, then

$$\int_0^\infty \mathrm{i}\,\tau^{d-2}\widehat{\psi}(\tau)\,\mathrm{d}\tau = \mathrm{i}\,\pi\big(D^{d-2}\psi\big)(0) = (d-2)\pi\big(D^{d-3}\phi\big)(0).$$

The Taylor expansion of ϕ about $t=0$ shows that, for ϕ even in t,

$$(d-2)\pi D^{d-3}\phi(0) = (-2)^{\frac{d-1}{2}}\pi^{\frac{1}{2}}\Gamma(\tfrac{d}{2})\int_0^\infty \partial_t(t^{-1}\partial_t)^{\frac{d-3}{2}}\phi(t)\,\mathrm{d}t.$$

For $d \geqslant 3$ odd this yields, assuming $\phi(t)$ is even in t,

$$\nu_d(\phi) = (-2\pi)^{\frac{1-d}{2}}\int_0^\infty \partial_t(t^{-1}\partial_t)^{\frac{d-3}{2}}\phi(t)\,\mathrm{d}t.$$

If $d=2$, then

$$\int_0^\infty \mathrm{i}\,\widehat{\psi}(\tau)\,\mathrm{d}\tau = -\int_0^\infty \partial_\tau\widehat{\phi}(\tau)\,\mathrm{d}\tau = 2\int_0^\infty \phi(t)\,\mathrm{d}t,$$

and if $d \geqslant 4$ is even, then

$$\int_0^\infty \mathrm{i}\,\tau^{d-2}\widehat{\psi}(\tau)\,\mathrm{d}\tau = (d-2)\int_0^\infty \tau^{d-3}\widehat{\phi}(\tau)\,\mathrm{d}\tau = (d-2)\pi\big(|D|^{d-3}\phi\big)(0).$$

Note that, for $\phi(t)$ even in t,

$$\int_{-\infty}^\infty t^{-1}\partial_t\phi(t)\,\mathrm{d}t = -\pi(|D|\phi)(0).$$

The following identity, which is valid for $k \geqslant 0$,

$$t\partial_t|D|^k\delta = -(k+1)|D|^k\delta,$$

shows that when $\phi(t)$ is even in t, and $k \geqslant 1$,

$$\int_0^\infty (t^{-1}\partial_t)^k\phi(t)\,\mathrm{d}t = \frac{(-1)^k\pi}{2^k(k-1)!}\big(|D|^{2k-1}\phi\big)(0).$$

Hence when $d \geqslant 4$ is even, and $\phi(t)$ is even in t,

$$\nu_d(\phi) = 2(-1)^{\frac{d-2}{2}}(2\pi)^{-\frac{d}{2}}\int_0^\infty (t^{-1}\partial_t)^{\frac{d-2}{2}}\phi(t)\,\mathrm{d}t.$$

From the above formula, this holds when $d=2$ as well.

5. Evaluation of the trace for $k \geqslant 2$ and $2k \geqslant d$

Let

$$M_k(\xi) = \int_{\Delta^{k-1}} \prod_{j=1}^k \left(\frac{\sin(s_j|\xi_j|)}{|\xi_j|}\right)\mathrm{d}\mathbf{s},$$

where Δ^{k-1} is the $k-1$-simplex,

$$\Delta^{k-1} = \{\mathbf{s} \in \mathbb{R}^k : s_1 + \cdots + s_k = 1\,,\ s_j \geqslant 0\ \ \forall j\},$$

and the measure $\mathrm{d}\mathbf{s}$ is the pullback of Lebesgue measure by the projection onto $(s_1, \dots, s_{k-1})$. Then by Lemma 3.1, we can express $\mathrm{Tr}\langle \phi, W_{k,V}\rangle$ as

$$\frac{2}{k(2\pi)^{dk}} \int_{\mathbb{R}^{dk}} \int_0^\infty t^{2k} \phi(t) M_k(t\xi) \left(\prod_{j=1}^k \widehat{V}(\xi_j - \xi_{j-1}) \right) \mathrm{d}t\, \mathrm{d}\xi.$$

Lemma 5.1. — *Suppose $V_j \in \widehat{L}^1 \cap H^m(\mathbb{R}^d)$, and let $V_j^{(m_j)} = \langle D\rangle^{m_j} V_j$. Assume that $\{m_j\} \in \mathbb{N}^k$ satisfy $m_j \leqslant m$, and $\sum_j m_j \leqslant 2m$. Then*

$$\sup_{\xi_1} \int \prod_{j=1}^k \left| \widehat{V_j^{(m_j)}}(\xi_j - \xi_{j-1}) \right| \mathrm{d}\xi_2 \cdots \mathrm{d}\xi_k \\ \leqslant (2\pi)^{d(k-1)} \Big(\sup_j \|V_j\|_{\widehat{L}^1} \Big)^{k-2} \Big(\sup_j \|V_j\|_{H^m} \Big)^2.$$

If $k=2$, the bound holds for $V_j \in H^m(\mathbb{R}^d)$.

Proof. — Note that $|\widehat{V_j^{(m_j)}}(\xi)| = \langle \xi\rangle^{m_j} |\widehat{V_j}(\xi)|$. Without loss of generality we assume $\sum_j m_j = 2m$. For each value of ξ_1, the quantity

$$\int \prod_{j=1}^k \langle \xi_j - \xi_{j-1}\rangle^{m_j} \left| \widehat{V_j}(\xi_j - \xi_{j-1}) \right| \mathrm{d}\xi_2 \cdots \mathrm{d}\xi_k$$

is a convex function of $\{m_j\}_{j=1}^k$ on the set $\sum_j m_j = 2m$, $0 \leqslant m_j \leqslant m$. By convexity, it suffices to prove the inequality in the extremal cases where $m_j = m$ for 2 values of j and $m_j = 0$ otherwise, thus $\widehat{V_j^{(m_j)}} \in L^2$ for two values of j, and $\widehat{V_j^{(m_j)}} \in L^1$ for all other values of j. For such a case the result follows by Young's inequality. □

Lemma 5.2.

$$M_k(\xi) = \sum_{j=1}^k \left(\prod_{i \neq j} \frac{1}{|\xi_i|^2 - |\xi_j|^2} \right) \frac{\sin(|\xi_j|)}{|\xi_j|}\,.$$

Proof. — We start with the equality

$$\int_0^s \sin\left((s-r)A\right)\, \sin\left(rB\right) \mathrm{d}r = \frac{B\sin(sA)}{B^2 - A^2} + \frac{A\sin(sB)}{A^2 - B^2}\,.$$

Let $r_j = s_1 + \cdots + s_j$ for $1 \leqslant j \leqslant k-1$, and $r_0 = 0$, $r_k = 1$. Repeated application of the above equality then yields

$$\int_0^1 \int_0^{r_{k-1}} \cdots \int_0^{r_2} \left(\prod_{j=1}^{k} \sin\big((r_j - r_{j-1})|\xi_j|\big) \right) \mathrm{d}r_1 \cdots \mathrm{d}r_{k-1} = \sum_{j=1}^{k} \left(\prod_{i \neq j} \frac{|\xi_i|}{|\xi_i|^2 - |\xi_j|^2} \right) \sin(|\xi_j|),$$

and we obtain the result. In evaluating the integral we use that

$$\sum_{j=1}^{k-1} \frac{1}{|\xi_j|^2 - |\xi_k|^2} \left(\prod_{i \neq j, i<k} \frac{1}{|\xi_i|^2 - |\xi_j|^2} \right) = \prod_{i=1}^{k-1} \frac{1}{|\xi_i|^2 - |\xi_k|^2}.$$

This is equivalent to

$$\sum_{j=1}^{k-1} \left(\prod_{i \neq j, i<k} \frac{|\xi_i|^2 - |\xi_k|^2}{|\xi_i|^2 - |\xi_j|^2} \right) = 1,$$

which can be seen by observing that replacing $|\xi_k|^2$ by z gives a polynomial of order $k-2$ in z that has value 1 at each of $z = |\xi_n|^2$, $n = 1, \ldots, k-1$. □

We introduce a family of functions $G_\nu(w)$ for $\nu > -1$, defined initially for $w \notin (-\infty, 0]$ by the rule

$$G_\nu(z^2) = \frac{\sqrt{\pi}}{(2z)^\nu} J_\nu(z), \quad \mathrm{Re}(z) > 0,$$

From the power series expansion of $J_\nu(z)$, see [18, 3.1(8)], we have

$$G_\nu(w) = 4^{-\nu}\sqrt{\pi} \sum_{m=0}^{\infty} \frac{(-1)^m (\frac{1}{4}w)^m}{m!\Gamma(\nu+m+1)}. \tag{5.1}$$

We remark that the function G_ν is a generalized hypergeometric function,

$$G_\nu(w) = \frac{4^{-\nu}\sqrt{\pi}}{\Gamma(\nu+1)}\, {}_0F_1\Big(\nu+1, -\frac{w}{4}\Big),$$

though we will not use this fact here. See [1, p. 362, 9.1.69].

From a standard integral formula for $J_\nu(z)$, see [18, 6.2(8)], we see that $G_\nu(z)$ is an entire function given by the following integral for any $c > 0$,

$$G_\nu(z) = \frac{4^{-\nu}\sqrt{\pi}}{2\pi\,\mathrm{i}} \int_{c-\infty\,\mathrm{i}}^{c+\infty\,\mathrm{i}} \mathrm{e}^{s - \frac{z}{4s}} \,\frac{\mathrm{d}s}{s^{\nu+1}}\,.$$

From this we easily derive the following relations,

$$\frac{\mathrm{d}}{\mathrm{d}z} G_\nu(z) = -G_{\nu+1}(z), \tag{5.2}$$

and

$$\int_0^\infty G_{\nu+\frac{1}{2}}(r^2+z)\,\mathrm{d}r = \frac{\sqrt{\pi}}{2}\,G_\nu(z). \tag{5.3}$$

We note the following special cases:

$$G_\nu(z^2) = \begin{cases} 2\cos(z), & \nu = -\frac{1}{2}, \\ \sqrt{\pi}\,J_0(z), & \nu = 0, \\ z^{-1}\sin z, & \nu = \frac{1}{2}. \end{cases} \tag{5.4}$$

Another formula for $G_\nu(z^2)$, for $\nu > -1/2$, follows from [18, 3.3(4)],

$$G_\nu(z^2) = \frac{1}{4^\nu\,\Gamma(\nu+\frac{1}{2})}\int_{-1}^1 (1-s^2)^{\nu-\frac{1}{2}}\,\mathrm{e}^{\mathrm{i}\,zs}\,\mathrm{d}s.$$

This leads to the following bound for $j \geqslant 0$ and $x \in \mathbb{R}$, which is also directly verified for $\nu = -1/2$ using (5.4).

$$\begin{aligned} \sup_{x\geqslant 0}\left|\frac{\mathrm{d}^j}{\mathrm{d}x^j}G_\nu(x^2)\right| &= \frac{2}{4^\nu\,\Gamma(\nu+\frac{1}{2})}\int_0^1 s^j(1-s^2)^{\nu-\frac{1}{2}}\,\mathrm{d}s \\ &= \frac{\Gamma(\frac{j+1}{2})}{4^\nu\,\Gamma(\frac{j}{2}+\nu+1)}. \end{aligned} \tag{5.5}$$

Lemma 5.3. — *For any smooth function* $f:\mathbb{R}\to\mathbb{C}$, *one has*

$$\sum_{j=1}^k f(x_j)\left(\prod_{i\neq j}\frac{1}{x_i-x_j}\right) = (-1)^{k-1}\int_{\Delta^{k-1}} f^{(k-1)}(s_1x_1+\cdots+s_kx_k)\,\mathrm{d}\mathbf{s}.$$

Proof. — For $k=2$, this reduces to the equality

$$\int_0^1 f'(s_1x_1+(1-s_1)x_2)\,\mathrm{d}s_1 = \frac{f(x_1)-f(x_2)}{x_1-x_2}.$$

We proceed by induction, and write

$$\begin{aligned} \int_{\Delta^k} f^{(k)}(s_1x_1+\cdots+s_kx_k+s_{k+1}x_{k+1})\,\mathrm{d}\mathbf{s} &= \frac{1}{x_k-x_{k+1}} \\ \times\int_{\Delta^{k-1}}\Big(f^{(k-1)}(s_1x_1+\cdots+s_kx_k) &- f^{(k-1)}(s_1x_1+\cdots+s_kx_{k+1})\Big)\mathrm{d}\mathbf{s} \end{aligned}$$

By the induction assumption, the latter equals

$$\frac{(-1)^{k-1}}{x_k - x_{k+1}} \sum_{j=1}^{k-1} f(x_j) \left(\prod_{\substack{i \neq j \\ i<k}} \frac{1}{x_i - x_j} \right) \left(\frac{1}{x_k - x_j} - \frac{1}{x_{k+1} - x_j} \right)$$
$$+ \frac{(-1)^{k-1}}{x_k - x_{k+1}} \left(f(x_k) \prod_{i<k} \frac{1}{x_i - x_k} - f(x_{k+1}) \prod_{i<k} \frac{1}{x_i - x_{k+1}} \right)$$
$$= (-1)^k \sum_{j=1}^{k+1} f(x_j) \left(\prod_{i \neq j} \frac{1}{x_i - x_j} \right). \quad \square$$

For $\mathbf{s} \in \Delta^{k-1}$ and $\xi \in \mathbb{R}^{dk}$, we will use the following notation,

$$\mathbf{s} \cdot \xi = \sum_{j=1}^{k} s_j \xi_j, \qquad |\xi|_{\mathbf{s}}^2 = \sum_{j=1}^{k} s_j |\xi_j|^2.$$

We can write

$$\begin{aligned} |\xi|_{\mathbf{s}}^2 &= |\mathbf{s} \cdot \xi|^2 + |\xi|_{\mathbf{s}}^2 - |\mathbf{s} \cdot \xi|^2 \\ &\equiv |\mathbf{s}\dot{\xi}|^2 + Q_{k,\mathbf{s}}(\xi). \end{aligned} \tag{5.6}$$

Note that by strict convexity of $|\cdot|^2$, for $\mathbf{s}$ in the interior of Δ^{k-1} we have $Q_{k,\mathbf{s}}(\xi) > 0$ unless $\xi_i = \xi_j$ for all i, j. Furthermore,

$$Q_{k,\mathbf{s}}(\xi_1, \xi_2, \dots, \xi_k) = Q_{k,\mathbf{s}}(0, \xi_2 - \xi_1, \dots, \xi_k - \xi_1), \tag{5.7}$$

and

$$Q_{2,\mathbf{s}}(\xi) = s_1(1 - s_1)|\xi_2 - \xi_1|^2. \tag{5.8}$$

Recalling (5.4), by Lemmas 5.2 and 5.3 we have

$$M_k(t\xi) = \int_{\Delta^{k-1}} G_{k-\frac{1}{2}}\left(t^2 |\xi|_{\mathbf{s}}^2\right) \mathrm{d}\mathbf{s}.$$

This leads to the following expression for $\mathrm{Tr}\langle \phi, W_{k,V} \rangle$, for ϕ even,

$$\frac{2}{k(2\pi)^{dk}} \int_{\Delta^{k-1}} \int_{\mathbb{R}^{dk}} \int_0^\infty t^{2k} \phi(t)\, G_{k-\frac{1}{2}}\left(t^2 |\xi|_{\mathbf{s}}^2\right) \left(\prod_{j=1}^{k} \widehat{V}(\xi_j - \xi_{j-1}) \right) \mathrm{d}t\, \mathrm{d}\xi\, \mathrm{d}\mathbf{s}.$$

For $k \geqslant 1$ and $t \geqslant 0$, we can write $G_{k-\frac{1}{2}}\big(t^2|\xi|_{\mathbf{s}}^2\big)$ as

$$\Big(\frac{-1}{2z}\frac{\mathrm{d}}{\mathrm{d}z}\Big)^{k-1}\Big(\frac{\sin z}{z}\Big)\Big|_{z=t|\xi|_{\mathbf{s}}} = \sum_{j=k}^{2k-1}\frac{1}{\big(t|\xi|_{\mathbf{s}}\big)^j}\Big(a_{k,j}\cos\big(t|\xi|_{\mathbf{s}}\big)+b_{k,j}\sin\big(t|\xi|_{\mathbf{s}}\big)\Big),$$

which shows that we can write

$$\int_0^\infty t^{2k}\phi(t)\,G_{k-\frac{1}{2}}\big(t^2|\xi|_{\mathbf{s}}^2\big)\,\mathrm{d}t = \Phi(|\xi|_{\mathbf{s}}),$$

for an even, Schwartz function Φ.

We make the volume preserving change of variables:

$$\eta_1 = \mathbf{s}\cdot\xi, \quad \eta_j = \xi_j - \xi_1 \ \text{ for } \ 2 \leqslant j \leqslant k.$$

Let $Q_{k,\mathbf{s}}(\eta') = Q_{k,\mathbf{s}}(0,\eta_2,\dots,\eta_k)$. Then by (5.7), the integrand becomes

$$t^{2k}\phi(t)G_{k-\frac{1}{2}}\Big(t^2|\eta_1|^2 + t^2 Q_{k,\mathbf{s}}(\eta')\Big)\widehat{V}(\eta_2)\widehat{V}(\eta_3-\eta_2) \times\cdots\times\widehat{V}(\eta_k-\eta_{k-1})\widehat{V}(-\eta_k).$$

This is radial in η_1. Consequently, we can express $\mathrm{Tr}\langle\phi, W_{k,V}\rangle$ as

$$\frac{4\pi^{\frac{d}{2}}}{k(2\pi)^{kd}\Gamma(\frac{d}{2})}\int_{\Delta^{k-1}}\int_{\mathbb{R}^{d(k-1)}}\int_0^\infty\int_0^\infty t^{2k}\phi(t) \times G_{k-\frac{1}{2}}\big(t^2r^2+t^2Q_{k,\mathbf{s}}(\eta')\big)\widehat{V}(\eta_2)\cdots\widehat{V}(-\eta_k)\,\mathrm{d}t\,r^{d-1}\,\mathrm{d}r\,\mathrm{d}\eta'\,\mathrm{d}\mathbf{s}. \tag{5.9}$$

By Lemma 5.1, we have that

$$\int\big|\widehat{V}(\eta_2)\widehat{V}(\eta_3-\eta_2)\cdots\widehat{V}(-\eta_k)\big|\,\mathrm{d}\eta' \leqslant (2\pi)^{d(k-1)}\|V\|_{\widehat{L}^1}^{k-2}\|V\|_{L^2}^2.$$

Assume now that $2k \geqslant d$. The above integral is oscillatory, and requires integration in t before r to be convergent. We proceed formally here and flip the integration order of t and r, but note that the following steps can be made rigorous by inserting a cutoff $\chi(\epsilon t r)$ and letting $\epsilon \to 0$. Write

$$t^d\int_0^\infty G_{k-\frac{1}{2}}\big(t^2r^2+t^2Q_{k,\mathbf{s}}(\eta')\big)\,r^{d-1}\,\mathrm{d}r = \int_0^\infty\Big(\frac{-1}{2r}\frac{\partial}{\partial r}\Big)^m G_{k-m-\frac{1}{2}}\big(r^2+t^2Q_{k,\mathbf{s}}(\eta')\big)\,r^{d-1}\,\mathrm{d}r.$$

If d is even, we take $m = \frac{d}{2}$ and integrate by parts to obtain

$$\frac{\Gamma(\frac{d}{2})}{2}G_{k-\frac{d+1}{2}}\big(t^2Q_{k,\mathbf{s}}(\eta')\big).$$

If d is odd, we take $m = \frac{d-1}{2}$, integrate by parts, and use (5.3) to obtain

$$\frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{1}{2})}\int_0^\infty G_{k-\frac{d}{2}}\big(r^2+t^2Q_{k,\mathbf{s}}(\eta')\big)\,\mathrm{d}r = \frac{\Gamma(\frac{d}{2})}{2}G_{k-\frac{d+1}{2}}\big(t^2Q_{k,\mathbf{s}}(\eta')\big).$$

We thus conclude the following.

Lemma 5.4. — *If $V \in \widehat{L}^1_{\mathrm{c}}(\mathbb{R}^d)$ and $2k \geqslant d$, then*

$$\operatorname{Tr}\langle\phi, W_{k,V}\rangle = \int_0^\infty t^{2k-d}a_{k,V}(t)\phi(t)\,\mathrm{d}t$$

where

$$(5.10)\quad a_{k,V}(t) = \frac{2\pi^{\frac{d}{2}}}{k(2\pi)^{dk}}\int_{\mathbb{R}^{d(k-1)}}\int_{\Delta^{k-1}} G_{k-\frac{d+1}{2}}\Big(t^2Q_{k,\mathbf{s}}(\eta')\Big) \times \widehat{V}(\eta_2)\widehat{V}(\eta_3-\eta_2)\cdots\widehat{V}(-\eta_k)\,\mathrm{d}\mathbf{s}\,\mathrm{d}\eta'.$$

We conclude this section with the following observation.

Lemma 5.5. — *If $2k \geqslant d$, then*

$$G_{k-\frac{d+1}{2}}(0) = \begin{cases} \frac{\pi^{\frac{1}{2}}}{2^{2k-d-1}(k-\frac{d+1}{2})!}, & d \text{ odd},\\ \frac{2(k-\frac{d}{2})!}{(2k-d)!}, & d \text{ even}.\end{cases}$$

Proof. — If d is even, we use (5.2) and (5.4) to write

$$G_{k-\frac{d+1}{2}}(0) = 2\Big(\frac{-1}{2r}\frac{\mathrm{d}}{\mathrm{d}r}\Big)^{k-\frac{d}{2}}\cos(r)\Big|_{r=0}.$$

If d is odd, we use (5.2) and (5.4) to write

$$G_{k-\frac{d+1}{2}}(0) = \sqrt{\pi}\Big(\frac{-1}{2r}\frac{\mathrm{d}}{\mathrm{d}r}\Big)^{k-\frac{d+1}{2}}J_0(r)\Big|_{r=0}.$$

The Taylor expansion for $J_0(r)$ is given by

$$J_0(r) = \sum_{j=0}^\infty \frac{(-1)^j}{(j!)^2}\Big(\frac{r}{2}\Big)^{2j},$$

which leads to the desired formula. □

6. Evaluation of the trace for $k \geqslant 2$ and $2k < d$

If $2k < d$ we cannot use Lemma 5.4. Instead, we recall (5.9) and write

$$\operatorname{Tr}\langle\phi, W_{k,V}\rangle = \int M_\phi(\eta')\,\widehat{V}(\eta_2)\widehat{V}(\eta_3-\eta_2)\cdots\widehat{V}(\eta_k-\eta_{k-1})\widehat{V}(-\eta_k)\,\mathrm{d}\eta',$$

where

$$M_\phi(\eta') = \frac{4\pi^{\frac{d}{2}}}{k(2\pi)^{kd}\Gamma(\frac{d}{2})} \times \int_{\Delta^{k-1}} \int_0^\infty \int_0^\infty t^{2k}\phi(t) G_{k-\frac12}\big(t^2r^2 + t^2 Q_{k,\mathbf{s}}(\eta')\big)\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r\,\mathrm{d}\mathbf{s}.$$

By (5.2) and (5.4) we can write

$$t^{2k} G_{k-\frac12}\big(t^2r^2 + t^2 Q_{k,\mathbf{s}}(\eta')\big) = 2\left(\frac{-1}{2r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^k \cos\left(t\sqrt{r^2 + Q_{k,\mathbf{s}}(\eta')}\right).$$

Since $\phi \in \mathcal{S}(\mathbb{R})$ we can integrate by parts in r to see that $M_\phi(\eta')$ equals

$$\frac{8\pi^{\frac{d}{2}}}{k(2\pi)^{kd}\Gamma(\frac{d-2k}{2})} \int_{\Delta^{k-1}} \int_0^\infty \int_0^\infty \phi(t)\cos\left(t\sqrt{r^2+Q_{k,\mathbf{s}}(\eta')}\right)\mathrm{d}t\, r^{d-2k-1}\,\mathrm{d}r\,\mathrm{d}\mathbf{s}$$
$$= \frac{4\pi^{\frac{d}{2}}}{k(2\pi)^{kd}\Gamma(\frac{d-2k}{2})} \int_{\Delta^{k-1}} \int_0^\infty \widehat{\phi}\left(\sqrt{r^2 + Q_{k,\mathbf{s}}(\eta')}\right) r^{d-2k-1}\,\mathrm{d}r\,\mathrm{d}\mathbf{s}.$$

A simple calculation shows the following, where $\phi \in \mathcal{S}(\mathbb{R})$ is even,

$$\frac{1}{\sigma}\frac{\mathrm{d}}{\mathrm{d}\sigma}\widehat{\left(\frac{1}{t}\frac{\mathrm{d}\phi}{\mathrm{d}t}\right)}(\sigma) = \widehat{\phi}(\sigma).$$

Hence, when $r \geqslant 0$,

$$\left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^j \left(\left(\frac{1}{t}\frac{\mathrm{d}}{\mathrm{d}t}\right)^j \phi\right)^\wedge \left(\sqrt{r^2+c}\right) = \widehat{\phi}\left(\sqrt{r^2+c}\right).$$

Consider first the case that d is even. We apply this with $j = \frac{d-2k}{2}$, and integrate by parts to see that $M_\phi(\eta')$ equals the following,

$$\frac{(-2)^{\frac{d-2k-2}{2}} 4\pi^{\frac{d}{2}}}{k(2\pi)^{kd}} \int_{\Delta^{k-1}} \int_0^\infty \frac{\mathrm{d}}{\mathrm{d}r}\Big((t^{-1}\partial_t)^{\frac{d-2k}{2}}\phi\Big)^\wedge \left(\sqrt{r^2 + Q_{k,\mathbf{s}}(\eta')}\right)\mathrm{d}r\,\mathrm{d}\mathbf{s}$$
$$= \frac{2(-1)^{\frac{d-2k}{2}}}{k2^k(2\pi)^{(k-\frac12)d}} \int_{\Delta^{k-1}} \Big((t^{-1}\partial_t)^{\frac{d-2k}{2}}\phi\Big)^\wedge \left(\sqrt{Q_{k,\mathbf{s}}(\eta')}\right)\mathrm{d}\mathbf{s}.$$

Thus, when $d \geqslant 2k$ is even, we can write

$$\mathrm{Tr}\langle \phi, W_{k,V}\rangle = \int_0^\infty a_{k,V}(t)(t^{-1}\partial_t)^{\frac{d-2k}{2}}\phi(t)\,\mathrm{d}t,$$

where

$$a_{k,V}(t) = \frac{4(-1)^{\frac{d-2k}{2}}}{k2^k(2\pi)^{(k-\frac{1}{2})d}} \times \int_{\mathbb{R}^{(k-1)d}} \int_{\Delta^{k-1}} \cos\left(t\sqrt{Q_{k,\mathbf{s}}(\eta')}\right) \widehat{V}(\eta_2)\widehat{V}(\eta_3-\eta_2)\cdots\widehat{V}(-\eta_k)\,\mathrm{d}\mathbf{s}\,\mathrm{d}\eta'. \tag{6.1}$$

Now suppose that d is odd. Similar steps, taking $j = \frac{d-2k-1}{2}$, lead to the following formula for $M_\phi(\eta')$,

$$\frac{4(-1)^{\frac{d-2k-1}{2}}}{k2^k(2\pi)^{(k-\frac{1}{2})d+\frac{1}{2}}} \int_{\Delta^{k-1}} \int_0^\infty \left((t^{-1}\partial_t)^{\frac{d-2k-1}{2}}\phi\right)^\wedge \left(\sqrt{r^2+Q_{k,\mathbf{s}}(\eta')}\right) \mathrm{d}r\,\mathrm{d}\mathbf{s}.$$

If $f \in \mathcal{S}(\mathbb{R})$ is an even function, for $c \geqslant 0$ we have

$$\begin{aligned}\widehat{f}\left(\sqrt{r^2+c}\right) &= -2\int_0^\infty f'(t)\,\frac{\sin\left(t\sqrt{r^2+c}\right)}{\sqrt{r^2+c}}\,\mathrm{d}t \\ &= -2\int_0^\infty tf'(t)\,G_{\frac{1}{2}}\left(t^2r^2+t^2c\right)\mathrm{d}t.\end{aligned}$$

Thus, by (5.3) and (5.4), we can write

$$\int_0^\infty \widehat{f}\left(\sqrt{r^2+c}\right)\,\mathrm{d}r = -\pi\int_0^\infty f'(t)J_0\left(t\sqrt{c}\right)\,\mathrm{d}t.$$

Consequently, when $d > 2k$ is odd, we can write

$$\operatorname{Tr}\langle\phi, W_{k,V}\rangle = \int_0^\infty a_{k,V}(t)\,\partial_t(t^{-1}\partial_t)^{\frac{d-2k-1}{2}}\phi(t)\,\mathrm{d}t,$$

where

$$a_{k,V}(t) = \frac{2(-1)^{\frac{d-2k+1}{2}}}{k2^k(2\pi)^{(k-\frac{1}{2})d-\frac{1}{2}}} \times \int_{\mathbb{R}^{(k-1)d}} \int_{\Delta^{k-1}} J_0\left(t\sqrt{Q_{k,\mathbf{s}}(\eta')}\right) \widehat{V}(\eta_2)\widehat{V}(\eta_3-\eta_2)\cdots\widehat{V}(-\eta_k)\,\mathrm{d}\mathbf{s}\,\mathrm{d}\eta'. \tag{6.2}$$

7. Proof of Theorem 2.3

Recall that if $k = 2$, then $Q_{2,\mathbf{s}}(\eta) = s_1(1-s_1)|\eta|^2$, where $\eta \in \mathbb{R}^d$. We begin the proof of Theorem 2.3 by analyzing the form of $a_{2,V}(t)$, and consider first the case of $1 \leqslant d \leqslant 3$, hence $2k \geqslant d$.

- If $d = 3$: we obtain from (5.10), (5.4) and (5.8) that

$$a_{2,V}(t) = \frac{1}{4(2\pi)^4}\int_{\mathbb{R}^3}\int_0^1 J_0\left(t|\eta|\sqrt{s-s^2}\right)|\widehat{V}(\eta)|^2\,\mathrm{d}s\,\mathrm{d}\eta.$$

We use the Taylor expansion of $J_0(z)$ to evaluate the integral,

$$\int_0^1 J_0\Big(t|\eta|\sqrt{s-s^2}\Big)\,\mathrm{d}s = \sum_{j=0}^{\infty}\frac{(-1)^j}{(j!)^2}\bigg(\int_0^1 s^j(1-s)^j\,\mathrm{d}s\bigg)\bigg(\frac{t|\eta|}{2}\bigg)^{2j}$$

$$= \frac{\sin(\frac12 t|\eta|)}{\frac12 t|\eta|}, \tag{7.1}$$

where we use the following special case of the beta integral

$$\int_0^1 s^j(1-s)^j\,\mathrm{d}s = \frac{(j!)^2}{(2j+1)!}\,.$$

Thus,

$$a_{2,V}(t) = \frac{1}{2(2\pi)^4}\int_{\mathbb{R}^3}\frac{\sin\big(\frac12 t|\eta|\big)}{t|\eta|}\,|\widehat V(\eta)|^2\,\mathrm{d}\eta, \qquad d=3.$$

- If $d=1$, then by (5.10),

$$a_{2,V}(t) = \frac{\pi^{\frac12}}{(2\pi)^2}\int_{\mathbb{R}}\int_0^1 G_1\big(t^2 s(1-s)|\eta|^2\big)|\widehat V(\eta)|^2\,\mathrm{d}s\,\mathrm{d}\eta.$$

Using (5.4), (5.2), and the expansion of J_0, this yields

$$a_{2,V}(t) = \frac{1}{2\pi}\int_{\mathbb{R}}\frac{1-\cos\big(\frac12 t|\eta|\big)}{t^2|\eta|^2}\,|\widehat V(\eta)|^2\,\mathrm{d}\eta, \qquad d=1.$$

- If $d=2$, then by (5.10),

$$a_{2,V}(t) = \frac{1}{2(2\pi)^3}\int_{\mathbb{R}^2}\int_0^1 G_{\frac12}\big(s(1-s)t^2|\eta|^2\big)|\widehat V(\eta)|^2\,\mathrm{d}s\,\mathrm{d}\eta.$$

- If $d\geqslant 5$ is odd, we use (6.2) and (7.1) to write $\mathrm{Tr}\langle\phi, W_{2,V}\rangle$ in the indicated form with

$$a_{2,V}(t) = \frac{(-1)^{\frac{d+1}{2}}}{2(2\pi)^{\frac{3d-1}{2}}}\int_{\mathbb{R}^d}\frac{\sin\big(\frac12 t|\eta|\big)}{t|\eta|}\,|\widehat V(\eta)|^2\,\mathrm{d}\eta. \tag{7.2}$$

Note that the same form for $a_{2,V}(t)$ holds when $d=3$, which is expected by formally writing $\partial_t(t\partial_t)^{-1}\phi = t\phi$.

- If $d\geqslant 4$ is even, we use (6.1) to write $\mathrm{Tr}\langle\phi, W_{2,V}\rangle$ in the indicated form with

$$a_{2,V}(t) = \frac{(-1)^{\frac{d}{2}}}{2(2\pi)^{\frac{3d}{2}}}\int_{\mathbb{R}^d}\int_0^1 \cos\Big(t|\eta|\sqrt{s-s^2}\Big)|\widehat V(\eta)|^2\,\mathrm{d}s\,\mathrm{d}\eta. \tag{7.3}$$

Proof of Theorem 2.3. — We present the proof for $d\geqslant 3$; the proof for $d=1,2$ follows similarly. We assume $V\in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$ is real valued.

If $d \geqslant 3$ is odd, by (7.2) the asserted form for the trace holds with

$$a_{2,V}(t) = \frac{(-1)^{\frac{d+1}{2}}}{4(2\pi)^{\frac{3d-1}{2}}} \int_{\mathbb{R}^d} G_{\frac{1}{2}}\left(t^2|\eta|^2/4\right) |\widehat{V}(\eta)|^2 \,\mathrm{d}\eta.$$

Since $|\widehat{V}(\eta)|^2$ is integrable, dominated convergence implies $a_{2,V} \in C^0\left(\overline{\mathbb{R}_+}\right)$. Furthermore, $|a_{2,V}(t)| \leqslant \|V\|_{L^2}^2/4(2\pi)^{\frac{d-1}{2}}$, and equality holds at $t = 0$.

Assume now that $V \in H^m(\mathbb{R}^d)$, where $m \geqslant 1$. Dominated convergence and differentiation under the integral shows that $a_{2,V} \in C^{2m}(\overline{\mathbb{R}_+})$. Furthermore, by (5.5),

$$|\partial_t^j a_{2,V}(t)| \leqslant \frac{1}{2^{j+2}(2\pi)^{\frac{d-1}{2}}(j+1)} \left\||D|^{\frac{j}{2}} V\right\|_{L^2}^2.$$

We note that this bound also holds for $d = 1$. For $m \geqslant 1$ we can write

$$G_{\frac{1}{2}}\left(t^2|\eta|^2/4\right) = \sum_{j=0}^{m-1} \frac{(-1)^j t^{2j}|\eta|^{2j}}{2^{2j}(2j+1)!} + (-1)^m r_{2m+1}(t|\eta|)\, t^{2m}|\eta|^{2m},$$

where $r_{2m+1}(s)$ is a nonnegative, even, real analytic function satisfying

$$r_{2m+1}(0) = \frac{1}{2^{2j}(2m+1)!}, \qquad \sup_{s\in\mathbb{R}} r_{2m+1}(s) \leqslant \frac{1}{2^{2j}(2m+1)!}.$$

By dominated convergence it follows that the expansion (2.8) holds, with

$$c_{2,j} = \frac{(-1)^{j+\frac{d+1}{2}} \||D|^j V\|_{L^2}^2}{2^{2j+2}(2\pi)^{\frac{d-1}{2}}(2j+1)!}. \tag{7.4}$$

Conversely, suppose that $V \in H^{m-1}$, and that (2.9) holds. Necessarily (7.4) holds for $0 \leqslant j \leqslant m-1$ by the above steps. We thus conclude that

$$\sup_{t\in[0,1]} \int_{\mathbb{R}^3} r_{2m+1}(t|\eta|)\, |\eta|^{2m} |\widehat{V}(\eta)|^2 \,\mathrm{d}\eta \leqslant C.$$

Since $r_{2m+1} \geqslant 0$ and $\lim_{t\to 0} r_{2m+1}(t|\eta|) = 1/2^{2j}(2m+1)!$ pointwise in η, an application of Fatou's lemma yields that $|\eta|^{2m}|\widehat{V}(\eta)|^2$ is integrable.

If $d \geqslant 4$ is even, we use (7.3) for $a_{2,V}(t)$. Dominated convergence implies $a_{2,V} \in C^0\left(\overline{\mathbb{R}_+}\right)$. Furthermore $|a_{2,V}(t)| \leqslant \|V\|_{L^2}^2/2(2\pi)^{\frac{d}{2}}$, with equality at $t = 0$.

If $V \in H^m(\mathbb{R}^d)$, differentiating under the integral sign and evaluating the beta integral shows that $a_{2,V} \in C^{2m}(\overline{\mathbb{R}_+})$, with

$$\begin{aligned}|\partial_t^j a_{2,V}(t)| &\leqslant \frac{\Gamma(\frac{j}{2}+1)^2}{2(2\pi)^{\frac{d}{2}}\Gamma(j+2)} \left\||D|^{\frac{j}{2}} V\right\|_{L^2}^2 \\ &\leqslant \frac{1}{2^{j+1}(2\pi)^{\frac{d}{2}}} \left\||D|^{\frac{j}{2}} V\right\|_{L^2}^2.\end{aligned}$$

We note that the same bounds hold for $d = 2$.

To control the remainder term in the Taylor expansion, we write

$$\cos(x) = \sum_{j=0}^{m-1} \frac{(-1)^j x^{2j}}{(2j)!} + (-1)^m r_{2m}(x^2) x^{2m}$$

where $r_{2m} \geqslant 0$, and

$$r_{2m}(0) = \frac{1}{(2m)!}, \qquad \sup_{s \in \mathbb{R}} r_{2m}(s) \leqslant \frac{1}{(2m)!}.$$

Then

$$\int_0^1 \cos\Big(t|\eta|\sqrt{s-s^2}\Big)\, \mathrm{d}s$$
$$= \sum_{j=0}^{m-1} \frac{(-1)^j (j!)^2}{(2j)!(2j+1)!}\, t^{2j}|\eta|^{2j} + (-1)^m \widetilde{r}_{2m}(t^2|\eta|^2)\, t^{2m}|\eta|^{2m},$$

where $\widetilde{r}_{2m}$ is the nonnegative function defined by

$$\widetilde{r}_{2m}(t^2|\eta|^2) = 2\int_0^1 s^m(1-s)^m r_{2m}\big(s(1-s)t^2|\eta|^2\big)\, \mathrm{d}s.$$

We conclude that

$$c_{2,j} = \frac{(-1)^{j+\frac{d}{2}}(j!)^2\, \||D|^j V\|_{L^2}^2}{2(2\pi)^{\frac{d}{2}}(2j)!(2j+1)!}\,.$$

Since $\widetilde{r}_{2m}(0) \geqslant 0$, the remainder of the proof follows as for d odd. $\square$

8. Proof of Theorem 2.4 when $d \geqslant 4$

For $d \geqslant 4$ we will deduce Theorem 2.4 from an expansion of the multiplier that determines $a_{k,V}(t)$. Recall that $Q_{k,\mathbf{s}}(\eta') = Q_{k,\mathbf{s}}(0, \eta_2, \ldots, \eta_k)$, where $Q_{k,\mathbf{s}}$ is defined in (5.6). In matrix form, $Q_{k,\mathbf{s}}$ takes the form

$$Q_{k,\mathbf{s}}(\eta') = [0, \eta_2, \ldots, \eta_k] \cdot [\mathrm{diag}(\mathbf{s}) - \mathbf{s} \otimes \mathbf{s}] \cdot [0, \eta_2, \ldots, \eta_k]^T,$$

where $\eta_i \cdot \eta_j$ is the dot product, and $\mathbf{s}$ acts by multiplying η_j by s_j. We express this in terms of the variables of $\widehat{V}$. For $1 \leqslant j \leqslant k$ let

$$\theta_j = \eta_{j+1} - \eta_j, \quad \text{where } \eta_1 = \eta_{k+1} = 0.$$

Then

$$\eta_i = \sum_{j<i} \theta_j = -\sum_{j \geqslant i} \theta_j.$$

We use these representations in the quadratic expression for $Q_{k,\mathbf{s}}(\eta')$, according to the upper or lower diagonal parts of $Q_{k,\mathbf{s}}(\eta')$, to see that

$$Q_{k,\mathbf{s}}(\eta') = \sum_{i<j} q_{k,\mathbf{s}}(i,j)\langle\theta_i,\theta_j\rangle,$$

where

$$q_{k,\mathbf{s}}(i,j) = \sum_{i<l\leqslant j}(s_\ell - s_\ell^2) - 2\sum_{i<\ell<m\leqslant j} s_\ell s_m.$$

In particular, $|q_{k,\mathbf{s}}(i,j)| \leqslant 1$. Therefore,

$$|Q_{k,\mathbf{s}}(\eta')| \leqslant \sum_{i<j}|\theta_i||\theta_j|, \qquad |Q_{k,\mathbf{s}}(\eta')|^{\frac12} \leqslant \sum_i |\theta_i|.$$

We thus conclude from Lemma 5.1 that

$$(8.1)\quad \int_{\Delta^{k-1}}\int_{\mathbb{R}^{d(k-1)}} Q_{k,\mathbf{s}}(\eta')^{\frac{j}{2}}|\widehat{V}(\eta_2)||\widehat{V}(\eta_3-\eta_2)|\cdots|\widehat{V}(-\eta_k)|\,\mathrm{d}\eta'\,\mathrm{d}\mathbf{s} \leqslant \frac{k^j(2\pi)^{d(k-1)}}{(k-1)!}\|V\|_{\widehat{L}^1}^{k-2}\|V\|^2_{H^{\lceil j/2\rceil}}.$$

Consider first the case where $2k \geqslant d$. We use (5.10) to express $a_{k,V}(t)$. Differentiation under the integral sign, together with (5.5) and (8.1), shows that if $V \in \widehat{L}^1 \cap H^m$, then $a_{k,V} \in C^{2m}(\overline{\mathbb{R}_+})$, and for $0 \leqslant j \leqslant 2m$,

$$|\partial_t^j a_{k,V}(t)| \leqslant \frac{2^{d+2-2k}\pi^{\frac{d}{2}}k^j\Gamma(\frac{j+1}{2})}{(2\pi)^d k!\Gamma(\frac{2k-d+j+1}{2})}\|V\|_{\widehat{L}^1}^{k-2}\|V\|^2_{H^{\lceil j/2\rceil}}.$$

We refer to (2.13)–(2.14), and use Lemma 2.5 to conclude that

$$\begin{aligned}|\partial_t^j \widetilde{a}_{k,V}(t)| &\leqslant \frac{k^j\,\Gamma\big(\frac{j+1}{2}\big)}{(2\pi)^{\frac{d}{2}}2^{2(k-2)}k!\Gamma\big(\frac{j+1}{2}+k-2\big)}\|V\|_{\widehat{L}^1}^{k-2}\|V\|^2_{H^{\lceil j/2\rceil}}\\ &\leqslant \frac{k^j\,\Gamma\big(\frac{1}{2}\big)}{(2\pi)^{\frac{d}{2}}2^{2(k-2)}k!\,\Gamma\big(k-\frac{3}{2}\big)}\|V\|_{\widehat{L}^1}^{k-2}\|V\|^2_{H^{\lceil j/2\rceil}}\\ &\leqslant \frac{C_d\,k^{j-2}}{(2k-4)!}\|V\|_{\widehat{L}^1}^{k-2}\|V\|^2_{H^{\lceil j/2\rceil}}. \qquad (8.2)\end{aligned}$$

If $2k < d$, then we express $\mathrm{Tr}\langle\phi, W_{k,V}\rangle$ in the form (2.10), where $a_{k,V}(t)$ is given by (6.1) or (6.2), respectively if d is even or odd. Lemma 2.5 leads to the bound (8.2) in this case as well.

We conclude that, when $V \in \widehat{L}^1 \cap H^m$, then for $j \leqslant 2m$,

$$(8.3)\qquad |\partial_t^j \alpha_V(t)| \leqslant C_d\,\|V\|^2_{\lceil j/2\rceil}\,p_j\Big(t\|V\|_{\widehat{L}^1}^{1/2}\Big)\cosh\Big(t\|V\|_{\widehat{L}^1}^{1/2}\Big),$$

where p_j is a polynomial of order at most $\max(0, j-2)$.

The Taylor polynomial for $a_{k,V}(t)$ of order $2m$ at $t=0$ is of the form

$$a_{k,V}(t) = \sum_{j=0}^{m} c_{k,j}\, t^{2j} \int_{\Delta^{k-1}} \int_{\mathbb{R}^{d(k-1)}} Q_{k,\mathbf{s}}(\eta')^j \widehat{V}(\eta_2)\cdots\widehat{V}(-\eta_k)\,\mathrm{d}\eta'\,\mathrm{d}\mathbf{s},$$

where the coefficients $c_{k,j}$ can be read off from (5.10) and (5.1). The Taylor polynomial of $\widetilde{a}_{k,V}$ can then be deduced from (2.13) and (2.14).

9. Proof of Theorem 2.4 when $d \leqslant 3$

To show that $\mathrm{Tr}\langle\phi, W_{k,V}\rangle$ admits an expansion when $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$ and $d \leqslant 3$, we establish a representation that involves a multilinear integral of V instead of $\widehat{V}$. Throughout this section we assume that $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^d)$.

Theorem 9.1. — *If $d = 1,2,3$, and $k \geqslant 2$, then one can write*

$$\mathrm{Tr}\langle\phi, W_{k,V}\rangle = \int_0^\infty t^{2k-d}\phi(t)\int_{\mathbb{R}^{dk}} \left(V(u_1)\prod_{j=2}^{k} V(u_1+tu_j)\right)\mathrm{d}\sigma_k(u')\,\mathrm{d}u_1\,\mathrm{d}t,$$

with $\mathrm{d}\sigma_k(u')$ a finite positive measure on $\mathbb{R}^{d(k-1)}$, supported in the set

$$|u_2| + |u_3-u_2| + \cdots + |u_k - u_{k-1}| + |u_k| \leqslant 1.$$

Furthermore,

$$\int \mathrm{d}\sigma_k(u') = \begin{cases} \left(2^{2k-2}k!(k-1)!\right)^{-1}, & d=1,\\ \left(\pi k(2k-2)!\right)^{-1}, & d=2,\\ \left(2^{2k-2}\pi k!(k-2)!\right)^{-1}, & d=3.\end{cases} \tag{9.1}$$

If $d=1,2$, then $\mathrm{d}\sigma_k(u')$ is absolutely continuous with respect to $\mathrm{d}u'$.

Corollary 9.2. — *For $d = 1,2,3$, and $k \geqslant 2$, one can write*

$$\mathrm{Tr}\langle\phi, W_{k,V}\rangle = \int_0^\infty t^{2k-d} a_{k,V}(t)\,\phi(t)\,\mathrm{d}t,$$

where $a_{k,V}(t) \in C(\overline{\mathbb{R}_+})$, and satisfies the following bound when $1 \leqslant p_j \leqslant \infty$ and $\sum_{j=1}^k p_j^{-1} = 1$,

$$|a_{k,V}(t)| \leqslant \left(\int \mathrm{d}\sigma_k(u')\right)\prod_{j=1}^{k}\|V\|_{p_j}.$$

Proof. — By Theorem 9.1, equality holds with

$$a_{k,V}(t)=\int_{\mathbb{R}^{3k}}\left(V(u_1)\prod_{j=2}^{k}V(u_1+tu_j)\right)\,\mathrm{d}u_1\,\mathrm{d}\sigma_k(u').$$

We apply Hölder's inequality to estimate the integral over u_1. Continuity follows by continuity of translation in L^p for $p<\infty$ and the compact support of $\mathrm{d}\sigma_k$. □

We remark that for $1\leqslant d\leqslant 3$, Corollary 9.2 and (9.1) imply

$$|a_{k,V}(t)|\leqslant\frac{\|V\|_{L^\infty}^{k-2}\|V\|_{L^2}^2}{(2k-2)!}.$$

and hence

$$\begin{aligned}|\alpha_V(t)|&=\left|\sum_{k=2}^{\infty}(-1)^k t^{2(k-2)}a_{k,V}(t)\right|\\&\leqslant\|V\|_{L^2}^2\,\cosh\Big(t\,\|V\|_{L^\infty}^{1/2}\Big).\end{aligned}$$

To prove Theorem 9.1, we recall from Section 3 that

$$\operatorname{Tr}\langle\phi,W_{k,V}\rangle=\lim_{\epsilon\to 0}\operatorname{Tr}\left(\frac{2}{k}\int_{\mathbb{R}_+^k}\psi(s_1+\cdots+s_k)\mathbf{S}_\epsilon(s_k)V\cdots V\mathbf{S}_\epsilon(s_1)V\,\mathrm{d}^k s\right).$$

For $1\leqslant d\leqslant 3$, the operator $\mathbf{S}_\epsilon(s)$ is convolution with respect to the measure $\rho_\epsilon*\mathbf{S}(s,x)$, where $\rho_\epsilon(x)=\epsilon^{-d}\rho(\epsilon^{-1}x)$, and

$$\mathbf{S}(s,x)=\begin{cases}\frac{1}{2}\mathbf{1}_{[-s,s]}(x), & d=1,\\ (2\pi)^{-1}\big(s^2-|x|^2\big)_+^{-1/2}, & d=2,\\ (4\pi|x|)^{-1}\delta(s-|x|), & d=3.\end{cases}$$

The kernel of $\mathbf{S}_\epsilon(s,x)$ is smooth and compactly supported, and for $V\in L^\infty_{\mathrm{c}}$ the trace is given by integrating the kernel of the composition over the diagonal. This leads to the following formula for $\operatorname{Tr}\langle\phi,W_{k,V}\rangle$,

$$\lim_{\epsilon\to 0}\frac{2}{k}\int_{\mathbb{R}^{dk}}\int_{\mathbb{R}_+^k}\psi(s_1+\cdots+s_k)\prod_{j=1}^{k}\mathbf{S}_\epsilon(s_j,x_{j+1}-x_j)V(x_j)\,\mathrm{d}^k s\,\mathrm{d}x.$$

We proceed to analyze the limit, starting with the case $d=3$.

9.1. The case $d = 3$

Lemma 9.3. — *Let $d = 3$ and $\psi(s) = s\phi(s)$, and assume $V \in L^\infty_{\mathrm{c}}(\mathbb{R}^3)$. Then $\mathrm{Tr}\langle \phi, W_{k,V}\rangle$ is equal to the following, where $x_{k+1} \equiv x_1$,*

$$\frac{2}{k(4\pi)^k}\int_{\mathbb{R}^{3k}} \psi\left(|x_2 - x_1| + \cdots + |x_1 - x_k|\right)\prod_{j=1}^{k}\frac{V(x_j)}{|x_{j+1} - x_j|}\,\mathrm{d}x.$$

Proof. — Let $\mathrm{d}\Gamma(s,y) = (4\pi|y|)^{-1}\delta(s - |y|)$ denote $2^{-\frac{1}{2}}|y|$ times surface measure on the forward light cone $|y| = s$. Then by the above, we can write $\mathrm{Tr}\langle \phi, W_{k,V}\rangle$ as $2k^{-1}$ times the following

$$\lim_{\epsilon\to 0}\int \psi(s_1 + \cdots + s_k)\prod_{j=1}^{k}\rho_\epsilon(x_{j+1} - x_j - y_j)\,V(x_j)\,\mathrm{d}\Gamma(s_j, y_j)\,\mathrm{d}y\,\mathrm{d}^k s\,\mathrm{d}x.$$

The integrand is bounded and of compact support, so we may integrate first over s to see this equals

$$\frac{2}{k(4\pi)^k}\lim_{\epsilon\to 0}\int \frac{\psi\big(|y_1| + \cdots + |y_k|\big)}{|y_1|\cdots|y_k|}\left(\prod_{j=1}^{k}\rho_\epsilon(x_{j+1} - x_j - y_j)\,V(x_j)\right)\mathrm{d}y\,\mathrm{d}x.$$

Consider the function

$$\mu_\epsilon(x) = \int \frac{\psi\big(|y_1| + \cdots + |y_k|\big)}{|y_1|\cdots|y_k|}\left(\prod_{j=1}^{k}\rho_\epsilon(x_{j+1} - x_j - y_j)\right)\mathrm{d}y.$$

From the bound

$$\sup_{\epsilon>0}\int_{\mathbb{R}^3}|\rho_\epsilon(z_j - y_j)|\,|y_j|^{-1} \leqslant C\,|z_j|^{-1},$$

we conclude that

$$|\mu_\epsilon(x)| \leqslant C\prod_{j=1}^{k}\frac{1}{|x_{j+1} - x_j|}.$$

The right hand side is integrable over bounded sets in $\mathbb{R}^{3k}$, as seen from the fact that $|x|^{-1} \in L^1_{\mathrm{loc}} \cap L^2_{\mathrm{loc}}(\mathbb{R}^3)$. Additionally,

$$\lim_{\epsilon\to 0}\mu_\epsilon(x) = \psi\left(|x_2 - x_1| + \cdots + |x_1 - x_k|\right)\prod_{j=1}^{k}\frac{1}{|x_{j+1} - x_j|}$$

at points where $x_{j+1} \neq x_j$. Lebesgue dominated convergence then implies the conclusion of the lemma. □

We introduce variables $x_1 = u_1$, and $x_j = u_1 + u_j$ for $2 \leqslant j \leqslant k$, to write the trace as

$$\frac{2}{k(4\pi)^k} \int_{\mathbb{R}^{3k}} \psi(f(u')) \frac{V(u_1)V(u_1+u_2)\cdots V(u_1+u_k)}{|u_2||u_3-u_2|\cdots|u_k-u_{k-1}||u_k|} \,\mathrm{d}u'\,\mathrm{d}u_1,$$

where

$$f(u') = |u_2| + |u_3 - u_2| \cdots + |u_k - u_{k-1}| + |u_k|.$$

The function f is smooth on the open subset of $\mathbb{R}^{3(k-1)}$ where $u_{j+1} \neq u_j$, and $u_2 \neq 0$, $u_k \neq 0$. Furthermore, with the convention $u_1 = u_{k+1} = 0$,

$$\nabla_{u_j} f(u') = \frac{u_j - u_{j-1}}{|u_j - u_{j-1}|} - \frac{u_{j+1} - u_j}{|u_{j+1} - u_j|},$$

which vanishes exactly when u_j lies in the convex hull $[u_{j-1}, u_{j+1}]$. Let Ω be the open subset of $\mathbb{R}^{3(k-1)}$ where $u_2, u_k \neq 0$, and no three u_j's are colinear. Then f has non-zero gradient with respect to each u_j at all points in Ω, and since the complement of Ω is measure 0 we may write

$$\operatorname{Tr}\langle \phi, W_{k,V}\rangle = \int_0^\infty \phi(t) \int_{\mathbb{R}^{3k}} \left(V(u_1) \prod_{j=2}^k V(u_1 + u_j) \right) \mathrm{d}\sigma_{k,t}(u')\,\mathrm{d}u_1\,\mathrm{d}t,$$

where $\mathrm{d}\sigma_{k,t}(u')$ is the following positive measure,

$$\mathrm{d}\sigma_{k,t}(u') = \frac{2}{k(4\pi)^k} \frac{t\delta\big(t - f(u')\big)\,\mathbf{1}_\Omega(u')}{|u_2||u_3-u_2|\cdots|u_k-u_{k-1}||u_k|}\,\mathrm{d}u'.$$

If we denote $\mathrm{d}\sigma_k(u') = \mathrm{d}\sigma_{k,1}(u')$, then by changing $u' \to tu'$, we obtain

$$\operatorname{Tr}\langle \phi, W_{k,V}\rangle = \int_0^\infty \phi(t)\, t^{2k-3} \int_{\mathbb{R}^{3k}} \left(V(u_1) \prod_{j=2}^k V(u_1 + tu_j) \right) \mathrm{d}\sigma_k(u')\,\mathrm{d}u_1\,\mathrm{d}t.$$

The above steps show more generally that

$$\begin{aligned}\operatorname{Tr}&\left(\frac{2}{k} \int_{\mathbb{R}^k_+} \psi(s_1 + \cdots + s_k)\mathbf{S}(s_k)V_k \cdots V_2\,\mathbf{S}(s_1)V_1\,\mathrm{d}^k s \right)\\ &\quad= \int_0^\infty \phi(t)\, t^{2k-3} \int_{\mathbb{R}^{3k}} \left(V_1(u_1) \prod_{j=2}^k V_j(u_1 + tu_j) \right) \mathrm{d}\sigma_k(u')\,\mathrm{d}u_1\,\mathrm{d}t.\end{aligned}$$

The proof of Lemma 5.4 shows that when $d \leqslant 2k$, this equals

$$\begin{aligned}\frac{2\pi^{\frac{d}{2}}}{k(2\pi)^{dk}} \int_0^\infty \phi(t)\, t^{2k-d} \int_{\mathbb{R}^{d(k-1)}} \int_{\Delta^{k-1}} G_{k-\frac{d+1}{2}}\big(t^2 Q_{k,\mathbf{s}}(\eta')\big)&\\ \times \widehat{V_2}(\eta_2)\widehat{V_3}(\eta_3 - \eta_2) \cdots \widehat{V_k}(\eta_k - \eta_{k-1})\widehat{V_1}(-\eta_k)\,\mathrm{d}\mathbf{s}\,\mathrm{d}\eta'\,\mathrm{d}t.&\end{aligned}$$

This yields the relation, with $d = 3$ in this case, and $k \geqslant 2$,

$$\widehat{\mathrm{d}\sigma_k}(-\eta') = \frac{2\pi^{\frac{d}{2}}}{k(2\pi)^d} \int_{\Delta^{k-1}} G_{k-\frac{d+1}{2}}\big(Q_{k,\mathbf{s}}(\widetilde{\eta})\big)\,\mathrm{d}\mathbf{s}, \tag{9.2}$$

where

$$\widetilde{\eta} = (0, \eta_2, \eta_2 + \eta_3, \ldots, \eta_2 + \cdots + \eta_{k-1} + \eta_k).$$

By Lemma 5.5, for $d = 3$ we deduce that

$$\int_{\mathbb{R}^{3(k-1)}} \mathrm{d}\sigma_k(u') = \frac{1}{2^{2k-2}\pi k!(k-2)!}\,.$$

9.2. The case $d = 1$

A similar analysis, using the formula for the case $d = 1$:

$$\mathbf{S}(s; x, y) = \frac{1}{2}\mathbf{1}_{[-s,s]}(x - y)$$

leads to the following formula,

$$\operatorname{Tr}\langle \phi, W_{k,V}\rangle = \int_0^\infty \phi(t)\, t^{2k-1} \int_{\mathbb{R}^k} \left(V(u_1) \prod_{j=2}^{k} V(u_1 + t u_j) \right) \rho_k(u')\,\mathrm{d}u'\,\mathrm{d}u_1,$$

where

$$\rho_k(u') = \frac{1}{2^{k-1}k!}\big(1 - f(u')\big)_+^{k-1}.$$

By (9.2) and Lemma 5.5, we have

$$\int_{\mathbb{R}^{k-1}} \rho_k(u')\,\mathrm{d}u' = \frac{1}{2^{2k-2}k!(k-1)!}.$$

9.3. The case $d = 2$

If $d = 2$ we do not have a closed form for $\mathrm{d}\sigma_k(u')$, but observe that it is an integrable function for $k \geqslant 2$. For this, we note that $\mathrm{d}\sigma_k(u') = \rho_k(u')\,\mathrm{d}u'$, where $\rho_k(u')$ equals $2/k(2\pi)^k$ times the following,

$$\int_{\Delta^{k-1}} \big(s_1^2 - |u_2|^2\big)_+^{-1/2} \big(s_2^2 - |u_3 - u_2|^2\big)_+^{-1/2} \cdots \big(s_k^2 - |u_k|^2\big)_+^{-1/2}\,\mathrm{d}\mathbf{s}.$$

For $k = 2$, one has the estimate for $|u_2| \leqslant \frac{1}{2}$,

$$\int_{|u_2|}^{1-|u_2|} \big(s^2 - |u_2|^2\big)^{-\frac{1}{2}} \big((1-s)^2 - |u_2|^2\big)^{-\frac{1}{2}}\,\mathrm{d}s \approx 1 + |\log(1 - 2|u_2|)|.$$

We next observe that

$$\Big\| \big(s^2 - |u|^2\big)_+^{-1/2} \Big\|_{L^p(\mathbb{R}^2,\, \mathrm{d}u)} = C_p\, s^{\frac{2}{p}-1}, \quad 1 \leqslant p < 2.$$

When $k \geqslant 3$ we take $p = k/(k-1)$, and use the Hölder and Young inequalities to see that

$$\int_{\mathbb{R}^{2(k-1)}} \big(s_1^2 - |u_2|^2\big)_+^{-1/2} \big(s_2^2 - |u_3 - u_2|^2\big)_+^{-1/2} \cdots \big(s_k^2 - |u_k|^2\big)_+^{-1/2} \,\mathrm{d}u' \leqslant C_k \prod_{j=1}^{k} s_j^{1-\frac{2}{k}}.$$

Tonelli's theorem now implies integrability of $\rho_k(u')$. Lemma 5.5 and (9.2) yield

$$\int \rho_k(u')\,\mathrm{d}u' = \frac{1}{\pi k(2k-2)!}\,.$$

Proof of Theorem 2.4 for $d \leqslant 3$. The first part of Theorem 2.4 follows from Corollary 9.2, so it remains to establish differentiability of $a_{k,V}$. We first consider the case $m = 1$, and show that $a_{k,V}(t) \in C^2(\overline{\mathbb{R}_+})$, with bounds

$$\begin{aligned} |\partial_t a_{k,V}(t)| &\leqslant (k-1)\Big(\int \mathrm{d}\sigma_k(u')\Big) \|\nabla V\|_{L^2} \|V\|_{L^2} \|V\|_{L^\infty}^{k-2}, \\ |\partial_t^2 a_{k,V}(t)| &\leqslant (k-1)^2\Big(\int \mathrm{d}\sigma_k(u')\Big) \|\nabla V\|_{L^2}^2 \|V\|_{L^\infty}^{k-2}. \end{aligned} \tag{9.3}$$

We present the details for $d = 3$. Assume $V \in L^\infty_{\mathrm{c}} \cap H^1(\mathbb{R}^3)$, and consider

$$a_{k,V}(t) = \int V(u_1) \left(\prod_{j=2}^{k} V(u_1 + t u_j) \right) \mathrm{d}u_1\, \mathrm{d}\sigma_k(u').$$

If we apply ∂_t to $a_{k,V}(t)$, we formally obtain the following

$$\sum_{j=2}^{k} \int V(u_1) \left(\prod_{i \neq 1, j} V(u_1 + t u_i) \right) \big(\langle u_j, \nabla\rangle V\big)(u_1 + t u_j)\, \mathrm{d}u_1\, \mathrm{d}\sigma_k(u').$$

That this equals $\partial_t a_{k,V}(t)$ can be proven rigorously by taking difference quotients, using Hölder's inequality as in Corollary 9.2, continuity of translation in L^p for $p < \infty$, and the following, which holds for $V \in H^1(\mathbb{R}^d)$,

$$\lim_{h \to 0} \sup_{|u_j| \leqslant 1} \left\| \frac{V(u_1 + h u_j) - V(u_1)}{h} - \big(\langle u_j, \nabla\rangle V\big)(u_1) \right\|_{L^2(\mathrm{d}u_1)} = 0. \tag{9.4}$$

Setting $u_1 = tx_1$, $u_i = x_i - x_1$ for $i > 1$, then expresses $\partial_t a_{k,V}(t)$ as

$$c_k \sum_{j=1}^{k} t^3 \int_{\mathbb{R}^{dk}} \frac{\Big(\prod_{i\neq j} V(tx_i)\Big)\big(\langle x_j - x_1, \nabla\rangle V\big)(tx_j)}{|x_2 - x_1|\cdots|x_k - x_{k-1}||x_1 - x_k|} \times \delta\left(1 - \sum_i |x_{i+1} - x_i|\right) \mathrm{d}x.$$

We make a cyclic relabeling of the indices that takes j to 1, and reverse the above change of variables to see that $\partial_t a_{k,V}(t)$ is equal to

$$-c_k \sum_{j=2}^{k} \int \big(\langle u_j, \nabla\rangle V\big)(u_1) \left(\prod_{i=2}^{k} V(u_1 + tu_i)\right) \mathrm{d}u_1 \, \mathrm{d}\sigma_k(u').$$

Differentiation in t now leads to the formula

$$\partial_t^2 a_{k,V}(t) = c_k \sum_{i,j=2}^{k} \int \big(\langle u_j, \nabla\rangle V\big)(u_1)\big(\langle u_i, \nabla\rangle V\big)(u_1 + tu_i) \times \left(\prod_{m\neq 1,i} V(u_1 + tu_m)\right) \mathrm{d}u_1 \, \mathrm{d}\sigma_k(u').$$

Since $|u_j| \leqslant 1$ on the support of $\mathrm{d}\sigma_k(u')$, this will imply the bound (9.3).

To prove that $\partial_t^2 a_{k,V}$ is continuous requires more care than for $\partial_t a_{k,V}$, as translation is not strongly continuous in $L^\infty(\mathbb{R}^d)$. Instead, we observe that, by absolute continuity of the Lebesgue integral, the integral of $|\nabla V|^2$ over any set of measure ϵ is less than δ, where $\delta \to 0$ as $\epsilon \to 0$. For each ϵ we can use Lusin's Theorem to write V as a sum of a continuous function plus a function supported in a set of measure ϵ. For the continuous part we can apply continuity of translation as before, and we conclude that the above integral is continuous in t. Similar steps and (9.4) justify convergence of the difference quotients of $\partial_t a_{k,V}$ to the above formula for $\partial_t^2 a_{k,V}$.

For $m \geqslant 2$, we can apply the above proof and induction to see that $a_{k,V} \in C^{2m}(\overline{\mathbb{R}_+})$. Additionally, $\partial_t^j a_{k,V}(t)$ can be written as a sum of at most $(k-1)^j$ terms, each of the form

$$\int \big(\langle u, \nabla\rangle^{j_1} V\big)(u_1) \left(\prod_{m=2}^{k} \big(\langle u, \nabla\rangle^{j_m} V\big)(u_1 + tu_m)\right) \mathrm{d}u_1 \, \mathrm{d}\sigma_k(u'),$$

where $\langle u, \nabla\rangle$ indicates some $\langle u_i, \nabla\rangle$, possibly different in each occurrence, and

$$\max j_i \leqslant \lceil j/2 \rceil, \qquad \sum_{i=1}^{k} j_i = j.$$

The Gagliardo–Nirenberg inequalities, see [15, Lemma 3.4] which follows from [16, (3.17) in §13.3], then bounds

$$|\partial_t^j a_{k,V}(t)| \leqslant C_{d,j}(k-1)^j \left(\int \mathrm{d}\sigma_k(u') \right) \|V\|_{L^\infty}^{k-2} \|V\|_{\lceil j/2 \rceil}^2 .$$

In particular, the identities (9.1) imply

$$|\partial_t^j a_{k,V}(t)| \leqslant \frac{C_{d,j}(k-1)^j}{(2k-2)!} \|V\|_{L^\infty}^{k-2} \|V\|_{\lceil j/2 \rceil}^2 . \tag{9.5}$$

We may then sum over k to obtain the bound (2.11) with $X_d = L^\infty_{\mathrm{c}}$. □

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