A DIXMIER TRACE FORMULA FOR THE DENSITY OF STATES

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Abstract. A version of Connes trace formula allows to associate a measure on the essential spectrum of a Schrödinger operator with bounded potential. In solid state physics there is another celebrated measure associated with such operators — the density of states. In this paper we demonstrate that these two measures coincide.

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1. Introduction

Let \( d \geq 2 \), and let

\[
H = -\Delta + M_V
\]

be a Schrödinger operator on \( \mathbb{R}^d \), where \( \Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \) is the Laplace operator and \( V \) is a bounded real-valued measurable potential \( V \in L_\infty(\mathbb{R}^d) \). The density of states (or DOS) is a Borel measure \( \nu_H \) on \( \mathbb{R} \) naturally associated to \( H \), see e.g. [1, 29], defined as follows. Let \( L > 0 \), and let \( H_L \) be the restriction of \( H \) to the cube \((-L, L)^d\) with Dirichlet boundary conditions (for a definition see e.g. [25, §VI.4.4], [32, §XIII.15]). Let \( I \subset \mathbb{R} \) be a bounded interval, and let \( N_L(I) \) be the number of eigenvalues with multiplicities of \( H_L \) in \( I \) (which is necessarily finite, since \( H_L \) has compact resolvent). The density of states measure \( \nu_H \) of \( I \) is defined as

\[
\nu_H(I) = \lim_{L \to \infty} \frac{N_L(I)}{\text{Vol}((-L, L)^d)}
\]

The DOS measure does not always exist, see e.g. [37, p. 513]. However, it is well known to exist for certain classes of Hamiltonians important for solid state physics such as those corresponding to periodic, almost periodic and ergodic potentials, see
Another point to mention here is that the density of states measure $\nu_H$ has several definitions. The difference is in the choice of domain in the limit (1.2): one can replace the cubes $\{(-L, L)^d\}_{L>0}$ with a family of balls or other domains. There is also some variation in the choice of boundary conditions used to define $H_L$ (such as Dirichlet, Neumann, periodic, etc.). For our purposes it will be convenient to use yet another definition (see e.g. [37, (C41)], [21, (1.2)]) in terms of the spectral projections of $H$, as follows

$$\nu_H(I) = \lim_{R \to \infty} \frac{1}{\text{Vol}(B(0, R))} \text{Tr} \left( M_{\chi_{B(0, R)}} \chi_I(H) M_{\chi_{B(0, R)}} \right),$$

where $B(0, R)$ is the ball of radius $R$ centred at zero, $M_f$ is the operator of multiplication by a function $f$ on $L^2(\mathbb{R}^d)$, $\text{Tr}$ is the standard operator trace and $\chi_A$ is the indicator function of a set $A$. It is known that, assuming existence, these different definitions of DOS coincide at least for such important classes of potentials as periodic or ergodic, see e.g. [37, Theorem C.7.4] and [21]. In this paper we will assume existence of the limit (1.3).

The second measure which can be associated with $H$ comes from a version of Connes’ trace formula [19], [23, Corollary 7.21], [28, Theorem 11.7.5]. One form of Connes trace formula asserts that for all continuous and compactly supported functions $f$ on $\mathbb{R}^d$, we have:

$$\text{Tr}_\omega \left( M_f (1 - \Delta)^{-d/2} \right) = \frac{\omega_d}{d(2\pi)^d} \int_{\mathbb{R}^d} f(t) \, dt,$$

where $\text{Tr}_\omega$ is a Dixmier trace on the ideal $L^1(L_2(\mathbb{R}^d))$, and

$$\omega_d = \frac{2\pi^{d/2}}{\Gamma \left( \frac{d}{2} \right)}$$

is the $(d-1)$-volume of the unit sphere $S^{d-1}$. For our purpose it is desirable to rewrite this formula in the Fourier transform picture, as follows:

$$\text{Tr}_\omega \left( f(-i\nabla) M^{-d}_{(x)} \right) = \frac{\omega_d}{d(2\pi)^d} \int_{\mathbb{R}^d} f(t) \, dt,$$

where $\nabla = (\partial_1, \ldots, \partial_d)$ is the gradient operator, $f(-i\nabla)$ is defined via functional calculus, and

$$(x) = (1 + |x|^2)^{1/2}.$$ 

We would like to rewrite this formula in terms of the Laplacian $-\Delta$ rather than the gradient operator $\nabla$. To this end, consider the case where $f$ is a radial function, and therefore $f(-i\nabla)$ can be written as $g(-\Delta)$ for some continuous compactly supported function $g$ on $[0, \infty)$. Then by switching to polar coordinates we have

$$\text{Tr}_\omega \left( g(-\Delta) M^{-d}_{(x)} \right) = \frac{\omega_d}{d(2\pi)^d} \int_{\mathbb{R}^d} g(|x|^2) \, dx$$

$$= \frac{\omega_d}{d(2\pi)^d} \int_{S^{d-1}} \int_0^\infty g(r^2) r^{d-1} \, dr \, ds$$

$$= \frac{\omega_d^2}{d(2\pi)^d} \int_0^\infty g(r^2) r^{d-1} \, dr$$

$$= \frac{\omega_d^2}{2d(2\pi)^d} \int_0^\infty g(\lambda) \lambda^{d-1} \, d\lambda.$$
Now, let $V \in L_\infty(\mathbb{R}^d)$ be a real-valued potential. Our main result is the following:

**Theorem 1.1.** Let $H = -\Delta + M_V$ be a Schrödinger operator on $L_2(\mathbb{R}^d)$, where $V$ is a bounded real-valued measurable potential. For any $g \in C_c(\mathbb{R})$ the operator

$$g(H)M_{(x)}^{-d}$$

belongs to the weak trace-class ideal $L_1,\infty(L_2(\mathbb{R}^d))$. If we assume that the density of states of $H$ (defined according to (1.3)) exists and is a Borel measure $\nu_H$ on $\mathbb{R}$, then for every Dixmier trace $\text{Tr}_\omega$ on $L_1,\infty$ there holds the equality

$$(1.5) \quad \text{Tr}_\omega \left( g(H)M_{(x)}^{-d} \right) = \frac{\omega_d}{d} \int_{\mathbb{R}} g \, d\nu_H.$$

It is instructive to consider the simplest case, $V = 0$, which also serves to compute the constant in (1.5).

**Example 1.2.** For $H_0 = -\Delta$ we have

$$\text{Tr}_\omega(g(H_0)M_{(x)}^{-d}) = \left( \frac{\omega_d}{d} \int_{\mathbb{R}} g(\lambda) d\nu_{H_0}(\lambda) \right)$$

for all $g \in C_c(\mathbb{R})$.

**Proof.** We shall verify that:

$$\text{Tr}_\omega(e^{-tH_0}M_{(x)}^{-d}) = \frac{\omega_d}{d} \int_0^\infty e^{-t\lambda} \, d\nu_{H_0}(\lambda), \quad t > 0.$$  

This suffices to ensure that the equality holds for all $g \in C_c(\mathbb{R})$ (see the argument in Remark 5.3) provided both sides exist. The existence of the left-hand side follows from classical Cwikel estimates, or may be derived from the Cwikel estimates given below in Section 3. That there is indeed an explicitly computable density of states measure for this case is well known (see e.g. [37, Theorem C.7.7]).

Connes’ integration formula in the form (1.4) yields:

$$\text{Tr}_\omega(e^{t\Delta}M_{(x)}^{-d}) = \frac{\omega_d}{d(2\pi)^d} \int_{\mathbb{R}^d} e^{-t|x|^2} \, dx = \frac{\omega_d}{d(2\pi)^d} \left( \frac{\pi}{t} \right)^{d/2} = \frac{\omega_d}{d} (4\pi t)^{-d/2}.$$  

We may compare this to $\int_0^\infty e^{-t\lambda} \, d\nu_{H_0}(\lambda)$ using (1.3). According to [37, Proposition C.7.2], it suffices to compute:

$$\lim_{R \to \infty} \frac{1}{|B(0, R)|} \text{Tr}(M_{x_B(0, R)} e^{-tH_0}).$$

The semigroup $e^{-tH_0}$ has integral kernel (see e.g. [31, §IV.7, Example 3]):

$$K_t(x, y) = (4\pi t)^{-d/2} e^{-\frac{|x-y|^2}{4t}}.$$  

Hence $K_t(x, x) = (4\pi t)^{-d/2}$ is constant, and we have:

$$\frac{1}{|B(0, R)|} \text{Tr}(M_{x_B(0, R)} e^{-tH_0}) = \frac{1}{|B(0, R)|} \int_{B(0, R)} (4\pi t)^{-d/2} \, dx = (4\pi t)^{-d/2}.$$  

$\square$
Theorem 1.1 observes a direct connection between two measures which can naturally be associated with the operator (1.1). Since these two measures a priori have very different definitions, this connection ought to be considered as somewhat surprising. At the same time, both measures do share some obvious common properties. Indeed, both measures are invariants of a Schrödinger operator (1.1), both are supported on the essential spectrum of $H$ and they both exhibit certain robustness. Namely, the Dixmier trace $\text{Tr}_\omega$, used in the definition of one of these measures, is insensitive to trace class perturbations, while the density of states measure $\nu_H$ is insensitive to localised perturbations $V_0 + V$ of the bounded potential $V_0$, [37, Theorem C.7.7, Theorem C.7.8] reflecting the fact that DOS is a property of the behaviour of the potential $V$ at infinity.

2. Preliminaries

2.1. Trace ideals. The following material is standard; for more details we refer the reader to [28, 36]. Let $\mathcal{H}$ be a complex separable Hilbert space, and let $\mathcal{B}(\mathcal{H})$ denote the set of all bounded operators on $\mathcal{H}$, and let $\mathcal{K}(\mathcal{H})$ denote the ideal of compact operators on $\mathcal{H}$. Given $T \in \mathcal{K}(\mathcal{H})$, the sequence of singular values $\mu(T) = \{\mu(k, T)\}_{k=0}^\infty$ is defined as:

\[ \mu(k, T) = \inf\{\|T - R\| : \text{rank}(R) \leq k\}. \]

Let $p \in (0, \infty)$. The Schatten class $\mathcal{L}_p$ is the set of operators $T$ in $\mathcal{K}(\mathcal{H})$ such that $\mu(T)$ is $p$-summable, i.e. in the sequence space $\ell_p$. If $p \geq 1$ then the $\mathcal{L}_p$ norm is defined as:

\[ \|T\|_p := \|\mu(T)\|_{\ell_p} = \left( \sum_{k=0}^\infty \mu(k, T)^p \right)^{1/p}. \]

With this norm $\mathcal{L}_p$ is a Banach space, and an ideal of $\mathcal{B}(\mathcal{H})$.

The weak Schatten class $\mathcal{L}_{p,\infty}$ is the set of operators $T$ such that $\mu(T)$ is in the weak $\mathcal{L}_p$-space $\ell_{p,\infty}$, with quasi-norm:

\[ \|T\|_{p,\infty} = \sup_{k \geq 0} (k+1)^{1/p}\mu(k, T) < \infty. \]

As with the $\mathcal{L}_p$ spaces, $\mathcal{L}_{p,\infty}$ is an ideal of $\mathcal{B}(\mathcal{H})$. We also have the following form of Hölder’s inequality,

\[ \|TS\|_{r,\infty} \leq c_{p,q} \|T\|_{p,\infty} \|S\|_{q,\infty} \]

where $\frac{1}{r} = \frac{1}{p} + \frac{1}{q}$, for some constant $c_{p,q}$. Indeed, this follows from the definition of the weak $\mathcal{L}_p$-quasinorms and the inequality $\mu(2n, TS) \leq \mu(n, T)\mu(n, S)$ for $n \geq 1$ [21, Proposition 1.6], [22, Corollary 2.2].

Note that if $r > p$, then we have the inequality:

\[ \|T\|_r^r = \sum_{k=0}^\infty \mu(k, T)^r \leq \sum_{k=0}^\infty (k+1)^{-\frac{r}{p}} \|T\|_{p,\infty} \|S\|_{q,\infty} = \zeta\left(\frac{r}{p}\right) \|T\|_{p,\infty} \]

where $\zeta$ is Riemann’s zeta function.

For $q \in (1, \infty)$, we also consider the ideal $\mathcal{L}_{q,1}$, defined as the set of compact operators $T$ on $\mathcal{H}$ satisfying:

\[ \|T\|_{\mathcal{L}_{q,1}} := \sum_{n \geq 0} \mu(n, T) \frac{\mu(n, T)^{q-1}}{(n+1)^{q-1}} < \infty. \]
We have the following Hölder-type inequality: if $\frac{1}{p} + \frac{1}{q} = 1$ then
\begin{equation}
\|TS\|_1 \leq \|T\|_{p,\infty} \|S\|_{q,1}
\end{equation}
(see e.g. [16, p. 303]).

For this paper, the relevant continuous embeddings between these ideals are
\begin{equation}
L_{p,\infty} \subset L_q, \quad L_{p,\infty} \subset L_{q,1}, \quad 0 < p < q \leq \infty
\end{equation}
(see e.g. [16, §IV.2.2, Proposition 1]).

Among ideals of particular interest is $L_{1,\infty}$, and we are concerned with traces on this ideal. For more details, see [28, Section 5.7] and [35]. A linear functional $\varphi : L_{1,\infty} \to \mathbb{C}$ is called a trace if it is unitarily invariant. That is, for all unitary operators $U$ and for all $T \in L_{1,\infty}$ we have that $\varphi(U^*TU) = \varphi(T)$. It follows that for all bounded operators $B$ we have $\varphi(BT) = \varphi(TB)$.

A Dixmier trace $\text{Tr}_\omega$ is a trace on $L_{1,\infty}$ defined in terms of an extended limit $\omega \in \ell_\infty(\mathbb{N})^*$ (i.e., a continuous extension of the limit functional to $\ell_\infty(\mathbb{N})$). Given a positive operator $T \in L_{1,\infty}$, $\text{Tr}_\omega(T)$ is defined as:
\begin{equation}
\text{Tr}_\omega(T) = \omega \left( \left\{ \frac{\sum_{k=0}^{\infty} \mu(k, T)}{\log(2 + N)} \right\}^{\infty}_{N=0} \right).
\end{equation}

If $\omega$ is dilation invariant, that is, if for all $n \geq 1$ we have $\omega \circ \sigma_n = \omega$, where $\sigma_n$ is the dilation semigroup $\sigma_n(\{a_j\}_{j=0}^{\infty}) = \{a_{jn}\}_{j=0}^{\infty}$, then $\text{Tr}_\omega$ is called a Dixmier trace and extends to a linear functional on $L_{1,\infty}$.

We note that it can however be proved that $\text{Tr}_\omega$ extends to a trace on $L_{1,\infty}$ with no extra invariance conditions on $\omega$ (see [34, Theorem 17])\footnote{Moreover it can be proved that $\text{Tr}_\omega$ is a Dixmier trace for every extended limit $\omega$. This will appear in the upcoming second edition of [28].}

More generally, an extended limit is a bounded linear functional $\omega$ on $L_\infty((0, \infty))$ which extends the limit functional from the subspace of functions having limit at $\infty$ to all of $L_\infty((0, \infty))$.

2.2. Double operator integrals. In this paper we will make brief use of the technique of double operator integrals for unitary operators. See e.g. [2, 4, 6, 9, 10, 19].

Given two unitary operators $U$ and $V$ on $\mathcal{H}$, a double operator integral with symbol $\phi \in L_\infty(\mathbb{T}^2)$ is a linear map $T^{U,V}_\phi : L_2 \to L_2$ defined as follows. The operators $U$ and $V$ also act as unitary operators of left and right multiplication on the Hilbert-Schmidt space $L_2$:
\begin{equation}
LUX = UX, \quad RVX = XV, \quad X \in L_2.
\end{equation}

As linear operators on $L_2$, $LU$ and $RV$ are commuting unitary operators and hence there is a joint functional calculus $\phi \to \phi(LU, LV) \in B(L_2)$ for $\phi$ a bounded function on the torus $\mathbb{T}^2$. Denote $T^{U,V}_\phi := \phi(LU, RV)$. For a Lipschitz class function $f$ on $\mathbb{T}$, denote by $f^{[1]}$ the divided difference function $f^{[1]}(z, w) = \frac{f(z) - f(w)}{z - w}$ set to an arbitrary value on the diagonal.

A short computation based on a Fourier decomposition of $f$ (see [2, Theorem 1.1.3]) shows that
\begin{equation}
\|T^{U,V}_{f^{[1]}}|_{L_2} - I_{L_1} \|_{L_1} \leq \|T^{f^{[1]}}_X|_{L_2(\mathbb{T})} + \|f''\|_{C(\mathbb{T})}.
\end{equation}
Provided the above right hand side is finite, we also have that $T_{f[1]}^{U,V}$ extends by duality to $B(H)$, and an interpolation argument (as described in e.g. [3, p. 5225]) implies that if $p > 1$ we have
\[ \|T_{f[1]}^{U,V}\|_{L_{p,\infty}} \leq \|f'\|_{L_2(\mathbb{T})} + \|f''\|_{L_2(\mathbb{T})} \]
and similarly if $q > 1$ we have
\[ \|T_{f[1]}^{U,V}\|_{L_{q,1}} \leq \|f'\|_{L_2(\mathbb{T})} + \|f''\|_{L_2(\mathbb{T})}. \]

If $X \in B(H)$, then we also have the following identity (see [10, Theorem 8.5], [2, Theorem 3.5.4] or [9, Theorem 4.1] for the related self-adjoint case):
\[ T_{f[1]}^{U,U}(U,X) = [f(U), X]. \]

If $g$ is a bounded function on the spectrum of $U$, then it follows from the definition of $T_{f[1]}^{U,U}$ that we also have:
\[ g(U)T_{f[1]}^{U,U}(X) = T_{f[1]}^{U,U}(g(U)X), \quad T_{f[1]}^{U,U}(X)g(U) = T_{f[1]}^{U,U}(Xg(U)), \quad X \in B(H). \]

3. CWIKEL TYPE ESTIMATES

We will extensively use the notation
\[ \langle x \rangle = (1 + |x|^2)^{1/2} \]
for $x \in \mathbb{R}^d$ and $|x|$ denotes the $\ell_2$-norm of $x$, so that $x \mapsto \langle x \rangle^{-1} \in L_{d,\infty}(\mathbb{R}^d)$. Recall that $V$ is a bounded measurable real valued function on $\mathbb{R}^d$, and $H = -\Delta + MV$ is the Schrödinger operator associated to the potential $V$. We exclusively consider $d \geq 2$.

This section is devoted to a proof of the claim that for integers $p \geq 1$ and $z \in \mathbb{C} \setminus \mathbb{R}$, we have that $(H + z)^{-p}M_{x|z}^{-p}$ is in the ideal $\mathcal{L}_{d/p,\infty}$. This is a crucial component to proving that the operator inside the Dixmier trace in Theorem 1.1 is indeed in the ideal $\mathcal{L}_{1,\infty}$. Somewhat similar estimates on the singular values of operators of the form $f(H)g(M_x)$ are also in [37, Section B.9].

Our proofs are based on the following classical Cwikel estimate (see [36, Theorem 4.2] or for the $p = 2$ case see the more recent [27, Corollary 1.2, Theorem 5.6]).

The function spaces $\ell_2,\infty(L_4)(\mathbb{R}^d)$ and $\ell_2,\log(L_{\infty})(\mathbb{R}^d)$ are defined by the norms:
\[ \|g\|_{\ell_2,\infty(L_4)(\mathbb{R}^d)} = \left\| \left\{ \|g\|_{L_4(\Delta + k)} \right\} \right\|_{\ell_2,\infty}, \]
\[ \|f\|_{\ell_2,\log(L_{\infty})(\mathbb{R}^d)} = \left( \sum_{k \in \mathbb{Z}^d} (1 + \log(1 + |k|))\|f\|_{L_{\infty}(\Delta + k)}^2 \right)^{1/2} \]
where $\Delta = [0,1)^d$ is the unit cube and $|k|$ denotes the $\ell_2$-norm of $k \in \mathbb{Z}^d$.

**Proposition 3.1.** Let $2 < p < \infty$. If $f \in L_p(\mathbb{R}^d)$ and $g \in L_{p,\infty}(\mathbb{R}^d)$, then the operator $f(M_x)g(-i\nabla)$ is in the ideal $L_{p,\infty}$. For $Mfg(-i\nabla) \in L_{2,\infty}(\mathbb{R}^d)$, we instead require that $g \in \ell_{2,\infty}(L_4)(\mathbb{R}^d)$ and $f \in \ell_{2,\log}(L_{\infty})(\mathbb{R}^d)$.

We begin with a lemma of elementary operator theory, required for the proof of the main result of this section (Theorem 3.4).

**Lemma 3.2.** Let $A, B, C$ be bounded operators such that $A = B - AC$. If $B \in \mathcal{L}_{p_0,\infty}$ and $C \in \mathcal{L}_{p_1,\infty}$, for $0 < p_0, p_1 < \infty$ then $A \in \mathcal{L}_{p_0,\infty}$.
Lemma 3.3. For all integers \( p \geq 0 \) and for any \( \epsilon > 0 \), we have:
\[
M_p \left( [H_0, M_{(x)}^{-p}] \right) (H_0 + 1)^{-1} \in L_{d+\epsilon, \infty}.
\]

Proof. By definition,
\[
H_0 = -\sum_{m=1}^{d} \partial_m^2.
\]
If \( f \in C^2(\mathbb{R}^d) \) is bounded, with all derivatives up to second order bounded, then a straightforward calculation shows that
\[
[\partial_m^2, M_f] = 2M_{\partial_m f} \partial_m + M_{\partial_m^2 f}, \quad 1 \leq m \leq d
\]
which gives
\[
[H_0, M_f] = -2 \sum_{m=1}^{d} M_{\partial_m f} \partial_m - M_{H_0 f}.
\]
Define the function \( f_p \) by \( f_p(x) := \langle x \rangle^{-p}, \ x \in \mathbb{R}^d \). For \( 1 \leq m \leq d \), we have (here \( x = (x_1, \ldots, x_d) \in \mathbb{R}^d \)):
\[
\partial_m f_p(x) = -px_m(x)^{-p-2},
\]
\[
\partial_m^2 f_p(x) = p(p+2)x_m^2(x)^{-p-4} - p(x)^{-p-2},
\]
\[
H_0 f_p(x) = -p(p + 2 - d)(x)^{-p-2}.
\]
Using (3.1), we write
\[
M_p \left( [H_0, M_{(x)}^{-p}] \right) = M_p^{-1}[H_0, M_{f_p}] = M_p^{-1}(-2 \sum_{m=1}^{d} M_{\partial_m f_p} \partial_m - M_{H_0 f_p})
\]
\[
= -2 \sum_{m=1}^{d} M_{f_p^{-1} \partial_m f_p} \partial_m - M_{f_p^{-1} H_0 f_p}.
\]
Since for any \( \epsilon > 0 \)
\[
f_p^{-1} \partial_m f_p(x) = -px_m(x)^{-2} \in L_{d, \infty}(\mathbb{R}^d) \cap L_{\infty}(\mathbb{R}^d) \subset L_{d+\epsilon, \infty}(\mathbb{R}^d)
\]
and \( \partial_m (H_0 + 1)^{-1} = g(-i\nabla) \) with
\[
g(t) = \frac{-it_m}{1 + |t|^2} \in L_{d, \infty}(\mathbb{R}^d) \cap L_{\infty}(\mathbb{R}^d) \subset L_{d+\epsilon, \infty}(\mathbb{R}^d)
\]
it follows from Proposition 3.1 that for any $\epsilon > 0$

\begin{equation}
\sum_{m=1}^{p} M_{f^{-1}_p \partial_m f} \partial_m (H_0 + 1)^{-1} \in \mathcal{L}_{d+\epsilon, \infty}.
\end{equation}

Since

\[ f^{-1}_p H_0 f_p = -p(p + 2 - d)\langle x \rangle^{-2} \in L_{d/2, \infty}(\mathbb{R}^d) \cap L_\infty(\mathbb{R}^d) \]

and $(H_0 + 1)^{-1} = g(-i\nabla)$ with $g(t) = \frac{1}{1 + |t|^2} \in L_{d/2, \infty}(\mathbb{R}^d) \cap L_\infty(\mathbb{R}^d)$, it follows from Proposition 3.1 that for any $\epsilon > 0$

\begin{equation}
M_{f^{-1}_p H_0 f_p} (H_0 + 1)^{-1} \in \mathcal{L}_{d/2+\epsilon, \infty}.
\end{equation}

Combining (3.3), (3.4) and (3.5) gives for any $\epsilon > 0$

\[ M_p^p [H_0, M_{(x)}^{-p}](H_0 + 1)^{-1} \in \mathcal{L}_{d+\epsilon, \infty}. \]

\[ \square \]

We now present the main Cwikel estimate of this section:

**Theorem 3.4.** For any $z \in \mathbb{C} \setminus \mathbb{R}$ and $p = 1, 2, \ldots$

\[ (H + z)^{-p} M_{(x)}^{-p} \in \mathcal{L}_{d/p, \infty}. \]

**Proof.** We introduce the notation:

\[ A_p(z) = (H + z)^{-p} M_{(x)}^{-p}, \]
\[ B_p(z) = (H + z)^{1-p} M_{(x)}^{-p} (H + z)^{-1}, \]
\[ C_p(z) = M_p^p [H_0, M_{(x)}^{-p}](H + z)^{-1}. \]

We prove the assertion by induction on $p$, our goal being to prove that $A_p(z) \in \mathcal{L}_{d/p, \infty}$ for all $p \geq 1$. The resolvent identity gives

\[ (H + z)^{-1}(H_0 + z) = 1 - (H + z)^{-1} M_V \in \mathcal{B}(\mathcal{H}). \]

Consider the base case $p = 1$. If $d > 2$, then since $x \mapsto \langle x \rangle^{-1} \in L_{d, \infty}(\mathbb{R}^d)$ and $y \mapsto (y^2 + z)^{-1} \in L_{d/2, \infty}(\mathbb{R}^d) \cap L_\infty(\mathbb{R}^d) \subset L_d(\mathbb{R}^d)$, the Fourier dual of Proposition 3.1 yields:

\[ (H_0 + z)^{-1} M_{(x)}^{-1} \in L_{d, \infty}. \]

On the other hand, if $d = 2$, then we shall verify that $x \mapsto \langle x \rangle^{-1} \in \ell_{2, \infty}(L_4)(\mathbb{R}^2)$, and that $y \mapsto (|y|^2 + z)^{-1} \in \ell_{2, \log}(L_{\infty})(\mathbb{R}^2)$. There is a constant $C_d$ such that for $k \in \mathbb{Z}^2$ we have:

\[ \|\langle x \rangle^{-1}\|_{L_4(\Delta + k)} \leq C_d(k)^{-1} \]

and therefore,

\[ \|\langle x \rangle^{-1}\|_{\ell_{2, \infty}(L_4)(\mathbb{R}^2)} \leq C_d \|\{\langle k \rangle^{-1}\}_{k \in \mathbb{Z}^2}\|_{\ell_{2, \infty}} < \infty. \]

Similarly, for $k \in \mathbb{Z}^2$, there is a constant $C_{d,z}$ such that:

\[ \|(|y|^2 + z)^{-1}\|_{L_\infty(\Delta + k)} \leq C_{d,z}(k)^{-4} \]

and therefore,

\[ \|(|y|^2 + z)^{-1}\|_{\ell_{2, \log}(L_{\infty})(\mathbb{R}^2)} \leq C_{d,z} \left( \sum_{k \in \mathbb{Z}^2} (1 + \log(1 + |k|))\langle k \rangle^{-4} \right)^{1/2} < \infty. \]
It then follows from Proposition 3.1 that \((H_0 + z)^{-1}M^{-1}_{(x)} \in \mathcal{L}_{2,\infty}(L_2(\mathbb{R}^2))\) when \(d = 2\). So in all cases \(d \geq 2\), we have \((H_0 + z)^{-1}M^{-1}_{(x)} \in \mathcal{L}_{d,\infty}\).

Hence,
\[
A_1(z) = (H + z)^{-1}(H_0 + z) \cdot (H_0 + z)^{-1}M^{-1}_{(x)} \in \mathcal{B}(\mathcal{H}) \cdot \mathcal{L}_{d,\infty} = \mathcal{L}_{d,\infty}.
\]
This proves the \(p = 1\) case.

Suppose the estimate holds for \(p \geq 1\). Let us prove it for \(p + 1\). Using the identity
\[
[X^{-1}, Y] = -X^{-1}[X, Y]X^{-1},
\]
we write
\[
A_{p+1}(z) - B_{p+1}(z) = (H + z)^{-p} \cdot [(H + z)^{-1}, M^{-p-1}_{(x)}]
= -(H + z)^{-p-1}[H_0, M^{-p-1}_{(x)}](H + z)^{-1}
= -A_{p+1}(z)C_{p+1}(z).
\]
We now verify that the operators \(A_{p+1}(z)\), \(B_{p+1}(z)\) and \(C_{p+1}(z)\) satisfy the assumptions in Lemma 3.2.

With the identity
\[
B_{p+1}(z) = A_p(z)A_1(\bar{z})^*,
\]
Hölder’s inequality (2.1) and the inductive assumption yield
\[
B_{p+1}(z) \in \mathcal{L}_{\frac{d}{p+1},\infty} : \mathcal{L}_{d,\infty} \subset \mathcal{L}_{\frac{d}{p+1},\infty}.
\]
Also,
\[
C_{p+1}(z) = M^{p+1}_{(x)}[H_0, M^{-p-1}_{(x)}](H_0 + z)^{-1} \cdot (H_0 + z)(H + z)^{-1}.
\]
Lemma 3.3 states that:
\[
M^{p+1}_{(x)}[H_0, M^{-p-1}_{(x)}](H_0 + z)^{-1} \in \mathcal{L}_{2d,\infty}.
\]
Since \((H_0 + z)(H + z)^{-1} = 1 - M_V(H + z)^{-1} \in \mathcal{B}(\mathcal{H})\) it follows that
\[
C_{p+1}(z) \in \mathcal{L}_{2d,\infty} : \mathcal{B}(\mathcal{H}) = \mathcal{L}_{2d,\infty}.
\]
That is, \(B_{p+1}(z) \in \mathcal{L}_{d/(p+1),\infty}\) and \(C_{p+1}(z) \in \mathcal{L}_{2d,\infty}\), so applying Lemma 3.2 to the operators \(A_{p+1}(z)\), \(B_{p+1}(z)\) and \(C_{p+1}(z)\) yields \(A_{p+1}(z) \in \mathcal{L}_{d/(p+1),\infty}\), so the assertion follows by induction on \(p\).

As a useful corollary, we also include the following:

**Proposition 3.5.** Let \(\epsilon > 0\). Then
\[
\limsup_{r \downarrow d} \|[M^{-r}_{(x)}, e^{-\epsilon(r-1)H}]\|_1 < \infty
\]
and
\[
\limsup_{r \downarrow d} \|[M^{1-r}_{(x)}, e^{-\epsilon(r-1)H}]\|_{\frac{d}{2r}+1} < \infty.
\]

**Proof.** Let \(U\) be the unitary operator \(\frac{H+i}{\sqrt{d}}\), and let \(\phi_r\) be a smooth function on the unit circle such that for \(t \geq -\|V\|_\infty\) we have
\[
\phi_r \left( \frac{t+i}{t-i} \right) = e^{-\frac{r}{2}(r-1)t}.
\]
Since \( \phi_s \) is smooth, the transformer \( T_{\phi_s}^{U} \) is bounded from \( L_1 \) to \( L_1 \) (see (2.5)), and one can compute that the \( L_2(T) \) norms of \( \phi_s' \) and \( \phi_s'' \) are bounded above by a constant multiple of \( r - 1 \) and \( (r - 1)^2 \) respectively, so in particular:

\[
\limsup_{r \to d} \| T_{\phi_s}^{U} \|_{L_1 \to L_1} < \infty.
\]

Similarly, (2.6) yields:

\[
\limsup_{r \to d} \| T_{\phi_s}^{U} \|_{L_\frac{d}{d-r} \to L_\frac{d}{d-r}} < \infty.
\]

Using the semigroup property of \( e^{-t(r-1)H} \) and the Leibniz rule, we have:

\[
[M_{(x)}^{r}, e^{-\frac{1}{2}t(r-1)H}] = e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{r}, e^{-\frac{1}{2}t(r-1)H}] + [M_{(x)}^{r}, e^{-\frac{1}{2}t(r-1)H}] e^{-\frac{1}{2}t(r-1)H}.
\]

Since \( e^{-\frac{1}{2}t(r-1)H} = \phi_s(U) \), from (2.7), we have:

\[
[M_{(x)}^{r}, e^{-\frac{1}{2}t(r-1)H}] = T_{\phi_s}^{U} ([M_{(x)}^{r}, U]).
\]

Combining the preceding two displays, from (2.8) it follows that

\[
[M_{(x)}^{r}, e^{-\frac{1}{2}t(r-1)H}] = T_{\phi_s}^{U} (e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{r}, U] + [M_{(x)}^{r}, U] e^{-\frac{1}{2}t(r-1)H}).
\]

Now (3.7) implies that there is a constant \( C_{d,e} \) such that:

\[
\| [M_{(x)}^{r}, e^{-\frac{1}{2}t(r-1)H}] \|_1 \leq C_{d,e} (\| e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{r}, U] \|_1 + \| [M_{(x)}^{r}, U] e^{-\frac{1}{2}t(r-1)H} \|_1).
\]

An identical argument yields:

\[
\| [M_{(x)}^{1-r}, e^{-\frac{1}{2}t(r-1)H}] \|_{L_1} \leq C_{d,e} (\| e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{1-r}, U] \|_{L_1} + \| [M_{(x)}^{1-r}, U] e^{-\frac{1}{2}t(r-1)H} \|_{L_1})
\]

for a possibly larger constant \( C_{d,e} \). We now concentrate on determining the \( L_1 \) and \( L_\frac{d}{d-r} \) norms of \( e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{r}, U] \) and \( e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{1-r}, U] \) respectively. Identical arguments will control the \( L_1 \) and \( L_\frac{d}{d-r} \) norms of \( [M_{(x)}^{r}, U] e^{-\frac{1}{2}t(r-1)H} \) and \( [M_{(x)}^{1-r}, U] e^{-\frac{1}{2}t(r-1)H} \) respectively.

Using (3.6), we have the following computations for the commutator \( [M_{(x)}^{r}, U] \):

\[
[M_{(x)}^{r}, \frac{H + i}{H - i}] = [M_{(x)}^{r}, 1 + 2i(H - i)^{-1}]
\]

\[
= 2i[M_{(x)}^{r}, (H - i)^{-1}]
\]

\[
= -2i(H - i)^{-1} [M_{(x)}^{r}, H](H - i)^{-1}
\]

\[
= -2i(H - i)^{-1} [M_{(x)}^{r}, H_0](H - 1)^{-1}.
\]

In view of (3.1) and the computations leading to (3.4), we have:

\[
(H - i)^{-1} [M_{(x)}^{r}, H_0](H - i)^{-1}
\]

\[
= 2r \sum_{m=1}^{d} (H - i)^{-1} M_{m(x)}^{r-2} \partial_m (H - i)^{-1} + r(r + 2 - d)(H - i)^{-1} M_{m(x)}^{r-2} (H - i)^{-1}.
\]

It follows now from the triangle inequality that:

\[
\| e^{-\frac{1}{2}t(r-1)H} [M_{(x)}^{r}, U] \|_1 \leq C_{d,e} (r \sum_{m=1}^{d} \| (H - i)^{-1} e^{-\frac{1}{2}t(r-1)H} M_{m(x)}^{r-1} M_{m(x)}^{r-1} \partial_m (H - i)^{-1} \|_1
\]

\[
+ r(r + d + 2) \| (H - i)^{-1} e^{-\frac{1}{2}t(r-1)H} M_{m(x)}^{r-2} (H - i)^{-1} \|_1).
\]
Using the fact that \( x_m \langle x \rangle^{-1} \), \( \partial_m (H - i)^{-1} \) and \( (H - i)^{-1} \) are bounded, we arrive at the bound:

\[
\| e^{-\frac{1}{2} (r-1)^{H} [M_{(x)}^{-1}, U]} \|_1 \leq C_{d,e} r^2 \| e^{-\frac{1}{2} (r-1)^{H} M_{(x)}^{-1}} \|_1.
\]

Here, once again the size of the constant may have increased. An identical argument, replacing the \( L_1 \) norm by the \( L_{\frac{d}{d-1},1} \) and using (3.8) leads to the bound:

\[
\| e^{-\frac{1}{2} (r-1)^{H} [M_{(x)}^{-1}, U]} \|_{\frac{d}{d-1},1} \leq C_{d,e} r^2 \| e^{-\frac{1}{2} (r-1)^{H} M_{(x)}^{-1}} \|_{\frac{d}{d-1},1}.
\]

Since \( r > d \), (3.9) yields

\[
\| e^{-\frac{1}{2} (r-1)^{H} [M_{(x)}^{-1}, U]} \|_1 \leq C_{d,e} r^2 \| e^{-\frac{1}{2} (r-1)^{H} M_{(x)}^{-1}} \|_1 \| M_{(x)}^{-r} \|_\infty \| e^{-\frac{1}{2} (d-1)^{H} M_{(x)}^{-d-1}} \|_1.
\]

and (3.10) yields

\[
\| e^{-\frac{1}{2} (r-1)^{H} [M_{(x)}^{-1}, U]} \|_{\frac{d}{d-1},1} \leq C_{d,e} r^2 \| e^{-\frac{1}{2} (r-1)^{H} M_{(x)}^{-1}} \|_{\frac{d}{d-1},1} \| M_{(x)}^{-r} \|_\infty \| e^{-\frac{1}{2} (d-1)^{H} M_{(x)}^{-d-1}} \|_{\frac{d}{d-1},1}.
\]

Using the fact that \( (H + i)^{N} e^{-\frac{1}{2} (d-1)^{H}} \) is bounded for any \( N \geq 0 \), we have:

\[
\| e^{-\frac{1}{2} (d-1)^{H} M_{(x)}^{-d-1}} \|_1 \leq C_{d,e} \| (H + i)^{-(d+1)} M_{(x)}^{-d-1} \|_1,
\]

for a potentially different constant \( C_{d,e} \). Theorem 3.4 now provides the desired bounds, since \( L_{\frac{d}{d-1},\infty} \subset L_1 \). Similarly,

\[
\| e^{-\frac{1}{2} (d-1)^{H} M_{(x)}^{-d}} \|_{\frac{d}{d-1},1} \leq C_{d,e} \| (H + i)^{-d} M_{(x)}^{-d} \|_{\frac{d}{d-1},1}.
\]

Since \( L_{1,\infty} \subset L_{\frac{d}{d-1},\infty} \), Theorem 3.4 again yields the desired bound.

\[\]

4. A residue formula

We now proceed to the proof of the claim that:

\[
\text{Tr}(e^{-s^{H} M_{(x)}^{-d}}) = \lim_{r \downarrow 1} (r - 1) \text{Tr}(e^{-s^{H} M_{(x)}^{-d}}).
\]

That the left hand side makes sense is ensured by Theorem 3.4; indeed, it implies that \( (H + i)^{-d} M_{(x)}^{-d} \in L_{1,\infty} \), and since the operator \( e^{-s^{H}} (H + i)^{d} \) has bounded extension it follows that \( e^{-s^{H}} M_{(x)}^{-d} \in L_{1,\infty} \). That the right hand side makes sense will be a consequence of the arguments in this section. The proofs of this section are achieved with some recently developed techniques in operator integration, developed originally in [18] and later extended in [40, Section 5.2].

4.1. Abstract result. The following is an abstract operator theoretic result. It is similar to [17, Theorem B.1], although the assumptions are slightly different and the result is stated with an explicit norm bound.

**Theorem 4.1.** Let \( d \geq 2 \), \( r > 1 \) let \( p > \frac{d}{2} \geq 1 \) and select \( q \in (1, \infty) \) such that \( \frac{1}{p} + \frac{1}{q} \leq 1 \). Let \( A, B \in B(H) \) be positive operators satisfying the following four conditions:

(i) \([BA^{\frac{1}{2}}, A^{\frac{1}{2}}] \in L_{p,\infty};
(ii) B^{-1}A^{-1} \in L_{q,1};
(iii) B^{-1}|B, A^{-1}|A \in L_1; 
(iv) (A^{1/2} BA^{1/2})^{-1} \in L_{q,1};

Lemma 4.4. Let $A$, $B$, $d$, $r$, $p$, and $q$ be as in Theorem 4.1. Then the map $s \mapsto T_r(s)$ takes values in the trace class, and there is a constant $c_p > 0$ such that for all $s \in \mathbb{R}$:

$$
\|T_r(s)\|_1 \leq c_p(1 + |s|)\|BA^{\frac{1}{2}}, A^{\frac{1}{2}}\|_{p, \infty}\|BA^r, A^r\|_{q, 1}
+ c_p(1 + |s|)\|BA^r, A^r\|_{p, \infty} + \|BA^r, A^r\|_{p, \infty}.
$$

The proof of Theorem 4.1 is based on the formula given in [40, Section 5.2], stated in terms of a mapping $T_r : \mathbb{R} \to \mathcal{B}(\mathcal{H})$ defined as follows:

Definition 4.2. Let $A$ and $B$ be positive bounded operators, and let

$$
Y := A^{1/2}BA^{1/2}.
$$

We define the mapping $T_r : \mathbb{R} \to \mathcal{B}(\mathcal{H})$ by,

$$
T_r(0) := B^{-1}[BA^{\frac{1}{2}}, A^{-\frac{1}{2}}] + [BA^{\frac{1}{2}}, A^{\frac{1}{2}}]Y^{-1},
$$

$$
T_r(s) := B^{-1+is}[BA^{\frac{1}{2}}, A^{-\frac{1}{2}+is}]Y^r - iB^{is}[BA^{\frac{1}{2}}, A^{\frac{1}{2}+is}]Y^{-1} - is, \quad s \neq 0.
$$

We now collect some auxiliary results for the proof of Theorem 4.1.

Lemma 4.3. Let $p$ and $d$ be as in the statement of Theorem 4.1. Suppose that $A$ and $B$ are bounded positive operators such that $[BA^{\frac{1}{2}}, A^{\frac{1}{2}}] \in L_{p, \infty}$. Then for all $s \in \mathbb{R}$, $[BA^{\frac{1}{2}}, A^{\frac{1}{2}+is}] \in L_{p, \infty}$, and we have:

$$
\|[BA^{\frac{1}{2}}, A^{\frac{1}{2}+is}]\|_{p, \infty} \leq c_p(1 + |s|)\|[BA^{\frac{1}{2}}, A^{\frac{1}{2}}]\|_{p, \infty}.
$$

Proof. The main result in [30] asserts that for every Lipschitz continuous function $f$ on $\mathbb{R}$ and every $1 < p' < \infty$, we have a constant $C_{p'}$ such that:

$$
\|[X, f(Y)]\|_{p'} \leq C_{p'}\|f'\|_{\infty}\|[X, Y]\|_{p'},
$$

whenever $Y$ is a self-adjoint operator and $X$ is a bounded operator such that $[X, Y] \in L_{p', \infty}$. The method of proof in [30] was to construct a linear operator $T_{f[Y]}^{Y}$ which is bounded from $L_{p'}$ to $L_{p}$ for every $1 < p' < \infty$ and such that $T_{f[Y]}^{Y}([X, Y]) = [X, f(Y)]$. Since $p > 1$, the ideal $L_{p, \infty}$ is an interpolation space between $L_{p'}$ and $L_{p''}$ for suitable $1 < p' < p'' < \infty$. An interpolation argument (see e.g. [3, p. 2255]) further implies that $T_{f[Y]}^{Y}$ is bounded from $L_{p, \infty}$ to $L_{p, \infty}$, and we have the inequality:

$$
\|[X, f(Y)]\|_{p, \infty} \leq c_p\|f'\|_{\infty}\|[X, Y]\|_{p, \infty}
$$

for some constant $c_p$.

Take $X = BA^{\frac{1}{2}}$, $Y = A^{\frac{1}{2}}$ and $f(t) = |t|^{1+2is}$, $t \in \mathbb{R}$. Since $\|f'\|_{\infty} \leq 1 + 2|s|$, the assertion follows. \(\square\)

Lemma 4.4. Let $A$, $B$, $d$, $r$, $p$ and $q$ be as in Theorem 4.1. Then the map $s \mapsto T_r(s)$ takes values in the trace class, and there is a constant $c_p > 0$ such that for all $s \in \mathbb{R}$:

$$
\|T_r(s)\|_1 \leq c_p(1 + |s|)\|BA^{\frac{1}{2}}, A^{\frac{1}{2}}\|_{p, \infty}\|Y^{-1}\|_{q, 1}
+ c_p(1 + |s|)\|B^{r-1}A^{r-1}\|_{q, 1}\|[BA^{\frac{1}{2}}, A^{\frac{1}{2}}]\|_{p, \infty}
+ \|B^{r-1}[BA^{\frac{1}{2}}, A^{r-1}]A^{\frac{1}{2}}\|_1.
$$
Proof. We prove this for $s \neq 0$, the proof for $s = 0$ is identical. By the triangle inequality, we have
\[
\|T_r(s)\|_1 \leq \|B^{-1} [BA^\frac{1}{2}, A^{-\frac{1}{2}+is}] Y^{-is}\|_1 + \|B[BA^\frac{1}{2}, A^\frac{1}{2}+is] Y^{-1} - is\|_1 \\
\leq \|B^{-1} [BA^\frac{1}{2}, A^{-\frac{1}{2}+is}]\|_1 + \|B[BA^\frac{1}{2}, A^\frac{1}{2}+is] Y^{-1}\|_1 \\
=: (I) + (II).
\]
Using the Leibniz rule, we have
\[
[BA^\frac{1}{2}, A^{-\frac{1}{2}+is}] = A^{-1} [BA^\frac{1}{2}, A^\frac{1}{2}+is] + [BA^\frac{1}{2}, A^{-1}] A^\frac{1}{2}+is.
\]
Therefore, using (2.3) we get
\[
(I) = \|B^{-1} [BA^\frac{1}{2}, A^{-\frac{1}{2}+is}]\|_1 \\
\leq \|B^{-1} A^{-1} [BA^\frac{1}{2}, A^\frac{1}{2}+is]\|_1 + \|B^{-1} [BA^\frac{1}{2}, A^{-1}] A^\frac{1}{2}+is\|_1 \\
\leq \|B^{-1} A^{-1}\|_{q,1} \|[BA^\frac{1}{2}, A^\frac{1}{2}+is]\|_{p,\infty} \\
+ \|B^{-1} [BA^\frac{1}{2}, A^{-1}] A^\frac{1}{2}\|_1.
\]
Using Lemma 4.3, we have
\[
(I) \leq c_p(1 + |s|) \|B^{-1} A^{-1}\|_{q,1} \|[BA^\frac{1}{2}, A^\frac{1}{2}]\|_{p,\infty} \\
+ \|B^{-1} [BA^\frac{1}{2}, A^{-1}] A^\frac{1}{2}\|_1.
\]
On the other hand, using (2.3), we have:
\[
(II) = \|([BA^\frac{1}{2}, A^\frac{1}{2}+is] Y^{-1}\|_1 \leq \|([BA^\frac{1}{2}, A^\frac{1}{2}+is]\|_{p,\infty} \|Y^{-1}\|_{q,1}.
\]
Again applying Lemma 4.3, it follows that:
\[
(II) \leq c_d(1 + |s|) \|[BA^\frac{1}{2}, A^\frac{1}{2}]\|_{p,\infty} \|Y^{-1}\|_{q,1}.
\]
Hence, $T_r(s) \in \mathcal{L}_1$ with the appropriate norm bound. 

By means of Lemma 4.4 and an integral formula from [40, Theorem 5.2.1], we obtain a proof of Theorem 4.1.

Proof of Theorem 4.1. Define the function $g_r : \mathbb{R} \to \mathbb{R}$ by
\[
g_r(0) := 1 - \frac{r}{2}, \\
g_r(2t) := 1 - \frac{\sinh(rt)}{2\sinh((r-1)t)}, \quad t \neq 0.
\]
The function $g_r$ is Schwartz class on $\mathbb{R}$ (see [40, Remark 5.2.2]). According to [40, Theorem 5.2.1], the mapping $T_r$ is continuous in the weak operator topology and
\[
\|B^r A^r - Y^r\|_1 \leq \|T_r(0)\|_1 + \int_\mathbb{R} \|T_r(s)\|_1 |\hat{g}_r(s)| ds.
\]
where the integral on the left converges in the weak operator topology, and $\hat{g}_r$ is the Fourier transform of $g_r$, scaled so that $g_r(t) = \int_\mathbb{R} \hat{g}_r(s) e^{its} ds$. Our result is based on the estimate:
\[
\|B^r A^r - Y^r\|_1 \leq \|T_r(0)\|_1 + \int_\mathbb{R} \|T_r(s)\|_1 |\hat{g}_r(s)| ds.
\]
We may evaluate each \( \partial_s \) the right hand side converges and the assertion follows.

Schwartz class function, then so is the Fourier transform \( \widehat{g_r} \). Hence, the integral on the right hand side converges and the assertion follows.

4.2. The main residue formula. To apply Theorem 4.1 to the problem at hand, we need to verify its assumptions for the relevant operators.

**Lemma 4.5.** Let \( A = e^{-\epsilon H} \) and \( B = M_{(x)}^{-1} \), where \( \epsilon > 0 \). Let \( Y = A^\dagger B A^\dagger \). Let \( p > \frac{d}{2} \) and \( q > \frac{d+1}{d-1} \). We have the following:

(i) \([BA^\dagger, A^\dagger] \in L_{p,\infty} \) and \( Y \in L_{d,\infty} \);

(ii) \( \|B^{-1}A^{-1}\|_{q,1} = O(1) \) as \( r \downarrow d \);

(iii) \( \|B^{-1}[B, A^{-1}]A\|_1 = O(1) \) as \( r \downarrow d \);

(iv) If \( r > d \), we have \( (A^{1/2}BA^{1/2})^{-1} \in L_{q,1} \).

**Proof.** First we verify (i). We begin by noting that:

\[ [M_{(x)}^{-1}e^{-\frac{d}{2}H}, H] = [M_{(x)}^{-1}, H]e^{-\frac{d}{2}H} = [M_{(x)}^{-1}, H_0]e^{-\frac{d}{2}H}. \]

As in the proof of Lemma 3.3, specifically (3.1), we have:

\[ [M_{(x)}^{-1}, H_0] = 2 \sum_{m=1}^{d} M_{\partial_m((x)^{-1})} \partial_m + M_{H_0((x)^{-1})}. \]

We may evaluate each \( \partial_m((x)^{-1}) \) and \( H_0((x)^{-1}) \) using (3.2), to arrive at:

\[ [M_{(x)}^{-1}, H_0] = -2 \left( \sum_{m=1}^{d} M_{x_m(x)^{-1}} M_{(x)^{-1}}^{-2} \partial_m \right) - (3 - d)M_{(x)^{-3}}. \]

It follows that

\[ [M_{(x)}^{-1}e^{-\frac{d}{2}H}, H] = [M_{(x)}^{-1}, H_0]e^{-\frac{d}{2}H} \]

\[ = -2 \left( \sum_{m=1}^{d} M_{x_m(x)^{-1}} M_{(x)^{-1}}^{-3} \partial_m \right) e^{-\frac{d}{2}H} - (3 - d)M_{(x)^{-3}}e^{-\frac{d}{2}H}. \]

The latter term is in \( L_{d,\infty} \), since \( (H + i)^3e^{-\frac{d}{2}H} \) is bounded and Theorem 3.4 with \( p = 3 \) applies. For the former term, we instead use the fact that \( (H + i)^3e^{-\frac{d}{2}H} \) is bounded, and then Theorem 3.4 with \( p = 2 \) implies that:

\[ [M_{(x)}^{-1}e^{-\frac{d}{2}H}, H] \in L_{d,\infty} \subset L_{p,\infty}. \]

Let \( U = \frac{H+i}{H-i} \). It follows that

\[ [M_{(x)}^{-1}e^{-\frac{d}{2}H}, U] = 2i[M_{(x)}^{-1}e^{-\frac{d}{2}H}, (H-i)^{-1}] = -2i(H-i)^{-1}[M_{(x)}^{-1}e^{-\frac{d}{2}H}, H](H-i)^{-1} \in L_{p,\infty}. \]
We now use the smooth function \( \phi_2 \) introduced in the proof of Proposition 3.5 and (2.7) to arrive at:
\[
[M^{-1}(x)e^{-\frac{\xi H}{2}}, e^{-\frac{\xi H}{2}}] = T_{\phi_2}^{U,U}(e^{-\frac{\xi H}{2}}, U).
\]
Since \( p > 1 \), the ideal \( L_{p,\infty} \) is an interpolation space between \( L_1 \) and \( L_{\infty} \), and hence (2.5) implies the boundedness of \( T_{\phi_2}^{U,U} \) from \( L_{p,\infty} \) to \( L_{p,\infty} \).

Thus,
\[
[M^{-1}(x)e^{-\frac{\xi H}{2}}, e^{-\frac{\xi H}{2}}] = [BA\hat{x}, A\hat{x}] \in L_{p,\infty}.
\]
This yields the first part of (i). To see the second part (that \( Y \in L_{d,\infty} \)), simply note that: \( AB = e^{-\xi H}(H+i)(H+i)^{-1}M^{-1}(x) \), so that Theorem 3.4 yields \( AB \in L_{d,\infty} \), and:
\[
Y = A\hat{x}BA\hat{x} = BA - [BA\hat{x}, A\hat{x}].
\]
By taking \( \frac{d}{2} < p < d \), we have already proved that \( [BA^{1/2}, A^{1/2}] \in L_{d,\infty} \). Hence \( Y \in L_{d,\infty} \).

Now we prove (ii). If \( r > d \), we have:
\[
\|B^{-1}A^{-1}\|_{q,1} \leq \|B^{-d}\|_{\infty} \|A^{-d}\|_{\infty} \|B^{-d}A^{-d}\|_{q,1}.
\]
Then
\[
\|B^{-d}A^{-d}\|_{q,1} \leq \|e^{-\xi(H+i)^{d-1}d-1}\|_{\infty} \|M^{-d}(x)(H+i)^{1-d}\|_{q,1}.
\]
Since \( q > \frac{d}{r-1} \), we have:
\[
\|M^{-d}(x)(H+i)^{1-d}\|_{q,1} \leq \|M^{-d}(x)(H+i)^{1-d}\|_{\frac{q}{r-1},\infty}
\]
The assertion (ii) follows now from Theorem 3.4.

Next we prove (iii). We write \( B^{-1}[B, A^{-1}]A \) as
\[
B^{-1}[B, A^{-1}]A = [B^r, A^{-r}] \cdot A - [B^{-1}, A^{-1}] \cdot BA.
\]
Thus, using (2.3) and our previous observation that \( BA \in L_{d,\infty} \), we have
\[
\|B^{-1}[B, A^{-1}]A\|_1 \leq \|B^r, A^{-r}\|_1 \|A\|_\infty + \|B^{-1}, A^{-1}\|_{\frac{d}{r-1},1} \|BA\|_{d,\infty}.
\]
Since \( r > d \), Proposition 3.5 yields the desired uniform control on \( \|B^r, A^{-r}\|_1 \) and \( \|B^{-1}, A^{-1}\|_{\frac{d}{r-1},1} \) as \( r \downarrow d \).

Finally, we prove (iv). We have already proved in (i) that \( Y \in L_{d,\infty} \). It follows that \( Y^{-1} \in L_{\frac{1}{d},\infty} \). If \( r > d \), then \( L_{\frac{1}{d},\infty} \subset L_{\frac{1}{r},\infty} \), and by our assumption on \( q \), (2.4) implies the inclusion \( L_{\frac{1}{d},\infty} \subset L_{q,1} \). This establishes (iv).

\[\square\]

**Lemma 4.6.** Let \( s > 0 \) and \( 0 < \epsilon < \frac{s}{2\epsilon} \). Denoting \( Y \) as in Lemma 4.5, we have
\[
\left\| e^{-sH}M^{r} - e^{-(s-c\epsilon)H}Y^{r} \right\|_1 = O(1), \quad r \in [d, \frac{s}{2\epsilon}]
\]

**Proof.** Let \( A \) and \( B \) as in Lemma 4.5. Splitting up \( e^{-sH} \) as \( e^{-(s-c\epsilon)H}A^{r} \), we have
\[
e^{-sH}M^{r}\frac{r}{(x)} = e^{-(s-c\epsilon)H}A^{r}B^{r}
\]
\[
= e^{-(s-c\epsilon)H} \cdot (A^{r}B^{r} - Y^{r}) + (e^{-(s-c\epsilon)H} - e^{-(s-c\epsilon)H})Y^{r}
\]
\[
+ e^{-(s-c\epsilon)H}Y^{r}.
\]
From the triangle inequality,
\[
\|e^{-sH}M^{-r}_{(x)} - e^{-(s-\epsilon r)H}Y^r\|_1 \\
\leq \|e^{-(s-\epsilon r)H}\|_{\infty} \|A^rB^r - Y^r\|_1 + \|e^{-(s-\epsilon r)H} - e^{-(s-\epsilon d)H}\|_{\infty} \|Y^r\|_1.
\]

Consider the first summand. In view of Lemma 4.5, Theorem 4.1 is applicable and, moreover, the right hand side in Theorem 4.1 is bounded in \(r \in [d, \frac{t}{2}]\). So, the first summand is bounded for \(r \in [d, \frac{t}{2}]\). The second summand vanishes at \(r = d\), and for \(r > d\), it is estimated via (2.2) as:
\[
\|e^{-(s-\epsilon r)H} - e^{-(s-\epsilon d)H}\|_{\infty} \cdot (r - d)\|Y^r\|_1
\leq \sup_{\epsilon > -\|Y\|_{\infty}} \left| e^{-(s-\epsilon r)t} - e^{-(s-\epsilon d)t} \right| \cdot (r - d)\|Y\|_{d, \infty}.
\]
Since \((r - d)\zeta(\frac{t}{d})\) is bounded in the interval \([d, \frac{t}{2}]\), the result follows. \(\square\)

The following theorem is the main result in this section.

**Theorem 4.7.** For any Dixmier trace \(\text{Tr}_{\omega}\) and all \(s > 0\) we have
\[
d^{-1}\lim_{r \downarrow d}(r - d)\text{Tr}(e^{-sH}M^{-r}_{(x)}) = \text{Tr}_{\omega}(e^{-sH}M^{-d}_{(x)}).
\]

**Proof.** Denote the left hand side of this equality by \(E\). Lemma 4.6 implies
\[
E = d^{-1}\lim_{r \downarrow d}(r - d)\text{Tr}(e^{-(s-\epsilon r)H}Y^r).
\]

Hence for every extended limit \(\omega(f) = \omega - \lim_{t \to \infty} f(t)\) on \(L_{\infty}(0, \infty)\), we have (taking \(\frac{t}{d} - 1 = \frac{1}{d}\))
\[
E = \omega\left(\frac{1}{d}\text{Tr}(e^{-(s-\epsilon d)H}Y^{d+\frac{1}{d}})\right).
\]

According to [28, Theorem 8.6.5] (with \(A = Y^d\) and \(B = e^{-(s-\epsilon d)H}\)), it follows that
\[
E = \zeta_{\omega}(e^{-(s-\epsilon d)H}Y^d),
\]
where \(\zeta_{\omega} : L_{1, \infty} \to \mathbb{C}\) is the zeta function associated with the extended limit \(\omega\) (see [28, Definition 8.6.1 and Theorem 8.6.4]). Appealing to Lemma 4.6 with \(r = d\) and taking into account that \(\zeta_{\omega}\) vanishes on \(L_1\), we obtain
\[
E = \zeta_{\omega}(e^{-sH}M^{-d}_{(x)}).
\]

Since \(\zeta_{\omega}\) is a trace (by [28, Theorem 8.6.4 and Lemma 2.7.4]), it follows that
\[
E = \zeta_{\omega}(e^{-\frac{1}{2}sH}M^{-d}_{(x)}e^{-\frac{1}{2}sH}).
\]

Combining this with [28, Theorem 9.3.1] gives
\[
E = \text{Tr}_{\omega}(e^{-\frac{1}{2}sH}M^{-d}_{(x)}e^{-\frac{1}{2}sH}).
\]

It follows that \(E = \text{Tr}_{\omega}(e^{-sH}M^{-d}_{(x)})\). \(\square\)
5. Formula for the density of states

Our next step is to show that for all \( s > 0 \) we have

\[
\lim_{R \to \infty} \frac{1}{|B(0, R)|} \text{Tr}(e^{-sH} M_{B(0, R)}) = \frac{d}{\omega_d r_{1+1}} \lim_{r \downarrow 1} (r - 1) \text{Tr}(e^{-sH} M_{(x)}) .
\]

For each \( s > 0 \), the operator \( e^{-sH} \) is an integral operator \([38, \text{Corollary 25.9}]\), denote its kernel by \( K_{s,V} \). We shall prove the equivalent statement that

\[
\lim_{R \to \infty} \frac{1}{|B(0, R)|} \int_{B(0, R)} K_{s,V}(x, x) \, dx = \frac{d}{\omega_d r_{1+1}} \lim_{r \downarrow 1} (r - 1) \int_{\mathbb{R}^d} \langle \rho \rangle^{-dr} K_{s,V}(x, x) \, dx .
\]

Although the kernel \( K_{s,V} \) is only \textit{a priori} defined pointwise-almost everywhere, we understand the meaning of \( K_{s,V}(x, x) \) in a Lebesgue averaged sense, as justified by Brislawn’s theorem \([13, \text{Theorem 3.1}]\). The following is a routine abelian theorem.

\textbf{Lemma 5.1.} Let \( F \) be a bounded measurable function on \( \mathbb{R}^d \) and assume that there is \( c \in \mathbb{C} \) such that:

\[
\int_{B(0, R)} F(t) \, dt = c R^d + o(R^d), \quad R \to \infty.
\]

Then:

\[
\int_{\mathbb{R}^d} \langle \rho \rangle^{-dr} F(t) \, dt = \frac{c}{r - 1} + o\left(\frac{1}{r - 1}\right), \quad r \downarrow 1.
\]

More concisely, we have:

\[
\lim_{R \to \infty} \frac{1}{|B(0, R)|} \int_{B(0, R)} F(t) \, dt = \frac{1}{|B(0, 1)|} \lim_{r \downarrow 1} (r - 1) \int_{\mathbb{R}^d} \langle \rho \rangle^{-dr} F(t) \, dt,
\]

whenever the left hand side exists.

\textbf{Proof.} Write \( \langle \rho \rangle^{-dr} \) as an integral of an indicator function:

\[
\langle \rho \rangle^{-dr} = \int_0^{\langle \rho \rangle^{-dr}} d\theta = \int_0^1 x_{[0, \langle \rho \rangle^{-dr})} (\theta) \, d\theta
\]

\[
= \int_0^1 x_{[0, (\theta - \frac{\theta}{r} - 1)^{1/2})} (|t|) \, d\theta.
\]

Thus by Fubini’s theorem:

\[
\int_{\mathbb{R}^d} \langle \rho \rangle^{-dr} F(t) \, dt = \int_0^1 \int_{\mathbb{R}^d} x_{[0, (\theta - \frac{\theta}{r} - 1)^{1/2})} (|t|) F(t) \, dt \, d\theta
\]

\[
= \int_0^1 \left( \int_{B(0, (\theta - \frac{\theta}{r} - 1)^{1/2})} F(t) \, dt \right) \, d\theta.
\]

With the change of variable \( \theta = \langle R \rangle^{-dr} \), we have:

\[
\int_{\mathbb{R}^d} \langle \rho \rangle^{-dr} F(t) \, dt = \int_0^{\infty} \frac{dr R}{\langle R \rangle^{dr+2}} \int_{B(0, R)} F(t) \, dt \, dR
\]

\[
= dR \int_0^{\infty} \frac{R^{d+1}}{\langle R \rangle^{dr+2}} \left( \frac{1}{R^d} \int_{B(0, R)} F(t) \, dt \right) \, dR.
\]

Our assumption is that:

\[
\frac{1}{R^d} \int_{B(0, R)} F(t) \, dt = c + \rho(R)
\]
where \( \rho(R) = o(1) \) as \( R \to \infty \). Therefore:
\[
\int_{\mathbb{R}^d} F(t) \, dt = drc \int_0^\infty \frac{R^{d+1}}{(R')^{d+2}} \, dR + dr \int_0^\infty \frac{R^{d+1}}{(R')^{d+2}} \rho(R) \, dR.
\]
The former integral evaluates to \( \frac{1}{2} \frac{\Gamma(d(r-1)/2)\Gamma(1+d/2)}{\Gamma(1+dr/2)} \). Since the gamma function has a pole with residue 1 at 0\(^2\), we have:
\[
\int_{\mathbb{R}^d} F(t) \, dt = \frac{c}{r - 1} + O(1) + dr \int_0^\infty \frac{R^{d+1}}{(R')^{d+2}} \rho(R) \, dR, \quad r \downarrow 1.
\]
By assumption, \( \rho(R) \to 0 \) as \( R \to \infty \). Let \( \varepsilon > 0 \) and choose \( N \) large enough such that \( |\rho(R)| < \varepsilon \) when \( R > N \). Then:
\[
\left| \int_0^\infty \frac{R^{d+1}}{(R')^{d+2}} \rho(R) \, dR \right| \leq \int_0^N \frac{R^{d+1}}{(R')^{d+2}} |\rho(R)| \, dR + \varepsilon \frac{1}{2} \frac{\Gamma(d(r-1)/2)\Gamma(1+d/2)}{\Gamma(1+dr/2)}
\]
\[
= O(1) + \varepsilon O(\frac{1}{r - 1}), \quad r \downarrow 1.
\]
Since \( \varepsilon \) is arbitrary, we have:
\[
\int_0^\infty \frac{R^{d+1}}{(R')^{d+2}} \rho(R) \, dR = o\left(\frac{1}{r - 1}\right).
\]
Thus,
\[
\int_{\mathbb{R}^d} F(t) \, dt = \frac{c}{r - 1} + o\left(\frac{1}{r - 1}\right), \quad r \downarrow 1
\]
as claimed. \( \square \)

Corollary 5.2. For all \( s > 0 \), if the density of states measure \( \nu_H \) exists, then:
\[
\int_{\mathbb{R}} e^{-s\lambda} \, d\nu_H(\lambda) = \frac{1}{|B(0,1)|} \lim_{r \downarrow 1} (r-1) \int_{\mathbb{R}^d} \langle x \rangle^{-dr} K_{s,V}(x,x) \, dx.
\]
That is,
\[
\int_{\mathbb{R}} e^{-s\lambda} \, d\nu_H(\lambda) = \frac{1}{|B(0,1)|} \lim_{r \downarrow 1} (r-1) \text{Tr}(e^{-sH}M_{(x)}^{-dr}).
\]
whenever \( \nu_H \) exists.

Proof. By definition (c.f. (1.3)), we have:
\[
\int_{\mathbb{R}} e^{-s\lambda} \, d\nu_H(\lambda) = \lim_{R \to \infty} \frac{1}{|B(0,R)|} \text{Tr}(M_{X,0(0,R)} e^{-sH})
\]
\[
= \lim_{R \to \infty} \frac{1}{|B(0,R)|} \int_{B(0,R)} K_{s,V}(x,x) \, dx.
\]
We now conclude the proof by an application of Lemma 5.1. The only condition of Lemma 5.1 which needs to be checked is that \( x \mapsto K_{s,V}(x,x) \) is essentially bounded on \( \mathbb{R}^d \). This is \cite[Corollary 25.9]{38}. \( \square \)

\( ^2 \)This follows from the identity \( \Gamma(z) = \frac{1}{z} \Gamma(z+1) \)
Remark 5.3. Our proof crucially relies on the following well-known property of the Laplace transform of measures [41, Theorem II.6.3]: if \( \nu \) and \( \mu \) are complex Borel measures supported on some semi-axis \([-C, \infty)\) such that:

\[
\int_{\mathbb{R}} e^{-st} \, d\nu(t) = \int_{\mathbb{R}} e^{-st} \, d\mu(t)
\]

for all \( s > 0 \) (in particular, both integrals as Lebesgue integrals for all \( s > 0 \)), then \( \nu = \mu \).

An easy way to see this is as a consequence of the Stone-Weierstrass theorem [33, §5.7]. Without loss of generality, \( C = 0 \) and \( \mu = 0 \). Then we have a measure \( \nu \) on \([0, \infty)\) such that \( \int_{0}^{\infty} e^{-st} \, d\nu(t) = 0 \) for all \( s > 0 \). It follows that \( \int_{0}^{\infty} g(t) \, d\nu(t) = 0 \) for all continuous functions \( g \) which are a finite linear span of functions in \( \{e^{-st}\}_{s>0} \).

However the linear span of \( \{e^{-st}\}_{s>0} \) is a subalgebra of the set \( C_{c}([0, \infty)) \) which separates points, hence every \( f \in C_{c}([0, \infty)) \) is a uniform limit of functions in the linear span of \( \{e^{-st}\}_{s>0} \). Let \( f \in C_{c}([0, \infty)) \) be a continuous compactly supported function, and select a sequence \( \{g_{n}\}_{n \geq 0} \) of functions in the linear span of \( \{e^{-st}\}_{s>0} \) which uniformly approximate the continuous compactly supported function \( t \mapsto f(t)e^{t} \) as \( n \to \infty \). Thus we have:

\[
\left| \int_{0}^{\infty} f \, d\nu - \int_{0}^{\infty} g_{n}(t)e^{-t} \, d\nu(t) \right| \leq \sup_{t \geq 0} |e^{t}f(t) - g_{n}(t)| \int_{0}^{\infty} e^{-t} \, d|\nu|(t).
\]

Since each \( \int_{0}^{\infty} g_{n}(t)e^{-t} \, d\nu \) vanishes and also \( \int_{0}^{\infty} e^{-t} \, d|\nu|(t) < \infty \) by the assumption that each \( e^{-st} \) is \( \nu \)-integrable in the Lebesgue sense, it follows that \( \int_{0}^{\infty} f(t) \, d\nu = 0 \) for all continuous compactly supported continuous functions \( f \). Hence by the Riesz theorem, \( \nu = 0 \).

Proof of Theorem 1.1. Corollary 5.2 yields:

\[
\int_{\mathbb{R}} e^{-s\lambda} \, d\nu_{H}(\lambda) = \frac{1}{|B(0, 1)|} \lim_{r \downarrow 1} (r - 1) \text{Tr}(e^{-sH} M_{(x)}^{-dr}).
\]

Theorem 4.7 identifies the limit above as being exactly:

\[
\lim_{r \downarrow 1} (r - 1) \text{Tr}(e^{-sH} M_{(x)}^{-dr}) = \frac{1}{d} \lim_{r \downarrow d} (r - d) \text{Tr}(e^{-sH} M_{(x)}^{-r}) = \text{Tr}_{\omega}(e^{-sH} M_{(x)}^{-d}).
\]

Therefore,

\[
\int_{\mathbb{R}} e^{-s\lambda} \, d\nu_{H}(\lambda) = \frac{1}{|B(0, 1)|} \text{Tr}_{\omega}(e^{-sH} M_{(x)}^{-d}).
\]

Theorem 3.4 implies that if \( f \) is a Borel function on \( \mathbb{R} \) such that \( t \mapsto |f(t)||t|^{d} \) is bounded, then:

\[
|\text{Tr}_{\omega}(f(H) M_{(x)}^{-d})| \leq C \sup_{t \in \mathbb{R}} |f(t)||t|^{d}
\]

for some constant \( C \). From the Riesz theorem, it follows that the functional \( f \mapsto \text{Tr}_{\omega}(f(H) M_{(x)}^{-d}) \) is represented by a Borel measure \( \mu \) on \( \mathbb{R} \),

\[
\text{Tr}_{\omega}(f(H) M_{(x)}^{-d}) = \int_{\mathbb{R}} f \, d\mu, \quad f \in C_{c}^{0}(\mathbb{R}).
\]
This identity is only \textit{a priori} valid for continuous compactly supported functions, but we may include the function \( f(t) = e^{-st} \), for \( s > 0 \), as follows. Select a sequence \( \{ f_n \}_{n=0}^\infty \subset C_c(\mathbb{R}) \) such that as \( n \to \infty \) we have:

\[
\sup_{t > -\|V\|_\infty} |e^{-st} - f_n(t)| < 0.
\]

It follows that \( \int_\mathbb{R} f_n \, d\mu \to \int_\mathbb{R} e^{-st} \, d\mu(t) \) and (5.1) implies that \( \text{Tr}_\omega(f_n(H)M^{-d}_{(x)}) \to \text{Tr}_\omega(e^{-sH}M^{-d}_{(x)}) \). Hence,

\[
\int_\mathbb{R} e^{-st} \, d\mu(t) = \text{Tr}_\omega(e^{-sH}M^{-d}_{(x)}) = |B(0,1)| \int_\mathbb{R} e^{-st} \, d\nu_H(t), \quad s > 0.
\]

Uniqueness for the Laplace transform (Remark 5.3) gives the equality of measures, \( \mu = |B(0,1)| \nu_H = \frac{\omega d}{d} \nu_H \), and this is the desired equality. \( \square \)



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