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Resolvent Expansions and Trace Regularizations for Schrödinger Operators

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Abstract. We provide a direct approach to a study of regularized traces for long range Schrödinger operators and small time asymptotics of the heat kernel on the diagonal. The approach does not depend on multiple commutator techniques and improves upon earlier treatments by Agmon and Kannai, Melin, and the authors.

1. Introduction

In this paper we continue our study of regularized traces and heat invariants for Schrödinger operators, initiated in [**7**]. In [**7**], we derived certain expansions for the heat kernel, and studied asymptotics of trace distributions for Schrödinger operators with long range potentials. Our results were based on [**12**], where expansions for functions of Schrödinger operators were obtained by means of a certain commutator technique (see also [**1**]). In [**7**], we have shown that the multiple commutators of [**12**] could be eliminated, and the expansions could be presented in a much simpler form. Eliminating the commutators in [**7**] allowed us to derive explicit formulas for the coefficients of the asymptotics of trace distributions for long range Schrödinger operators. A similar approach was used earlier for computing the heat invariants of Riemannian manifolds in [**14**], [**16**]. However, the proofs in [**7**], as well as in [**14**], [**16**], still relied on the commutator techniques of [**1**] and [**12**].

Our purpose here is to reexamine [**7**], as well as [**1**] and [**12**], and to provide proofs of some of the basic results in these papers, which do not depend on the commutator techniques. Apart from the technical simplifications that this approach accomplishes, it also seems that one gains more insight into the nature of the expansions of [**1**], [**12**], and [**7**]. In particular,

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here the intuition that the above mentioned expansions are instances of a "noncommutative Taylor's formula", in the sense of [**9**], is justified.

The key ingredient of our approach is a version of the iterated resolvent identity that we state in Proposition 2.1 below (see also [**11**]). Using this identity, we study regularized traces in Section 2, and heat kernel expansions are then derived in Section 3. We remark that combining the proofs of Section 3 together with the combinatorial analysis of [**16**], we get a direct proof of the formulas for the heat invariants for Schrödinger operators, which improves the proofs from [**15**], [**16**]. In Section 4 we have collected additional results and remarks pertinent to heat kernel expansions and trace regularizations. In particular, we point out how the formulas for the heat invariants of [**16**] can be generalized to the case of matrix Schrödinger operators.

Throughout the paper, we shall make use of some estimates for the free resolvent, established in [**1**] and [**12**]. These estimates are as basic for us as they were in those papers. Apart from these results, our note is self-contained.

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2. Trace regularizations for long range potentials

The purpose of this section is to give a direct commutator independent approach to the expansions and regularized traces for functions of Schrödinger operators, studied in [**12**] and [**7**].

Let $H = -\Delta + V(x)$ in $L^2(\mathbf{R}^n)$, where $V \in C^\infty(\mathbf{R}^n)$ is a real-valued potential which is bounded on $\mathbf{R}^n$ together with all its derivatives. We shall write $H_0 = -\Delta$. Introduce the operators X_m, $m \geq 0$, recursively by

$$X_0 = I, \quad X_m = -VX_{m-1} + [X_{m-1}, H_0], \;\; m \geq 1. \tag{2.1}$$

An induction argument shows that X_m are differential operators of orders $\leq m-1$, $m \geq 1$, with coefficients that are bounded on $\mathbf{R}^n$ together with all derivatives.

Let $R(\lambda) = (H-\lambda)^{-1}$ and $R_0(\lambda) = (H_0 - \lambda)^{-1}$ be the resolvents of H and H_0, respectively. The following expansion for $R(\lambda)$ will play the crucial role throughout the present paper.

Proposition 2.1. *For each $M = 0, 1, 2, \dots,$ we have*

$$R(\lambda) = \sum_{m=0}^{M} X_m R_0(\lambda)^{m+1} + R(\lambda) X_{M+1} R_0(\lambda)^{M+1}. \tag{2.2}$$

Here

$$R(\lambda)X_{M+1}R_0(\lambda)^{M+1} = \mathcal{O}_M(1)\frac{\langle\lambda\rangle^{M/2}}{|\mathrm{Im}\,\lambda|^{M+2}} : L^2 \to L^2, \quad \mathrm{Im}\,\lambda \neq 0, \qquad (2.3)$$

and we write $\langle\lambda\rangle = (1+|\lambda|^2)^{1/2}$.

Proof: For $M = 0$, (2.2) becomes the resolvent equation. When proving (2.2), we may therefore assume that $M \geq 1$ and that (2.2) is already proved for lower values of this number. Thus,

$$R(\lambda) = \sum_{m=0}^{M-1} X_m R_0(\lambda)^{m+1} + R(\lambda)X_M R_0(\lambda)^M, \qquad (2.4)$$

and we only have to check that

$$R(\lambda)X_M R_0(\lambda)^M = X_M R_0(\lambda)^{M+1} + R(\lambda)X_{M+1}R_0(\lambda)^{M+1}.$$

In doing so we consider

$$\begin{aligned} &R(\lambda)X_M R_0(\lambda)^M - R(\lambda)X_{M+1}R_0(\lambda)^{M+1} \qquad (2.5)\\ = &\Big(R(\lambda)X_M - R(\lambda)X_{M+1}R_0(\lambda)\Big)R_0(\lambda)^M, \end{aligned}$$

and using the recursive definition (2.1), we see that the expression in the brackets in the right-hand side of (2.5) is equal to $X_M R_0(\lambda)$. This completes the proof of (2.2). When proving the L^2-remainder estimate (2.3), we shall make use of some results of [**12**]. Since the order of the differential operator X_{M+1} is $\leq M$, when estimating the norm on L^2 of $X_{M+1}R_0(\lambda)^{M+1}$, it suffices to estimate the norm of the operator

$$R_0(\lambda)^{M+1} : L^2 \to H^M.$$

Here H^M is the standard Sobolev space on $\mathbf{R}^n$. An application of Proposition 3.3 in [**12**] shows that this norm can be bounded from above by

$$\mathcal{O}_M(1)\frac{\langle\lambda\rangle^{M/2}}{|\mathrm{Im}\,\lambda|^{M+1}}, \quad \mathrm{Im}\,\lambda \neq 0.$$

Since the norm on L^2 of $R(\lambda)$ does not exceed $|\mathrm{Im}\,\lambda|^{-1}$, the estimate (2.3) follows. □

Remark. The iterated resolvent identity (2.2) was proved in [**9**] in the context of Banach algebras, and it can also be extracted from the book [**13**]. In the terminology of [**13**], the expansion (2.2) is an instance of a "noncommutative Taylor's formula", see also [**9**]. The connection between (2.2) and expansions for the heat kernel of H has been explained in [**7**], see also Section 3, and the recent paper [**11**].

Remark. The identity (2.2) should be compared with the standard Neumann expansion for the resolvent,

$$R(\lambda) = \sum_{m=0}^{M} (-1)^m R_0(\lambda)\,(V R_0(\lambda))^m + (-1)^{M+1} R(\lambda)\,(V R_0(\lambda))^{M+1}\,, \quad (2.6)$$

which holds for $M = 0, 1, 2, \ldots$. The point of (2.2), as compared to (2.6), is in rewriting the sum in (2.6), so that powers of the free resolvent $R_0(\lambda)$ appear there. The important thing, exploited in this paper, is a simple and explicit expression for the remainder in (2.2). It is precisely this expression that allows us to give short and direct proofs of some of the results of [**7**], [**1**], and [**12**].

In the remainder of this section, we shall assume that V is in the symbol space $S^{-\varepsilon}(\mathbf{R}^n)$ for some $0 < \varepsilon \leq 1$, so that

$$\partial^\alpha V(x) = \mathcal{O}_\alpha(1)\langle x\rangle^{-\varepsilon-|\alpha|}, \quad x \in \mathbf{R}^n.$$

A simple proof by induction using (2.1) shows that then,

$$X_m = \sum_{|\alpha|\leq m-1} b_{m\alpha}(x) D_x^\alpha,$$

where

$$b_{m\alpha}(x) \in S^{-\varepsilon m}(\mathbf{R}^n). \quad (2.7)$$

Moreover, as in [**7**], we find,

$$X_m = \sum_{k=0}^{m} (-1)^k \binom{m}{k} H^k H_0^{m-k}. \quad (2.8)$$

We shall prove the following result.

Theorem 2.2. *Let $V \in S^{-\varepsilon}(\mathbf{R}^n)$ for some $\varepsilon \in (0,1]$, and set $N(\varepsilon) = [n/\varepsilon]$, the integer part of n/ε. Then the operator*

$$\varphi(H) - \sum_{m=0}^{N(\varepsilon)} (-1)^m \frac{X_m \varphi^{(m)}(H_0)}{m!} \quad (2.9)$$

is of trace class on L^2, when $\varphi \in C_0^\infty(\mathbf{R})$.

The proof of Theorem 2.2 will consist of combining Proposition 2.1 with estimates for the resolvents and the functional calculus. Our starting point is the operator Cauchy's formula of Helffer and Sjöstrand. If $\varphi \in C_0^\infty(\mathbf{R})$, then

$$\varphi(H) = \frac{1}{\pi} \int \overline{\partial}\widetilde{\varphi}(\lambda) R(\lambda) L(d\lambda). \quad (2.10)$$

Here $L(d\lambda)$ is the Lebesgue measure in $\mathbf{C}$, and $\widetilde{\varphi} \in C_0^\infty(\mathbf{C})$ is an almost analytic extension of φ with support close to that of φ — see Chapter 8 in [**6**] and references given there. An application of functional calculus in this form allows us to conclude that

$$\frac{1}{\pi}\int \overline{\partial}\widetilde{\varphi}(\lambda)R_0(\lambda)^{m+1}L(d\lambda) = (-1)^m\varphi^{(m)}(H_0)/m!,$$

so that the contribution to $\varphi(H)$ from the sum in (2.2) is equal to

$$\sum_{m=0}^{M}\frac{1}{\pi}X_m\int \overline{\partial}\widetilde{\varphi}(\lambda)R_0(\lambda)^{m+1}L(d\lambda) = \sum_{m=0}^{M}\frac{(-1)^m X_m\varphi^{(m)}(H_0)}{m!}.$$

We get

$$\varphi(H) = \sum_{m=0}^{M}\frac{(-1)^m X_m\varphi^{(m)}(H_0)}{m!} + \frac{1}{\pi}\int \overline{\partial}\widetilde{\varphi}(\lambda)R(\lambda)X_{M+1}R_0(\lambda)^{M+1}L(d\lambda). \tag{2.11}$$

Here the last integral converges in the L^2-operator norm, in view of (2.3) and the fact that $\overline{\partial}\widetilde{\varphi}(\lambda) = \mathcal{O}(|\mathrm{Im}\,\lambda|^{\infty})$.

When establishing trace class properties of the operator in (2.9), we shall take M in (2.11) sufficiently large.

LEMMA 2.3. *Let us put $M = N := N(\varepsilon)$. Then the expression*

$$R(\lambda)X_{N+1}R_0(\lambda)^{N+1} \tag{2.12}$$

is an analytic family of trace class operators on L^2, for $\mathrm{Im}\,\lambda \neq 0$, *of the trace class norm*

$$\mathcal{O}_{\varepsilon}(1)\frac{\langle\lambda\rangle^{N/2+\varepsilon(N+1)}}{|\mathrm{Im}\,\lambda|^{N+2+\varepsilon(N+1)/2}}.$$

Proof: It follows from (2.7) and the pseudodifferential calculus used in [**12**], that

$$\{R(\lambda)X_{N+1}R_0(\lambda)^{N+1}; \mathrm{Im}\,\lambda \neq 0\}$$

is an analytic family of pseudodifferential operators whose symbols $p(x,\xi,\lambda)$ satisfy the estimates

$$\partial_x^{\alpha}\partial_{\xi}^{\beta}p(x,\xi,\lambda) = \mathcal{O}_{\alpha,\beta}(1)m(x,\xi)\langle x\rangle^{-|\alpha|}\langle\xi\rangle^{-|\beta|},$$

locally unformly in λ. Here the order function

$$m(x,\xi) = \langle x\rangle^{-\varepsilon(N+1)}\langle\xi\rangle^{-N-4} \in L^1(\mathbf{R}^{2n}),$$

since $\varepsilon(N+1) > n$, $N+4 > n$. The trace class properties of (2.12) follow.

When estimating the trace class norm of (2.12), we shall again make use of some results of Section 3 of [**12**], where estimates are derived for the norms of powers of $R_0(\lambda)$, considered as mappings between weighted Sobolev spaces. Let us recall from [**12**] that the weighted space $H_{(\mu,\nu)}$ is defined as the set of distributions $u \in \mathcal{S}'(\mathbf{R}^n)$ such that $\langle x\rangle^{\mu}\langle D\rangle^{\nu}u \in L^2$. Set

$$s = \frac{\varepsilon(N+1)}{2} > \frac{n}{2}.$$

It is then true that the trace class norm of the operator $X_{N+1}R_0(\lambda)^{N+1}$ on L^2 can be estimated from above by a constant (depending on ε) times the norm of the operator

$$X_{N+1}R_0(\lambda)^{N+1} : H_{(-s,-s)} \to H_{(s,s)}. \tag{2.13}$$

Now (2.7) shows that

$$X_{N+1} = \mathcal{O}(1) : H_{(-s,s+N)} \to H_{(s,s)},$$

and when estimating the norm in (2.13), it suffices therefore to estimate the norm of the mapping

$$R_0(\lambda)^{N+1} : H_{(-s,-s)} \to H_{(-s,s+N)}.$$

An application of Proposition 3.3 in [**12**] shows that the latter norm can be bounded from above by a constant times

$$\frac{\langle\lambda\rangle^{N/2+2s}}{|\operatorname{Im}\lambda|^{N+s+1}}, \quad \operatorname{Im}\lambda \neq 0.$$

It follows that the trace class norm of $R(\lambda)X_{N+1}R_0(\lambda)^{N+1}$ is

$$\mathcal{O}(1)\frac{\langle\lambda\rangle^{N/2+2s}}{|\operatorname{Im}\lambda|^{N+s+2}},$$

and recalling the definition of s, we complete the proof. □

An application of Lemma 2.3 shows that the integral

$$\int \overline{\partial}\widetilde{\varphi}(\lambda)R(\lambda)X_{N+1}R_0(\lambda)^{N+1}L(d\lambda)$$

converges in the space of trace class operators, due to the almost analyticity of $\widetilde{\varphi}$. The proof of Theorem 2.2 is complete, in view of (2.11).

Remark. An inspection of the arguments in this section shows that the operator

$$e^{-tH} - \sum_{m=0}^{N(\varepsilon)} \frac{t^m X_m e^{-tH_0}}{m!}, \quad t > 0. \tag{2.14}$$

is of trace class — see also Theorem 1.2 in [**7**]. This follows by combining Proposition 2.3 with Cauchy's integral formula, expressing e^{-tH} in terms of $R(\lambda)$. The asymptotic behaviour of the trace of (2.14), as $t \to 0^+$, has been described in [**7**].

3. Heat kernel expansions

In this section it will be assumed that $V \in C^\infty(\mathbf{R}^n)$ is a bounded real-valued function all of whose derivatives are bounded. Our purpose here is to give a direct proof of Theorem 1.1 of [**7**], relying upon the iterated resolvent equation (2.2). We recall that in [**7**], the proof of this result made use of the explicit expressions for the local heat invariants, derived in [**16**]. Since the proof in this section does not depend on the results of [**16**], we therefore obtain a more direct and transparent way of computing the above mentioned invariants for Schrödinger operators.

We shall prove the following result, which is Theorem 1.1 of [**7**].

Theorem 3.1. *For $M = 0, 1, 2, \ldots$, the following asymptotic representation of the heat kernel is true, as $t \to 0^+$,*

$$e^{-tH}(x,x) = \sum_{m=0}^{M} \frac{t^m}{m!} \left(X_m e^{-tH_0}\right)(x,x) + \mathcal{O}(t^{(M+2)/2-n/2}), \tag{3.1}$$

uniformly in x.

In proving (3.1), let us fix $A < 0$, $A < \inf \operatorname{Spec}(H)$. Multiplying the identity (2.2) by $e^{-t\lambda}$ and integrating over λ from $c - i\infty$ to $c + i\infty$, for any $c \le A$, we get:

$$e^{-tH} = \sum_{m=0}^{M} \frac{t^m X_m e^{-tH_0}}{m!} + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} R(\lambda) X_{M+1} R_0(\lambda)^{M+1} e^{-t\lambda} d\lambda, \quad t > 0. \tag{3.2}$$

In order to estimate the error term in (3.2), we apply the following result.

Lemma 3.2. *If the dimension $n = 1$, then the kernel of*

$$R(\lambda) X_{M+1} R_0(\lambda)^{M+1}, \quad M = 0, 1, \ldots,$$

is a continuous bounded function on $\mathbf{R}^2$ depending analytically on λ with $\operatorname{Re}\lambda \le A$*, and such that*

$$R(\lambda) X_{M+1} R_0(\lambda)^{M+1}(x,x) = \mathcal{O}(1) \langle\lambda\rangle^{(M+1)/2} |\lambda|^{-M-2}, \quad \operatorname{Re}\lambda \le A,$$

uniformly in x.

Proof: This follows directly from Theorem 4.2 of [**1**]. □

For any $t \in (0,1)$, we choose now $c = A/t$ in (3.2), so that $\lambda = (A/t)(1 + i\eta)$, $\eta \in \mathbf{R}$. A direct estimate of the kernel of the remainder in (3.2), making use of Lemma 3.2, then gives

$$e^{-tH}(x,x) = \sum_{m=0}^{M} \frac{t^m}{m!} \left(X_m e^{-tH_0}\right)(x,x) + \mathcal{O}(t^{(M+2)/2-1/2}). \tag{3.3}$$

This proves Theorem 3.1 in the one-dimensional case.

In the case of higher dimensions, we could have followed the idea of [**16**] and studied expansions of derivatives of $R(\lambda)$ with respect to the spectral parameter — see also the remark at the end of this section. We prefer a different approach, which has an advantage of being more direct. A straightforward computation, performed in Section 2 of [**7**], shows that, uniformly in x, we have

$$t^m \left(X_m e^{-tH_0}\right)(x,x) = \mathcal{O}(t^{(m+1)/2-n/2}), \quad m = 1, 2, \ldots,$$

and therefore it suffices to prove Theorem 3.1 only for sufficiently large M. We shall take $M > n-2$.

PROPOSITION 3.3. *Assume that* $M \in \mathbf{N}$ *is such that* $M > n-2$. *Then the distribution kernel of the operator*

$$R(\lambda) X_{M+1} R_0(\lambda)^{M+1} \tag{3.4}$$

is a continuous and bounded function on $\mathbf{R}^{2n}$ *depending analytically on* λ, *with* $\operatorname{Re}\lambda \leq A$. *We have, uniformly in* x,

$$\left(R(\lambda) X_{M+1} R_0(\lambda)^{M+1}\right)(x,x) = \mathcal{O}(1) \frac{\langle\lambda\rangle^{(M+n)/2}}{|\lambda|^{M+2}}, \quad \operatorname{Re}\lambda \leq A. \tag{3.5}$$

In the proof we shall need some estimates for the full resolvent $R(\lambda)$, considered as a mapping between the standard Sobolev spaces H^s.

PROPOSITION 3.4. *Let* $s \geq 0$ *be a real number and* $1 \leq j$ *be an integer. For any* $t \in [0, 2j]$, *we have*

$$R(\lambda)^j = \mathcal{O}_{s,t,j}(1) \frac{\langle\lambda\rangle^{t/2}}{|\lambda|^j} : H^s \to H^{s+t}, \quad \operatorname{Re}\lambda \leq A. \tag{3.6}$$

Proof: It suffices to show that

$$R(\lambda) = \mathcal{O}_{s,t}(1) \frac{\langle\lambda\rangle^{t/2}}{|\lambda|} : H^s \to H^{s+t}, \quad t \in [0,2], \quad \operatorname{Re}\lambda \leq A. \tag{3.7}$$

In doing so, it will be convenient to apply the adjoint equation of (2.2) with $M = [s]+1$,

$$R(\lambda) = \sum_{m=0}^{M} R_0(\lambda)^{m+1} X_m^* + R_0(\lambda)^{M+1} X_{M+1}^* R(\lambda), \quad \operatorname{Re}\lambda \leq A. \tag{3.8}$$

Here X_i^* is the formal adjoint of the differential operator X_i, $i = 0, 1, \ldots M+1$, and we have also used that $R(\lambda)^* = R(\overline{\lambda})$, and similarly for $R_0(\lambda)$. An application of Lemma 4.1 of [**1**] shows that

$$R_0(\lambda) = \mathcal{O}_{s,t}(1) \frac{\langle\lambda\rangle^{t/2}}{|\lambda|} : H^s \to H^{s+t}, \quad \operatorname{Re}\lambda \leq A,$$

and

$$R_0(\lambda)^{m+1} X_m^* = \mathcal{O}_{s,t,m}(1) \frac{\langle\lambda\rangle^{t/2} |\lambda|^{(m-1)/2}}{|\lambda|^{m+1}} : H^s \to H^{s+t}, \quad 1 \leq m \leq M.$$

Another application of the same lemma from [**1**] together with the standard L^2-bound on $R(\lambda)$ gives

$$R_0(\lambda)^{M+1} X_{M+1}^* R(\lambda) = \mathcal{O}_{s,t}(1) \frac{\langle\lambda\rangle^{t/2}}{|\lambda|^2} : H^s \to H^{s+t}, \quad M = [s]+1.$$

In view of (3.8), this establishes (3.7) and completes the proof of the proposition. □

Remark. It follows from (2.1), or, alternatively, from (2.8) that the operators $W_m := (-1)^m X_m^*$ satisfy $W_0 = I$, $W_m = W_{m-1}V + [W_{m-1}, H_0]$. An application of Proposition 4.1 of [**7**] shows that $W_m = V_m$, where the operators V_m were introduced in [**12**] using the multiple commutator technique, see also [**7**].

We now come to the proof of Proposition 3.3. It is clear that the operator in (3.4) has a bounded and continuous kernel, since it is a pseudodiferential operator of order $\leq -M-2 < -n$. In order to derive pointwise estimates for the kernel, we shall make use of Theorem 2.1 in [**1**]. We must therefore estimate the operator norms of the mappings:

$$R(\lambda)X_{M+1}R_0(\lambda)^{M+1} : L^2 \to L^2, \tag{3.9}$$

and

$$R(\lambda)X_{M+1}R_0(\lambda)^{M+1} : L^2 \to H^{M+2}. \tag{3.10}$$

As in Proposition 2.1, we see that the operator norm in (3.9) can be estimated from above by a constant times

$$\frac{\langle\lambda\rangle^{M/2}}{|\lambda|^{M+2}}, \quad \operatorname{Re}\lambda \leq A.$$

When estimating the norm in (3.10), we notice that an application of Lemma 4.1 of [**1**] shows that the operator norm of

$$X_{M+1}R_0(\lambda)^{M+1} : L^2 \to H^{M+2}$$

can be estimated by

$$\mathcal{O}_M(1)\frac{\langle\lambda\rangle^{M+1}}{|\lambda|^{M+1}}.$$

Now an application of Proposition 3.4 shows that

$$R(\lambda) = \mathcal{O}_M(1)\frac{1}{|\lambda|} : H^{M+2} \to H^{M+2}, \quad \operatorname{Re}\lambda \leq A,$$

and we conclude that the operator norm in (3.10) does not exceed

$$\mathcal{O}_M(1)\frac{\langle\lambda\rangle^{M+1}}{|\lambda|^{M+2}}, \quad \operatorname{Re}\lambda \leq A.$$

Furthermore, it follows by similar arguments that we have the same bound on the norm of the L^2-adjoint of the operator in (3.10), viewed as mapping $L^2 \to H^{M+2}$. An application of Theorem 2.1 of [**1**] then shows that the kernel of (3.4) is

$$\mathcal{O}(1)\left(\frac{\langle\lambda\rangle^{M/2}}{|\lambda|^{M+2}}\right)^{1-\frac{n}{M+2}}\left(\frac{\langle\lambda\rangle^{M+1}}{|\lambda|^{M+2}}\right)^{\frac{n}{M+2}}, \quad \operatorname{Re}\lambda \leq A,$$

which is

$$\mathcal{O}(1)\frac{\langle\lambda\rangle^{(M+n)/2}}{|\lambda|^{M+2}},$$

uniformly on $\mathbf{R}^{2n}$. This completes the proof of Proposition 3.3.

Applying (3.2), we get, for $M > n-2$,

$$e^{-tH}(x,x) = \sum_{m=0}^{M} \frac{t^m}{m!} \left(X_m e^{-tH_0}\right)(x,x) \tag{3.11}$$
$$+ \quad \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \left(R(\lambda) X_{M+1} R_0(\lambda)^{M+1}\right)(x,x) e^{-t\lambda}\, d\lambda, \quad t > 0, \quad c \leq A.$$

It follows from Proposition 3.3 that the integral in (3.11) converges absolutely for any $t \geq 0$, since $M + 2 - M/2 - n/2 > 1$ for $M > n-2$. When deriving a bound on the integral, we choose $c = A/t$, $0 < t < 1$, as in the first part of the proof. Another application of Proposition 3.3 shows that the remainder in (3.11) is

$$\mathcal{O}\left(t^{(M+2)/2 - n/2}\right), \quad t \to 0^+,$$

uniformly on $\mathbf{R}^n$. This completes the proof of Theorem 3.1.

Remark. Let $l \in \mathbf{N}$ be such that $l > n/2 - 1$. Since

$$\left(\frac{d}{d\lambda}\right)^l R(\lambda) = l! R(\lambda)^{l+1},$$

it is true that the kernel of the l-th derivative of $R(\lambda)$ is a continuous bounded function. Differentiating (2.2) with respect to λ we get

$$l! R(\lambda)^{l+1} = \sum_{m=0}^{M} \frac{(m+l)!}{m!} X_m R_0(\lambda)^{m+l+1} + \left(\frac{d}{d\lambda}\right)^l R(\lambda) X_{M+1} R_0(\lambda)^{M+1}. \tag{3.12}$$

Developing further the arguments used in this section, and, in particular, making use of the full power of Proposition 3.4, we can also show that for $M = 0, 1, 2, \dots$, the kernel of the remainder in the right-hand side of (3.12) is a continuous and bounded function on $\mathbf{R}^{2n}$ depending analytically on λ with $\operatorname{Re}\lambda \leq A$, such that, uniformly in x,

$$\left(\left(\frac{d}{d\lambda}\right)^l R(\lambda) X_{M+1} R_0(\lambda)^{M+1}\right)(x,x) = \mathcal{O}(1) \frac{\langle\lambda\rangle^{(M+n)/2}}{|\lambda|^{M+l+2}}, \quad \operatorname{Re}\lambda \leq A. \tag{3.13}$$

In the case of Schrödinger operators, the identity (3.12) together with (3.13) establishes therefore an explicit remainder estimate in the expansion, stated in Theorem 2.3.1 in [**16**].

4. Additional results and remarks

In the first part of this section we shall briefly discuss relations between the trace regularization of Section 2 and a different approach to regularized traces for long range Schrödinger operators, developed in [**4**], [**5**], following [**10**]. When $V \in S^{-\varepsilon}(\mathbf{R}^n)$, for some $\varepsilon > 0$, it is proved in [**4**] that the operator

$$\varphi(H_0+V)-\sum_{m=0}^{N(\varepsilon)}\frac{1}{m!}\frac{d^m}{d\varepsilon^m}\bigg|_{\varepsilon=0}\varphi(H_0+\varepsilon V),\quad N(\varepsilon)=[n/\varepsilon], \tag{4.1}$$

is of trace class, for $\varphi\in C_0^\infty(\mathbf{R})$. (More general perturbations are considered in [**4**]). We remark that if we choose $\varphi(t)=\varphi_\lambda(t)=(t-\lambda)^{-1}$, then an application of (2.6) shows that the operator in (4.1) is equal to

$$(-1)^{N(\varepsilon)+1}R(\lambda)\left(VR_0(\lambda)\right)^{N(\varepsilon)+1},$$

and for $\varepsilon\le 1$, this clearly is a trace class operator, depending analytically on λ, $\operatorname{Im}\lambda\neq 0$. The number of terms that one subtracts from $\varphi(H)$ in (4.1) to get a trace class operator agrees with that in (2.9) precisely when $\varepsilon\le 1$, while for $1<\varepsilon\le n$, one has to replace $N(\varepsilon)$ in (2.9) by n. This follows from the arguments of Section 2, if one observes that for $V\in S^{-\varepsilon}(\mathbf{R}^n)$, $\varepsilon>0$, it is true that the coefficients of the differential operator X_m are in $S^{-\overline{\varepsilon}m}(\mathbf{R}^n)$, where $\overline{\varepsilon}=\min(\varepsilon,1)$. The regularization (4.1) is therefore essentially different from the one in Theorem 2.2. In the terminology of [**13**], the regularization (4.1) corresponds to a "noncommutative Newton's formula", while (2.9) is related to Taylor's formula in the operator setting, see [**13**].

There is no difficulty in generalizing the results of the previous sections and of [**16**] to the case of matrix Schrödinger operators. To formulate the precise statement, let us consider

$$H=-\Delta\otimes I+V,$$

acting on $L^2(\mathbf{R}^n,\mathbf{C}^d)$, where I is the identity operator on $\mathbf{C}^d$ and where, for simplicity, we assume that V is a smooth compactly supported function on $\mathbf{R}^n$ with values in the set of Hermitian $d\times d$ matrices. The heat operator e^{-tH}, $t>0$, is a smoothing operator on $L^2(\mathbf{R}^n,\mathbf{C}^d)$, and the heat invariants $A_j(x)$ are the smooth $d\times d$ matrix-valued functions on $\mathbf{R}^n$, arising in the expansion

$$e^{-tH}(x,x)\sim(4\pi t)^{-n/2}\sum_{j=0}^{\infty}A_j(x)t^j,\quad t\to 0^+. \tag{4.2}$$

An inspection of the arguments in Section 3 shows that Theorem 3.1 remains valid in the case of H — see also [**8**] for resolvent expansions for much more general elliptic systems. Indeed, in our case, the operator H has a scalar constant coefficient principal part $H_0=-\Delta\otimes I$, and therefore the operation of commuting with H_0 increases the order of a $d\times d$ matrix operator by at most one unit. It follows, as in the scalar case, that the order of the matrix operator X_m, defined in (2.1), does not exceed $m-1$. Combining heat kernel expansions for H with the combinatorial analysis of [**16**] leads to the following closed expressions for the coefficients $A_j(x)$, cf. [**2**].

Theorem 4.1. *For any integer $r \geq j-1$, the $d \times d$ matrices $A_j(x)$, defined in* (4.2) *, are given by*

$$A_j(x) = (-1)^j \sum_{k=0}^{r} \binom{r+n/2}{k+n/2} \frac{1}{4^k k!(j+k)!} H_y^{j+k} \left(d(x,y)^{2k} I \right) |_{y=x} \quad j \geq 1. \tag{4.3}$$

Here I is the identity operator on $\mathbf{C}^d$ and $d(x,y)$ is the Euclidean distance in $\mathbf{R}^n$.

In particular, when $n=1$, we get formulas for the matrix KdV hierarchy—see [**15**] for the scalar case.

We shall finally point out how Theorem 4.1 can be generalized to the case of Laplace type operators, acting on sections of a d-dimensional vector bundle over some Riemannian manifold M of dimension n. We recall that an operator of Laplace type $\mathcal{L}$ has a scalar leading symbol, and the computation of the local heat invariants $A_j(x)$ in this case uses (2.2), and proceeds similarly to the case of the Laplacian on functions in [**16**]. When applying (2.2), one replaces the unperturbed part H_0 by $\mathcal{L}_0$, where $\mathcal{L}_0$ is the principal part of $\mathcal{L}$, with the coefficients frozen at the point $x \in M$, and the perturbation V is replaced by $\mathcal{L} - \mathcal{L}_0$. The main difficulty in applying (2.2) in this case lies in the fact that the principal part of $\mathcal{L}$ has variable coefficients, so that the order of $\mathcal{L} - \mathcal{L}_0$ is in general no less than the order of $\mathcal{L}$. This difficulty is resolved in [**16**] by a more careful study of the orders of the operators X_m, using results of [**1**]. As a consequence of this, a formula for the local heat invariants for the Laplacian, similar to (4.3), is obtained in [**16**]. There, instead of $r \geq j-1$, one assumes that $r \geq 3j$, and the Euclidean distance $d(x,y)$ in (4.3) is replaced by a Riemannian distance function — see Theorem 1.2.1 in [**16**]. The same formula is then also valid in the case of Laplace type operators.

Remark. It was proved recently in [**17**], that one can take $r \geq j$ in the case of the heat invariants for Laplace type operators. This could also be seen by our methods, working in geodesic polar coordinates near the point x, and using that the radial component of $\mathcal{L} - \mathcal{L}_0$ is an operator of order one — see [**3**]. We take this into account in a heat kernel expansion as in Theorem 3.1, and observe that the heat kernel associated to the operator $\mathcal{L}_0$ is a radial function, since in normal coordinates, $\mathcal{L}_0 = -\Delta \otimes I$, where Δ is the Euclidean Laplacian. Using these observations, one can infer the fact that we only need $r \geq j$ for Laplace type operators.

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