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On the heat kernel and the Korteweg–de Vries hierarchy

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ON THE HEAT KERNEL AND
THE KORTEWEG-DE VRIES HIERARCHY

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1. Introduction and examples.

Consider the one-dimensional Schrödinger (or Sturm-Liouville) operator

\[ L = \frac{\partial^2}{\partial x^2} + u(x). \]  

(1.1)

Its heat kernel \( H(x, y, t) \) is the fundamental solution of the heat equation

\[ \left( \frac{\partial}{\partial t} - L \right) f = 0. \]  

(1.2)

It is well known that \( H(t, x, y) \) has an asymptotic expansion of the form

\[ H(x, y, t) \sim e^{-\frac{(x-y)^2}{4t}} \left( 1 + \sum_{n=1}^{\infty} H_n(x, y)t^n \right) \]  

(1.3)

as \( t \to 0^+ \).

The differential equation (1.2) for \( H(x, y, t) \) implies the recursion-differential equations for the coefficients \( H_n = H_n(x, y) \):

\[ H_0 = 1 \]  

(1.4)

\[ (x - y) \frac{\partial H_n}{\partial x} + nH_n = LH_{n-1} \]  

for \( n \geq 1 \).

(1.5)

This system is known to admit unique smooth solutions \( H_n = H_n(x, y) \) in some neighborhood of the diagonal \( x = y \). The coefficients \( H_n \) are named after J. Hadamard [13], who constructed them for the first time.

**Keywords:** Heat kernel expansions, KdV hierarchy, tau functions.

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Computation of heat invariants of self-adjoint elliptic operators is a well known problem in spectral theory which has many applications, in particular to geometry and theoretical physics [5, 6, 10, 11, 17, 18]. The asymptotics of the one-dimensional Schrödinger operator are of particular interest due to their relations to the Korteweg-de Vries (KdV) hierarchy. More precisely, it is known that the restriction of the heat coefficients on the diagonal gives the right-hand sides of the KdV hierarchy, see [19, 21].

In the present paper we show that there are simple formulas for the Hadamard’s coefficients \( H_n(x,y) \) in terms of the \( \tau \)-function of the KdV hierarchy (see the next section for a precise definition of the \( \tau \)-function).

Remarkable explicit formulas for the coefficients of the Taylor expansion of \( H_n(x,y) \) around the diagonal \( x = y \) were previously constructed in [4], Theorem 1.3. However, these formulas have a rather complicated combinatorial structure and it is practically impossible to write a closed formula for the coefficients even for simple potentials \( u \). One advantage of the formulas derived in this paper is that they give finite expressions for the heat coefficient if the \( \tau \)-function is known (e.g. the solitons, or the more general algebro-geometric solutions of KdV).

To see the importance of the KdV equations, let us compute the first few coefficients using the defining relations (1.4)–(1.5). Anticipating the appearance of the \( \tau \)-function, let us write

\[
u(x) = 2 \frac{\partial^2 \log(\tau(x))}{\partial x^2}.
\]

From (1.5) one can easily obtain simple formulas for \( H_1 \) and \( H_2 \)

\[
H_1(x, y) = \frac{2}{x - y} \left( \frac{\tau'(x)}{\tau(x)} - \frac{\tau'(y)}{\tau(y)} \right)
\]

and

\[
H_2(x, y) = \frac{2}{(x - y)^2} \left( \left( \frac{\tau''(x)}{\tau(x)} + \frac{\tau''(y)}{\tau(y)} \right) - H_1(x, y) - 2 \frac{\tau'(x)\tau'(y)}{\tau(x)\tau(y)} \right).
\]

For the third coefficient we have the following formula

\[
(x - y)^3 H_3(x, y) = -6(x - y)H_2(x, y)2 \left( \frac{\tau'''(x)}{\tau(x)} - \frac{\tau'''(y)}{\tau(y)} \right)
- 2 \left( \frac{\tau''(x)\tau'(x)}{\tau^2(x)} - \frac{\tau''(y)\tau'(y)}{\tau^2(y)} \right)
+ 4 \left( \frac{\tau'(x)}{\tau(x)} \frac{\tau''(y)}{\tau(y)} - \frac{\tau'(y)}{\tau(y)} \frac{\tau''(x)}{\tau(x)} \right)
+ \frac{4}{3} \left( \left( \frac{\tau'(x)}{\tau(x)} \right)^3 - \left( \frac{\tau'(y)}{\tau(y)} \right)^3 \right) + \int_x^y u^2(\xi)d\xi.
\]
Notice that the integral cannot be computed explicitly, unless something remarkable happens. This is the place where the KdV equation comes in. Assume that \( u(x) \) depends on an additional parameter \( s_3 \) and it satisfies the KdV equation

\[
4 \partial_3 u = u''' + 6uu',
\]

where \( \partial_3 = \partial/\partial s_3 \) stands for the partial derivative with respect to \( s_3 \), and \( u' \) is the derivative with respect to \( x \). Then one can easily see that

\[
\int_y^x u^2(\xi)d\xi = -\frac{2}{3} \left( \frac{\tau'''(x)}{\tau(x)} - \frac{\tau'''(y)}{\tau(y)} \right) + \frac{2}{3} \left( \frac{\tau''(x)\tau'(x)}{\tau^2(x)} - \frac{\tau''(y)\tau'(y)}{\tau^2(y)} \right)
\]

\[
-\frac{4}{3} \left( \left( \frac{\tau'(x)}{\tau(x)} \right)^3 - \left( \frac{\tau'(y)}{\tau(y)} \right)^3 \right) + \frac{8}{3} \partial_3 \log \frac{\tau(x)}{\tau(y)},
\]

which combined with (1.8) leads to a simple formula for \( H_3(x, y) \).

We'll extend these computations by showing that if \( u \) is a solution of the KdV hierarchy and \( \tau \) is the corresponding \( \tau \)-function, then there are simple explicit formulas for \( H_n(x, y) \) in terms of \( \tau \).

The paper is organized as follows. In the next section we recall some basic facts about the KdV hierarchy and Sato theory, which are needed for the formulation and the proof of the main result. In Section 3, we prove a general formula for \( H_n(x, y) \). It is interesting that the smoothness of the coefficient \( H_n(x, y) \) on the diagonal is related to the Gegenbauer polynomials. As a corollary of the main theorem, we see the symmetry of the coefficients about the diagonal \( x = y \) as well as the connection between \( H_n(x, x) \) and KdV equations.

As another application of the explicit formula, we show in [16] that the expansion is finite if and only if the potential \( u(x) \) is a rational solution of the KdV hierarchy decaying at infinity studied in [1, 2]. Equivalently, one can characterize the corresponding operators as the rank one bispectral family in [9]. For related results concerning the finiteness property of the heat kernel expansion on the integers and rational solutions of the Toda lattice hierarchy see [12]. For solitons of the Toda lattice and purely discrete versions of the heat kernel see [14].
2. Korteweg-de Vries hierarchy and Sato theory.

In this section we recall some basic facts about KdV hierarchy and Sato theory. For more details on this and the more general Kadomtsev-Petviashvili hierarchy we refer the reader to the papers [20, 7] or the more detailed expositions [8, 22].

Let

\[ L = \frac{\partial^2}{\partial x^2} + u(x) \]

be a second order differential operator. The KdV hierarchy is defined by the Lax equations

\[
\frac{\partial L}{\partial s_j} = [(L^{j/2})_+, L],
\]

where \( j = 1, 3, 5, \ldots \) is an odd positive integer and \((L^{j/2})_+\) is the differential part of the pseudo-differential operator \(L^{j/2} \). The first equation (for \( j = 1 \)) simply means that \( u(x, s_1, s_3, s_5, \ldots) = u(x + s_1, s_3, s_5, \ldots) \), giving us the convenience to occasionally identify \( x \) and \( s_1 \). The next equation (for \( j = 3 \)) is exactly the KdV equation (1.9). Let us represent \( L \) in a dressing form

\[
L = W \partial^2 W^{-1},
\]

where \( W \) is a pseudo-differential operator of the form

\[
W = \sum_{k=0}^{\infty} \psi_k \partial^{-k}, \quad \psi_0 = 1.
\]

The wave (Baker) function \( \Psi(x, s, z) \) and the adjoint wave function \( \Psi^*(x, s, z) \) are defined as

\[
\Psi(x, s, z) = W \exp \left( xz + \sum_{i=1}^{\infty} s_{2i-1} z^{2i-1} \right)
\]

\[
= \left( \sum_{k=0}^{\infty} \psi_k z^{-k} \right) \exp \left( xz + \sum_{i=1}^{\infty} s_{2i-1} z^{2i-1} \right)
\]

and

\[
\Psi^*(x, s, z) = (W^*)^{-1} \exp \left( -xz - \sum_{i=1}^{\infty} s_{2i-1} z^{2i-1} \right)
\]

\[
= \left( \sum_{k=0}^{\infty} \psi_k^* z^{-k} \right) \exp \left( -xz - \sum_{i=1}^{\infty} s_{2i-1} z^{2i-1} \right),
\]

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where $W^*$ is the formal adjoint to the pseudo-differential operator $W$. Using (2.2) one can easily see that

\begin{equation}
L\Psi(x, s, z) = z^2\Psi(x, s, z) \quad \text{and} \quad L\Psi^*(x, s, z) = z^2\Psi^*(x, s, z).
\end{equation}

We shall also use the reduced wave function $\bar{\Psi}$ and the reduced adjoint wave function $\bar{\Psi}^*$ obtained from $\Psi$ and $\Psi^*$, respectively, by omitting the exponential factor, i.e.

\begin{equation}
\bar{\Psi}(x, s, z) = \sum_{k=0}^{\infty} \psi_k z^{-k}
\end{equation}

and

\begin{equation}
\bar{\Psi}^*(x, s, z) = \sum_{k=0}^{\infty} \psi_k^* z^{-k}.
\end{equation}

Equations (2.6) imply

\begin{equation}
L\bar{\Psi}(x, s, z) + 2z\partial_x \bar{\Psi}(x, s, z) = 0 \quad \text{and} \quad L\bar{\Psi}^*(x, s, z) - 2z\partial_x \bar{\Psi}^*(x, s, z) = 0.
\end{equation}

Using equations (2.2)–(2.5) one can show that the wave and the adjoint wave function satisfy the following bilinear identities

\begin{equation}
\text{res}_z \left( z^{2n} \Psi^{(l)}(x, s, z)\Psi^*(x, s, z) \right) = 0,
\end{equation}

for all nonnegative integers $n$ and $l$, where $\Psi^{(l)}(x, s, z)$ is the $l$th derivative of $\Psi$ with respect to $x$, and the residue is around $z = \infty$.

The remarkable discovery of the Kyoto school was that the KdV hierarchy (2.1) could be described by a function $\tau(x, s)$. This goes back to an earlier work of Hirota, see [15]. The reduced wave and the reduced adjoint wave functions can be expressed in terms of $\tau(x, s)$ by the following formulas

\begin{equation}
\bar{\Psi}(x, s, z) = \frac{\tau(x; s - [z^{-1}])}{\tau(x, s)} \quad \text{and} \quad \bar{\Psi}^*(x, s, z) = \frac{\tau(x; s + [z^{-1}])}{\tau(x, s)},
\end{equation}

where $[z] = (z, z^3/3, z^5/5, \ldots)$.

Finally, let us denote by $W_n(x, y)$ the coefficients of the function\(^1\)

\begin{equation}
\bar{\Psi}(x, s, z)\bar{\Psi}^*(y, s, z), \quad \text{i.e.}
\end{equation}

\begin{equation}
\bar{\Psi}(x, s, z)\bar{\Psi}^*(y, s, z) = \sum_{n=0}^{\infty} W_n(x, y)z^{-n}.
\end{equation}

\(^1\) This function is closely related to the Green function for $L$. 

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Using (2.11) we can easily write an explicit formula for \( W_n \) in terms of the \( \tau \)-function. If we denote by \( \mathcal{S}_k(s) \) the elementary Schur polynomials defined by

\[
\sum_{k=0}^{\infty} \mathcal{S}_k(s)z^k = \exp\left(\sum_{k=1}^{\infty} s_{2k-1}z^{2k-1}\right),
\]

then we have

\[
W_n(x, y) = \sum_{k=0}^{n} \left[ \mathcal{S}_k(-\tilde{\partial}) \tau(x, s) \right] \left[ \mathcal{S}_{n-k}(\tilde{\partial}) \tau(y, s) \right] \tau(x, s) \tau(y, s),
\]

where

\[
\tilde{\partial} = (\partial_1, \partial_3/3, \ldots, \partial_{2k-1}/(2k-1), \ldots).
\]

### 3. Explicit formulas for Hadamard’s coefficients.

The main result of the paper is the following theorem.

**Theorem 3.1.** — The Hadamard’s coefficients can be computed from the following relation

\[
H_n(x, y) = (-1)^n \sum_{k=0}^{n-1} \frac{2^{n-k}(n-k)_{2k} W_{n-k}(x, y)}{k!(x-y)^{n+k}},
\]

where \( (\alpha)_k = \alpha(\alpha+1)\ldots(\alpha+k-1) \) denotes the Pochhammer symbol, and \( W_n(x, y) \) are defined by (2.14).

**Proof.** — To prove that the Hadamard’s coefficients are given by (3.1) we need to check that (1.5) holds and that \( H_n(x, y) \) are smooth on the diagonal \( x = y \).

To see that (1.5) holds, let us denote

\[
f_n(x, y, z) = (-1)^n \sum_{k=0}^{n-1} \frac{2^{n-k}(n-k)_{2k} z^{n-k-1}}{k!(x-y)^{n+k}}.
\]

Then (3.1) can be rewritten as

\[
H_n(x, y) = \text{res}_z \left[ f_n(x, y, z) \bar{\Psi}(x, s, z) \bar{\Psi}^*(y, s, z) \right].
\]
Using the last equation together with (2.9) one can easily see that
\[(x - y)\partial_x + n] H_n(x, y) - L(x, \partial_x)H_{n-1}(x, y)\]
\[= \text{res}_z \left[ ((x - y)\partial_x f_n(x, y, z) + nf_n(x, y, z) \right.\]
\[- \partial_x^2 f_{n-1}(x, y, z) \bar{\Psi}(x, s, z) \bar{\Psi}^*(y, s, z)\]
\[+ \left. ((x - y)f_n(x, y, z) + 2zf_n-1(x, y, z) \right] \]
\[- 2\partial_x f_{n-1}(x, y, z))\partial_x \bar{\Psi}(x, s, z) \bar{\Psi}^*(y, s, z) \right].\]

A direct computation now shows that
\[(x - y)\partial_x f_n(x, y, z) + nf_n(x, y, z) - \partial_x^2 f_{n-1}(x, y, z) = 0\]
\[(x - y)f_n(x, y, z) + 2zf_n-1(x, y, z) - 2\partial_x f_{n-1}(x, y, z) = 0,\]
which proves (1.5).

Next we need to show that $H_n(x, y)$ is well defined on the diagonal.
Writing $H_n(x, y)$ as
\[(3.4) \quad H_n(x, y) = \frac{2(-1)^n}{(x - y)^{2n-1}} \sum_{k=0}^{n-1} \frac{2^k(x - y)^k(k + 1)_{2n-2k-2}}{(n - k - 1)!} W_{k+1}(x, y),\]
and applying L'Hôpital's rule we see that we need to prove that for
\[j = 0, 1, \ldots, 2n - 2\]
we have
\[(3.5) \quad \sum_{k=0}^{n-1} 2^k \binom{j}{k} \binom{2n - 2 - k}{n - k - 1} \partial_x^{j-k} W_{k+1}(x, y)|_{x=y} = 0.\]
Using (2.12) and
\[\partial_x^n \bar{\Psi}(x, s, z) = \exp \left( -xz - \sum_{i=1}^{\infty} s_{2i-1} z^{2i-1} \right) (\partial_x - z)^j \Psi(x, s, z)\]
we see that (3.5) is equivalent to the following identities
\[(3.6) \quad \text{res}_z \left[ \sum_{k=0}^{n-1} 2^k \binom{j}{k} \binom{2n - 2 - k}{n - k - 1} \Psi(x, s, z) \right] = 0.\]
Equation (3.6) will follow from the bilinear identities (2.10) if we can show that the polynomial
\[(3.7) \quad P_{n,j}(w) = \sum_{k=0}^{n-1} 2^k \left( \binom{j}{k} \binom{2n - 2 - k}{n - k - 1} \right) (w - 1)^{j-k},\]
is an even/odd function when $j$ is an even/odd number, respectively. It is
a pleasant surprise to see that these polynomials are closely related to very

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well known classical orthogonal polynomials – the so called Gegenbauer polynomials.

The Gegenbauer (or ultraspherical) polynomials are defined by
\[
(3.8) \quad C^\lambda_n(w) = \sum_{k=0}^{n} 2^k \binom{\lambda + k - 1}{k} \binom{2\lambda + n + k - 1}{n - k} (w - 1)^k,
\]
see for example [3], pages 302–303. Notice that this definition can be used for arbitrary $\lambda$. If $\lambda > -1/2$ and $\lambda \neq 0$ these polynomials are orthogonal on the interval $(-1, 1)$ with respect to $(1 - x^2)^{\lambda - \frac{1}{2}}$ which, in particular, implies that $C^\lambda_n(w)$ is an even/odd function when $n$ is even/odd, respectively.

However, we need these polynomials also for negative values of $\lambda$. In this case, we can use the three term recurrence relation
\[
(3.9) \quad 2(n + \lambda)wC^\lambda_n(w) = (n + 1)C^\lambda_{n+1}(w) + (n + 2\lambda - 1)C^\lambda_{n-1}(w).
\]
and $C^\lambda_0 = 1$ and $C^\lambda_1 = 2\lambda w$ to deduce that $C^\lambda_n(w)$ is an even/odd polynomial when $n$ is even/odd, respectively.

Changing the summation index in (3.7) we can rewrite $P_{n,j}(w)$ as
\[
(3.10) \quad P_{n,j}(w) = \sum_{k=\max(0,j-n+1)}^{j} 2^{j-k} \binom{j}{k} \frac{(2n - j - 2 + k)!}{(n - j + k - 1)!} (w - 1)^k.
\]

From the last equation and the defining relation (3.8) for the Gegenbauer polynomials one can see that\footnote{\((−1)!! = 1\) and \((2k − 1)!! = 1 \cdot 3 \cdots (2k − 1)\) for \(k \geq 1\).}
\[
(3.11) \quad P_{n,j}(w) = j!2^{n-1}(2n - 2j - 3)!! C^{n-j-\frac{1}{2}}_{j}(w) \quad \text{for} \quad 0 \leq j \leq n - 1,
\]
\[
(3.12) \quad P_{n,j}(w) = \frac{(-1)^{j-n+1}j!2^{n-1}}{(2j - 2n + 1)!!} C^{n-j-\frac{1}{2}}_{j}(w) \quad \text{for} \quad n \leq j \leq 2n - 2,
\]
which completes the proof. \(\square\)

From (2.14) and (3.1) we obtain the following

COROLLARY 3.2. — The Hadamard’s coefficients $H_n(x, y)$ are symmetric functions of $x$ and $y$, i.e. we have
\[
H_n(x, y) = H_n(y, x).
\]

Finally, we show that the heat coefficients $\{H_n(x, x)\}$ determine the right-hand sides of KdV equations (2.1).

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Corollary 3.3. — We have
\begin{equation}
H_n(x, x) = \frac{2^n}{(2n-1)!!} W_{2n}(x, x)
\end{equation}
and
\begin{equation}
[(L_{2n-1})^+, L] = 2\partial_x W_{2n}(x, x).
\end{equation}
Thus, the KdV hierarchy (2.1) is equivalent to the following equations
\begin{equation}
\partial_{2n-1} u = \frac{(2n-1)!!}{2^{n-1}} \partial_x H_n(x, x), \text{ for } n = 1, 2, \ldots.
\end{equation}

Proof. — Using (3.1) and applying L'Hôpital's rule 2n − 1 times we see that
\begin{equation}
H_n(x, x) = (-1)^n \frac{2}{(2n-1)!} \times \sum_{k=0}^{n-1} 2^k \binom{2n-1}{k} \frac{(2n-k-2)!}{(n-k-1)!} \partial_x^{2n-1-k} W_{k+1}(y, x)|_{y=x}
\end{equation}
\begin{equation}
= (-1)^n \frac{2}{(2n-1)!} \times \text{res}_z [z^{2n-1} (P_{n,2n-1}(z^{-1}\partial_x) \Psi(x, s, z)) \Psi^*(x, s, z)],
\end{equation}
where $P_{n,2n-1}(w)$ is the polynomial defined by (3.10) for $j = 2n - 1$
\begin{equation}
P_{n,2n-1}(w) = \sum_{k=n}^{2n-1} 2^{2n-1-k} \binom{2n-1}{k} \frac{(k-1)!}{(k-n)!} (w-1)^k.
\end{equation}
Notice that this time we have
\begin{equation}
P_{n,2n-1}(w) = (-1)^n 2^{n-1}(2n-2)!! \left(C_{2n-1}^{-n+\frac{1}{2}}(w) + 1\right),
\end{equation}
and using the same argument (the bilinear identity and the fact that $C_{2n-1}^{-n+\frac{1}{2}}(w)$ is an odd polynomial) we obtain (3.13) from (3.16).

From (2.2), (2.4), (2.5) and (2.11) it follows that
\begin{equation}
L_{2n-1} = W \partial_x^{2n-1} W^{-1} = \sum_{i,j=0}^{\infty} \frac{S_i(-\tilde{\partial}) \tau(x, s)}{\tau(x, s)} \partial_x^{2n-1-i-j} S_j(\tilde{\partial}) \tau(x, s).
\end{equation}
Combining this formula with (2.14) we find that the coefficient of $\partial_x^{-1}$ in $L_{2n-1}^{2n-1}$ is $W_{2n}(x, x)$. If we denote by $(L_{2n-1})^-$ the integral (Volterra) part of the pseudo-differential operator $L_{2n-1}^{2n-1}$ we obtain
\begin{equation}
[(L_{2n-1}^{2n-1})^+, L] = [(L_{2n-1}^{2n-1})^-, L]^+ = [L, (L_{2n-1}^{2n-1})^-]^+ = [\partial_x^2 + u(x), W_{2n}(x, x) \partial_x^{-1} + O(\partial_x^{-2})]^+ = 2\partial_x (W_{2n}(x, x)),
\end{equation}
which gives (3.14) and completes the proof. \qed
BIBLIOGRAPHY


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