Heat Kernel Coefficients for Periodic Schrödinger Operators

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1. Introduction

For an *n*-dimensional Schrödinger operator

(1.1)
$$\mathfrak{L} = \left(\frac{\partial}{\partial x_1}\right)^2 + \dots + \left(\frac{\partial}{\partial x_n}\right)^2 - u(x)$$

with $x = (x_1, \dots, x_n)$ and locally smooth potential u(x), we define its heat kernel $\Phi(x, \xi, t)$ to be the fundamental solution of the heat equation

(1.2)
$$\left(\frac{\partial}{\partial t} - \mathfrak{L}\right) \Phi(x, \xi, t) = 0, \quad \Phi(x, \xi, 0) = \delta(x - \xi).$$

It is well-known (see e.g. [12, 23]) that $\Phi(x,\xi,t)$ has an asymptotic expansion of the form

(1.3)
$$\Phi(x,\xi,t) \sim \frac{e^{-\frac{|x-\xi|^2}{4t}}}{(4\pi t)^{\frac{n}{2}}} \left(1 + \sum_{\nu=1}^{\infty} U_{\nu}(x,\xi)t^{\nu} \right) \quad \text{as } t \to 0^+.$$

In can be directly shown from (1.2) that the coefficients U_{ν} of this expansion satisfy the following transport equations

$$(1.4) (x - \xi, \partial_x) U_{\nu}(x, \xi) + \nu U_{\nu}(x, \xi) = \mathfrak{L}[U_{\nu-1}(\cdot, \xi)](x), \nu = 1, 2, \dots$$

with a convention $U_0 \equiv 1$. It turns out that the differential-recurrence system (1.4) has a unique solution if one requires that $U_{\nu}(x,\xi)$ is bounded as $x \to \xi$. Following [14], we will refer to the heat kernel coefficients $U_{\nu}(x,\xi)$ as the *Hadamard coefficients* of the operator \mathfrak{L} .

The problem of calculating the Hadamard coefficients has appeared in many different contexts in mathematics. For example, the heat kernel expansion of the Laplacian on Riemannian manifolds is one of the main objects of study in Spectral Geometry. In this paper we consider the Schrödinger operator $\mathfrak L$ on flat space, in which case the Hadamard coefficients are directly connected to Huygens' principle as well as the theory of solitons.

The paper is organized as follows: In section 2, we explain the connection between the heat kernel expansion and Huygens' principle. We give examples of non-trivial "Huygens operators," including the subject of the paper, the operator (2.12). We also state the main result of the paper, which is an explicit formula for the Hadamard coefficients of the operator (2.12). In section 3, we describe Darboux transformations and their relationship with the Hadamard coefficients. This is used to show that there are a finite number of non-zero Hadamard coefficients of (2.12) and is used later in Section 6 to prove the main result. In sections 4 and 5, we show how the Hadamard coefficients can be expressed in terms of the asymptotics of the resolvent kernel. Finally, in section 6, we derive explicit formulas for both the Hadamard coefficients U_{ν} of (2.12) and the asymptotics of its resolvent kernel. While sections 2-3 are mostly review, sections 4-6 are essentially new results.

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2. Finite Heat Kernel Expansions and Hadamard's problem

The study of the Hadamard coefficients goes back to Jacques Hadamard in his investigation of Huygens' principle [16]. A hyperbolic operator is said to satisfy Huygens' principle if the solution of any Cauchy problem at time t depends only on the initial data on a sphere of radius t centered at the point (x, y, z), i.e. the fundamental solution is supported on the surface of the characteristic conoid. In his "Lectures on the Cauchy problem", Jacques Hadamard proposed the problem of determining all second-order hyperbolic operators with this special property. He also gave a very useful criterion for a given hyperbolic operator

(2.1)
$$\square_{n+1} + u(x) = \left(\frac{\partial}{\partial t}\right)^2 - \left(\frac{\partial}{\partial x_1}\right)^2 - \dots - \left(\frac{\partial}{\partial x_n}\right)^2 + u(x)$$

to satisfy Huygens' principle. Explicitly, Hadamard's criterion states that such an operator satisfies Huygens' principle if and only if n > 1 is odd and

$$(2.2) U_p(x,\xi) = 0$$

where p = (n-1)/2 and the Hadamard coefficients $U_{\nu}(x,\xi)$ of the operator (2.1), which appear in the fundamental solution of the wave equation, are exactly the heat kernel coefficients of the corresponding Schrödinger operator

(2.3)
$$\left(\frac{\partial}{\partial x_1}\right)^2 + \dots + \left(\frac{\partial}{\partial x_n}\right)^2 - u(x).$$

Note that if $U_p(x,\xi) = 0$, then $U_{\nu}(x,\xi) = 0$ for all $\nu \geq p$, as is clear from the transport equation once we require that $U_{\nu}(x,\xi)$ is bounded as $x \to \xi$. Thus, we have the following

Proposition 1. If the hyperbolic operator (2.1) satisfies Huygens' principle then the operator (2.3) has a finite heat kernel expansion.

We will refer to an operator (2.3) with property (2.2) as terminating at the level p. Note that the restriction on p by the dimension n is not essential to the problem of finding Huygens operators, since given any p-terminating hyperbolic operator \mathfrak{L} , it is always possible to lift to a higher-dimensional hyperbolic operator

(2.4)
$$\mathfrak{L}' := \mathfrak{L} - \sum_{i=1}^{l} \left(\frac{\partial}{\partial y_i} \right)^2$$

with the same U_k as \mathfrak{L} . So in fact, Hadamard's problem reduces to the problem of finding terminating operators.

Hadamard conjectured that all second-order hyperbolic operators were equivalent to the standard d'Alembertian up to change of variables. This conjecture turned out to be false, with the first class of non-trivial Huygens operators being given by K. Stellmacher and J. Lagnese ([19, 20, 21, 26, 27]). This class of operators had the form

$$\square_{n+1} + u(x)$$

where u(x) is a rational function of one variable defined by

$$(2.6) u(z) = 2\frac{d^2}{dz^2} \log P_k(z)$$

and the sequence of polynomials $P_k(z)$ is defined by the differential-recurrence relation

$$(2.7) P'_{k+1}(z)P_{k-1}(z) - P'_{k-1}(z)P_{k+1}(z) = (2k+1)P_k^2(z)$$

starting from $P_0 = 1$, $P_1 = z$. In fact, it was proved that all operators of the form (2.5) with potential u(x) depending on one variable which satisfied Huygens' principle were of this form ([20]). The polynomials $P_k(z)$ first appeared in the works of Burchnall and Chaundy ([11]) and were discovered independently in the context of Hadamard's problem by Stellmacher and Lagnese ([21]) and in the context of integrable systems by Adler, Airault, McKean, and Moser [1, 2].

Another class of Huygens' operators in Minkowski space was discovered by Y. Berest and A. Veselov ([8, 9]) in which the potential u(x) depends on several variables. For a fixed Coxeter group W with root system \mathfrak{R} and a W-invariant, integer-valued function $m: \mathfrak{R} \to \mathbf{Z}_{\geq 0}$, we can associate a "Calogero-Moser" potential

(2.8)
$$u(x) = \sum_{\alpha \in \mathfrak{R}_{+}} \frac{m_{\alpha}(m_{\alpha} + 1)(\alpha, \alpha)}{(\alpha, x)^{2}}.$$

In ([8]), it was shown that the hyperbolic operator

$$\square_{n+1} + u(x)$$

satisfies Huygens' principle provided that n is odd and $n \geq 3 + 2 \sum_{\alpha \in \Re_+} m_{\alpha}$.

Finally, a third class of hyperbolic operators satisfying Huygens' principle was discovered by Y. Berest and I. Loutsenko ([6]) in which case the potential u(x) depends on two variables. Given a strictly increasing sequence of positive integers

$$(2.10) 0 \le k_1 < k_2 < \dots < k_{m-1} < k_m = N$$

we define a sequence of functions $\chi_j(\varphi)$ by

(2.11)
$$\chi_j(\varphi) := \cos(k_j \varphi + \varphi_j)$$

where $\varphi_j \in \mathbf{R}$ are arbitrary phases. Then the operator

(2.12)
$$\mathfrak{L} := \Box_{n+1} - \frac{2}{r^2} \left(\frac{\partial}{\partial \varphi} \right)^2 \log \mathcal{W}[\chi_1(\varphi), \chi_2(\varphi), ..., \chi_m(\varphi)]$$

satisfies Huygens' principle provided that $n \geq 3$ is odd and

$$(2.13) N \le \frac{n-3}{2}$$

Here (r, φ) denote polar coordinates in the Euclidean 2-plane (x_1, x_2) and $W[\chi_1(\varphi), \chi_2(\varphi), ..., \chi_m(\varphi)]$ is the Wronskian of the functions $\chi_1(\varphi), \chi_2(\varphi), ..., \chi_m(\varphi)$. These operators are an extension of the operators (2.9) with potentials (2.8) corresponding to the dihedral group $I_2(q)$ (see [4, 6])

In fact, it was shown ([4]) that any linear, second-order, normal hyperbolic operator

$$\mathfrak{L} = \square_{n+1} + u(x_1, x_2)$$

with locally analytic potential $u(x_1, x_2)$ homogeneous of degree -2 that satisfies Huygens' principle must be of the form (2.12). The aim of this paper is to complete the investigation

of the operators (2.12) by computing explicitly their Hadamard coefficients: to be precise, our main result can be stated as follows.

Theorem 1. The Hadamard coefficients of the operator (2.12) can be presented in simple closed form in terms of polar coordinates:

$$U_0 = 1$$

$$(2.14) U_{\nu} = \frac{(-2)^{\nu}}{(r\rho)^{\nu}} \frac{1}{\mathcal{W}(\varphi)\mathcal{W}(\phi)} \sum_{i=1}^{m} c_{i} \mathcal{W}_{i}(\varphi)\mathcal{W}_{i}(\phi) T_{k_{i}}^{(\nu)}(\cos(\varphi - \phi)) , \quad \nu \geq 1 ,$$

where c_i and W_i are defined, respectively, as

(2.15)
$$c_i := \begin{cases} 1 & \text{if } m = 1\\ \prod_{\substack{j=1\\j\neq i}}^m (k_i^2 - k_j^2) & \text{if } m > 1 \end{cases}$$

$$\mathcal{W}_i := \mathcal{W}[\chi_1, \dots, \chi_{i-1}, \chi_{i+1}, ..., \chi_m]$$

and $T_N(z) := \cos(N \arccos(z)), z \in [-1, 1]$, is the N^{th} Chebyshev polynomial, with $T_N^{(\nu)}(z)$ its derivative of order ν with respect to z.

3. Darboux transformations

Both the potentials in (2.6) and (2.12) can be obtained from ∂^2 by a sequence of classical Darboux transformations. By Darboux transformation we mean the following: Starting with a Sturm-Liouville operator

(3.1)
$$L_0 := -\frac{\partial^2}{\partial \omega^2} + v_0(\varphi)$$

we fix an eigenfunction $\Psi_1(\varphi)$ with eigenvalue λ_1 . This gives rise to a factorization

(3.2)
$$L_0 - \lambda_1 = -\left(\frac{\partial}{\partial \varphi} + f_1(\varphi)\right) \left(\frac{\partial}{\partial \varphi} - f_1(\varphi)\right)$$

where $f_1(\varphi)$ is the logarithmic derivative of $\Psi_1(\varphi)$, i.e.

(3.3)
$$f_1(\varphi) = \frac{\partial}{\partial \varphi} \log \Psi_1(\varphi) = \frac{\Psi'_1(\varphi)}{\Psi_1(\varphi)}$$

We then define

(3.4)
$$A_0 := \frac{\partial}{\partial \varphi} - f_1(\varphi)$$

and

(3.5)
$$A_0^* := -\frac{\partial}{\partial \varphi} - f_1(\varphi).$$

So, writing

$$(3.6) L_0 = \lambda_1 + A_0^* A_0,$$

we then define the Darboux transformation of L_0 with respect to λ_0 as

$$(3.7) L_1 := \lambda_1 + A_0 A_0^*.$$

This new operator is of the form

(3.8)
$$L_1 = -\frac{\partial^2}{\partial \varphi^2} + v_1(\varphi)$$

where

(3.9)
$$v_1(\varphi) = v_0(\varphi) - 2\left(\frac{\partial}{\partial \varphi}\right)^2 \log \Psi_1(\varphi)$$

Given another eigenfunction $\Psi(\varphi)$ of L_0 with eigenvalue $\lambda \neq \lambda_1$, the function

(3.10)
$$A_0[\Psi(\varphi)] = \frac{\mathcal{W}[\Psi_1, \Psi]}{\Psi_1}$$

is an eigenfunction of L_1 with the same eigenvalue. This is clear from the relation

$$(3.11) L_1 \circ A_0 = A_0 \circ L_0.$$

We see therefore that the Darboux transformation L_1 of L_0 with respect to λ_1 has the same spectrum as L_0 , with the exception of the point λ_1 . Fixing another eigenfunction $\Psi_2(\varphi)$ of L_0 with eigenvalue $\lambda_2 \neq \lambda_1$, we get an eigenfunction of L_1 which we can use to apply a Darboux transformation to L_1 . Continuing this process N times, we end up with an operator

(3.12)
$$L_N = -\frac{\partial^2}{\partial \varphi^2} + v_N(\varphi)$$

with $v_N(\varphi)$ related to $v_0(\varphi)$ by the equation

(3.13)
$$v_N(\varphi) = v_0(\varphi) - 2\left(\frac{\partial}{\partial \varphi}\right)^2 \log \mathcal{W}[\Psi_1(\varphi), \Psi_2(\varphi), \cdots \Psi_N(\varphi)].$$

 L_0 and L_N are again intertwined by the relation

$$(3.14) L_N \circ (A_{N-1} \circ \cdots A_1 \circ A_0) = (A_{N-1} \circ \cdots A_1 \circ A_0) \circ L_0.$$

Here the operators A_i take the form

(3.15)
$$A_i := \frac{\partial}{\partial \varphi} - f_{i+1}(\varphi)$$

where

(3.16)
$$f_{i+1}(\varphi) = \frac{\partial}{\partial \varphi} \log \frac{\mathcal{W}[\Psi_1(\varphi), \cdots, \Psi_{i+1}(\varphi)]}{W[\Psi_1(\varphi), \cdots, \Psi_i(\varphi)]}$$

and an arbitrary eigenfunction $\Psi(\varphi)$ of L_0 of eigenvalue $\lambda \neq \lambda_1, \lambda_2, \dots, \lambda_n$ is transformed to the eigenfunction

$$(3.17) (A_{N-1} \circ \cdots A_1 \circ A_0) \Psi(\varphi) = \frac{\mathcal{W}[\Psi_1(\varphi), \cdots, \Psi_N(\varphi), \Psi(\varphi)]}{W[\Psi_1(\varphi), \cdots, \Psi_N(\varphi)]}$$

of L_N of eigenvalue λ .

In suitably chosen cylindrical coordinates, the operator (2.12) can be written explicitly as follows

(3.18)
$$\mathfrak{L} = \Delta_{n-2} + \left(\frac{\partial}{\partial r}\right)^2 + \frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}L$$

where (r,φ) are the polar coordinates in the corresponding Euclidean plane and

(3.19)
$$L := -\left(\frac{\partial}{\partial \varphi}\right)^2 + v(\varphi)$$

is a one-dimensional Schrödinger operator with $v(\varphi) = u(\cos \varphi, \sin \varphi)$. The operator (3.19) is then the N-th Darboux transformation of the operator $-\left(\frac{\partial}{\partial \varphi}\right)^2$ obtained by taking (2.11) as our eigenfunctions. Moreover, the Hadamard coefficients have the form

(3.20)
$$U_{\nu}(x,\xi) = \frac{1}{(r\rho)^{\nu}} \sigma_{\nu}(\varphi,\phi), \quad \nu = 0, 1, 2, ...,$$

where (ρ, ϕ) is the polar coordinates of ξ . The above transport equation (1.4) in this case is equivalent to the system of equations ([4, Lemma 3.1])

(3.21)
$$\sin(\varphi - \phi) \frac{\partial}{\partial \varphi} \sigma_{\nu}(\varphi, \phi) + \nu \cos(\varphi - \phi) \sigma_{\nu}(\varphi, \phi) = -(L - (\nu - 1)^{2}) [\sigma_{\nu - 1}(\cdot, \phi)](\varphi), \quad \nu \ge 1,$$

which has a unique solution $(\sigma_0, \sigma_1, \sigma_2, ...)$ such that $\sigma_0(\varphi, \phi) \equiv 1$ and $\sigma_{\nu}(\varphi, \phi)$ are bounded as $\varphi \to \phi$. For convenience, we will also refer to the functions $\sigma_{\nu}(\varphi, \phi)$ as Hadamard coefficients. We now state a proposition concerning Hadamard coefficients and the Darboux transformation.

Proposition 2. Let L_0 and L_1 be two operators where L_1 is obtained from L_0 by a single Darboux transformation as in (3.6) and (3.7). Let (σ_{ν}^0) and (σ_{ν}^1) be the sequences of Hadamard coefficients of L_0 and L_1 , respectively. Then the following identity holds:

(3.22)
$$\sigma_{\nu+1}^{1}(\varphi,\phi) + \frac{2}{\sin(\varphi-\phi)} A_{0}^{*}[\sigma_{\nu}^{1}(\cdot,\phi)](\varphi)$$
$$= \sigma_{\nu+1}^{0}(\varphi,\phi) + \frac{2}{\sin(\varphi-\phi)} A_{0}[\sigma_{\nu}^{0}(\varphi,\cdot)](\phi)$$

where A_0 and A_0^* are as in (3.6) and (3.7).

This result is essentially due to Berest ([4, 6]) and we state it without proof. It is not hard to see from the proposition that if an operator \tilde{L} can be obtained from $-\partial^2$ by a finite sequence of Darboux transformations, as in the case of (3.19), then it will have a finite number of non-zero Hadamard coefficients. We will refer back to (3.22) in our proof of Theorem 1 in Section 6.

Darboux transformations have widely been used as a means to generate non-trivial solutions to linear and non-linear partial differential equations such as the nonlinear Schrödinger and sine-Gordon equations. Starting with the trivial potential u(z) = 0, Darboux transformations can be used to produce what are known as "finite-gap" solutions to the KdV equation

$$(3.23) u_t = 6uu_x - u_{xxx}.$$

Written as a compatibility condition on the system of linear partial differential equations

(3.24)
$$\begin{cases} L\Psi = \lambda \Psi \\ \Psi_t = (L^{3/2})_+ \Psi \end{cases}$$

it is easy to verify that any Darboux transformation $L \to \tilde{L}$ and $\Psi \to \tilde{\Psi}$ preserves the system of equations (3.24) and hence (3.23). Both the Stellmacher-Lagnese potentials (2.7) and the Berest-Loutsenko potentials (2.11) are directly related to "finite-gap" solutions to the KdV equation. The Stellmacher-Lagnese potentials are known as *rational solutions* of the KdV equation decreasing at infinity. Similarly, if we set $\varphi_i = 4k_i^3t + \varphi_{0i}$ for some $\varphi_{0i} \in \mathbb{R}$, then v satisfies

$$(3.25) v_t = -v_{\varphi\varphi\varphi} + 6vv_{\varphi}$$

Such a function is known as a *singular periodic* solution, which is a periodic analogue of the *reflectionless*, *N-soliton* solution.

The Calogero-Moser potentials (2.9) cannot be obtained from classical Darboux transformations, however the operators (2.9) with these potentials are known to satisfy the intertwining identity $\mathfrak{L}D = D\square_{n+1}$ where

$$D = \sum_{|\alpha| \le N} q_{\alpha}(x) \partial^{\alpha}$$

is a differential operator depending only on the space variables (x_1, \dots, x_n) . Although the exact relationship between Huygens' principle and the theory of solitions is unclear, physical intuition seems to support the view that they are connected in some fundamental way. In the same sense that soliton equations are the result of a perfect balance between dispersion and nonlinearity, Huygens operators are deformations of the standard wave operator which maintain a balance between the diffusive effect of the operator and the reactive effect of the potential. Following ([5]), we may interpret the Calogero-Moser potentials as a higher-dimensional analogue of the reflectionless soliton potentials.

4. Asymptotics of the Resolvent Kernel

Let us define a two-index functional sequence $\{f_{l,k}(\varphi,\phi)\}_{l\in\mathbb{Z},k\in\mathbb{Z}_+}$ by the recurrence rule

$$(4.1) f_{l,0}(\varphi,\phi) := \delta_{l0}, \quad l \in \mathbb{Z}$$

$$(4.2) f_{l,k}(\varphi,\phi) := -\frac{\partial}{\partial \varphi} f_{l,k-1}(\varphi,\phi) - \frac{1}{2} \sin(\varphi-\phi) f_{l-1,k-1}, \quad k \ge 1,$$

where δ_{l0} stands for a standard Kronecker symbol, and we set

(4.3)
$$\hat{\sigma}_k(\varphi, \phi) := \sum_{l \in \mathbb{Z}} f_{l,k}(\varphi, \phi) \, \sigma_l(\varphi, \phi) \,, k \in \mathbb{Z}_+.$$

It is clear from (4.1)-(4.2) that for any $k \in \mathbb{Z}_+$ and l > k we have $f_{l,k} \equiv 0$ and hence the right-hand of (4.3) is a well-defined expression. In fact, it can be easily shown that $(\hat{\sigma}_k)$ satisfies the following differential-recurrence relation

(4.4)
$$\frac{\partial}{\partial \varphi} \hat{\sigma}_k(\varphi, \phi) = \frac{1}{2} L[\hat{\sigma}_{k-1}(\cdot, \phi)](\varphi), \quad k \ge 1.$$

The condition that $\sigma_k(\varphi, \phi)$ is bounded as $\varphi \to \phi$ is equivalent to conditions

(4.5)
$$\hat{\sigma}_{2\mu+1}(\phi,\phi) = 0 \text{ for all } \mu = 0, 1, 2, \dots,$$

(4.6)
$$\hat{\sigma}_{2\mu}(\phi,\phi) + \hat{\sigma}'_{2\mu-1}(\cdot,\phi)(\phi) = 0, \quad \mu \ge 1$$

and hence $\hat{\sigma}_k$'s can be uniquely determined from (4.4)-(4.6).

The meaning of $\hat{\sigma}_k(\varphi, \phi)$ is clarified in [4]:

Theorem 2. ([4, Lemma 4.2]) Let $\zeta \in \mathbb{C}$ be a complex parameter, and let $G(\varphi, \phi)$ be a resolvent kernel of the Sturm-Liouville operator L, i.e.,

$$(4.7) (L+\zeta^2) [G(\cdot,\phi;\zeta)](\varphi) = 0,$$

(4.8)
$$G(\varphi, \phi; \zeta)|_{\varphi = \phi} = 0,$$

(4.9)
$$\frac{\partial}{\partial \varphi} \left[G(\varphi, \phi; \zeta) \right]_{\varphi = \phi} = 1,$$

Then the coefficients $\hat{\sigma}_k(\varphi, \phi)$ determine the asymptotics of the kernel $G(\varphi, \phi; \zeta)$ along the imaginary axis in the complex ζ -plane at $\pm i\infty$. More precisely, for $\zeta = im, m \in \mathbb{R}$, we have an asymptotic expansion

(4.10)
$$G(\varphi, \phi; im) \sim \text{Re}\left[e^{im(\varphi-\phi)} \sum_{k=0}^{\infty} \frac{\hat{\sigma}_k(\varphi, \phi)}{(im)^{k+1}}\right]$$

We will hereby refer to the sequence $(\hat{\sigma}_k)$ as the asymptotics of the resolvent kernel. Now we will show how this sequence is related to the Baker-Akhiezer function of the Schrödinger operator L.

Let W be a pseudo-differential operator such that

(4.11)
$$L = W \left(-\frac{\partial^2}{\partial \varphi^2} \right) W^{-1} ,$$

then by definition the Baker-Akhiezer function of L is

(4.12)
$$\Psi(\varphi, z) = W e^{\varphi z} = \left(1 + \sum_{i=1}^{\infty} \psi_i z^{-i}\right) e^{\varphi z}.$$

This function is unique up to multiplication by a series with constant coefficients of the form $1 + c_1 z^{-1} + c_2 z^{-2} + \dots$ Similarly, we can introduce the notion of the *adjoint* Baker-Akhiezer function as

(4.13)
$$\Psi^*(\varphi, z) = (W^*)^{-1} e^{-\varphi z} = \left(1 + \sum_{i=1}^{\infty} \psi_i^* z^{-i}\right) e^{-\varphi z},$$

where W^* is the formal adjoint to the operator W. One can easily check that these functions are solutions of the equation

$$(4.14) L\psi = -z^2 \psi.$$

Let $W_n(\varphi, \phi)$ be coefficients of the product

(4.15)
$$\Psi(\varphi, z)\Psi^*(\phi, z) = \sum_{n=0}^{\infty} W_n(\varphi, \phi) z^{-n} e^{(\varphi - \phi)z}.$$

Now, applying L to (4.15) and using (4.14) we get the following system of equations:

$$LW_{n-1}(\varphi,\phi) = 2\frac{\partial}{\partial\varphi}W_n(\varphi,\phi)$$
 , $n \ge 1$.

Finally, comparing the last equation with (4.4), we obtain

Lemma 1. Let $\{\hat{\sigma}_n(\varphi, \phi)\}$ be the functional sequence given by (4.4)-(4.6). Then there exists unique set of constants c_m (m = 1, 2, ...) such that

$$W_k(\varphi, \phi) = \sum_{m+n=k} c_m \hat{\sigma}_n(\varphi, \phi), k \ge 1.$$

In fact, the set of polynomials associated with the quasipolynomials (4.12) forms a principal ideal in $\mathbf{C}[z]$, and if we choose W such that the polynomial part of (4.12) generates this ideal, then $W_k(\varphi, \phi) = \hat{\sigma}_k(\varphi, \phi)$ for all k.

In the next theorem we derive the inverse to the formula (4.3):

Theorem 3. The Hadamard's coefficients of \mathcal{L} can be computed as follows

(4.16)
$$\sigma_k(\varphi, \phi) := \sum_{l \in \mathbb{Z}} h_{l,k}(\varphi, \phi) \,\hat{\sigma}_l(\varphi, \phi) \,, k \in \mathbb{Z}_+ \,,$$

where the sequence $\{h_{l,k}(\varphi,\phi)\}_{l\in\mathbb{Z},k\in\mathbb{Z}_+}$ is defined by the following rule

$$(4.17) h_{l,0}(\varphi,\phi) := \delta_{l0}, \quad l \in \mathbb{Z}$$

$$(4.18) h_{l,k}(\varphi,\phi) := \frac{2}{\sin(\varphi-\phi)} \left(\frac{\partial}{\partial \varphi} h_{l,k-1}(\varphi,\phi) - h_{l-1,k-1}(\varphi,\phi) \right), \quad k \ge 1.$$

Proof. We make the ansatz

(4.19)
$$\sigma_k(\varphi,\phi) := \sum_{l=0}^k \tilde{h}_{l,k}(\varphi,\phi) \,\hat{\sigma}_l(\varphi,\phi) \,, k \in \mathbb{Z}_+ \,,$$

and substitute (4.19) into (3.21).

Using (4.4) and assuming that $\tilde{h}_{l,k}(\varphi,\phi) = 0$ for l > k, we obtain, by equating coefficients of the same σ -terms on both sides of equation (3.21),

$$\tilde{h}_{k,k}(\varphi,\phi) = \frac{(-2)^k}{\sin^k(\varphi - \phi)},\,$$

(4.20)
$$\tilde{h}_{l,k}(\varphi,\phi) = \frac{2}{\sin(\varphi-\phi)} \left(\frac{\partial}{\partial \varphi} \, \tilde{h}_{l,k-1}(\varphi,\phi) - \tilde{h}_{l-1,k-1}(\varphi,\phi) \right),$$

$$\sin(\varphi - \phi) \frac{\partial}{\partial \varphi} \tilde{h}_{l,k}(\varphi, \phi) + k \cos(\varphi - \phi) \tilde{h}_{l,k}(\varphi, \phi) = \left(\frac{\partial^2}{\partial \varphi^2} + (k - 1)^2\right) [\tilde{h}_{l,k-1}(\varphi, \phi)].$$

The consistency of the last two relations yields

(4.21)
$$\left(\frac{\partial^2}{\partial \varphi^2} - (k-1)^2\right) \left[\tilde{h}_{l,k-1}(\varphi,\phi)\right] + 2(k-1) \cot(\varphi-\phi) \frac{\partial}{\partial \varphi} \,\tilde{h}_{l,k-1}(\varphi,\phi)$$

$$= \frac{\partial}{\partial \varphi} \,\tilde{h}_{l-1,k-1} + 2(k-1) \cot(\varphi-\phi) \,\tilde{h}_{l-1,k-1}(\varphi,\phi)$$

To finish the proof of the lemma we only need to check that the sequence defined by the relations (4.17)-(4.18) will satisfy (4.21). This can easily verified by induction on k.

The relation (4.16) gives an explicit formula for computation of Hadamard coefficients, provided that we have a simple description of coefficients $h_{l,k}(\varphi,\phi)$. Using (4.18), one can easily show that

$$(4.22) h_{l,k}(\varphi,\phi) = \begin{cases} \frac{(-2)^k}{\sin^{2k-l}(\varphi-\phi)} \sum_{i=0}^{\frac{k-l}{2}} c_{l,k}^i \sin^{2i}(\varphi-\phi) & | & \text{if } k-l \text{ is even} \\ \frac{(-2)^k \cos(\varphi-\phi)}{\sin^{2k-l}(\varphi-\phi)} \sum_{i=0}^{\frac{k-l-1}{2}} c_{l,k}^i \sin^{2i}(\varphi-\phi) & | & \text{if } k-l \text{ is odd} \end{cases}$$

where $\{c_{l,k}^i\}$ is a three-index numerical sequence satisfying the corresponding recurrence relation. For instance, when l=1 we can find from this relation

$$(4.23) c_{1,k}^{i} = \begin{cases} \frac{(-1)^{i}(2k-2i-3)!!}{(2i)!!} \prod_{j=1}^{i} (k-2j+1)^{2} & | & \text{if } k \text{ is odd} \\ \frac{(-1)^{i}(2k-2i-3)!!}{(2i)!!} \prod_{j=1}^{i} (k-2j)^{2} & | & \text{if } k \text{ is even} \end{cases}.$$

However, we do not have such simple combinatorial presentation for all $\{c_{l,k}^i\}$ and this leads us to the next section.

5. Generating Functions

We consider the following two generating series defined by the sequences obtained from $\{h_{l,k}(\varphi,\phi)\}$ by fixing indices l and k respectively:

$$H_k(\varphi, \phi; z) = \sum_{l=0}^{\infty} h_{l,k}(\varphi, \phi) z^l$$
.

$$\tilde{H}_k(\varphi, \phi; \lambda) = \sum_{k=0}^{\infty} h_{l,k}(\varphi, \phi) \lambda^k,$$

The following lemma gives a nice description of H_k .

Lemma 2. Let Ω be the linear operator, depending on the parameter z, defined by

$$\Omega := \frac{2}{\sin(\varphi - \phi)} \left(\frac{\partial}{\partial \varphi} - z \right)$$

then H_k is a polynomial of order k in z such that

$$H_k(\varphi, \phi; z) = \Omega^k[1]$$
.

Proof. Multiplying both sides of the defining relation (4.18) by z^l and summing up with respect to l, we obtain

(5.1)
$$\sum_{l=0}^{\infty} h_{l,k}(\varphi,\phi) z^{l} := \frac{2}{\sin(\varphi-\phi)} \left(\frac{\partial}{\partial \varphi} \sum_{l=0}^{\infty} h_{l,k-1}(\varphi,\phi) z^{l} - z \sum_{l=0}^{\infty} h_{l,k-1}(\varphi,\phi) z^{l} \right), \quad k \ge 1.$$

Since $h_{l,k}(\varphi, \phi) = 0$ for l > k, $H_k(\varphi, \phi; z)$ is a polynomial with respect to z and the last equation can be rewritten as

$$H_k = \frac{2}{\sin(\varphi - \phi)} \left(\frac{\partial}{\partial \varphi} - z \right) H_{k-1}.$$

In order to complete the proof this lemma we notice that the relation (4.17) implies that $H_0 = 1$.

Remark. In the future we will also use the following presentation of the operator Ω

$$\Omega := \frac{2}{\sin(\varphi - \phi)} \cdot e^{(\varphi - \phi)z} \circ \frac{d}{d\varphi} \circ e^{-(\varphi - \phi)z}$$

Similarly, one can prove

Lemma 3. For the generating function $\tilde{H}_l(\varphi, \phi; \lambda)$ we have :

(5.2)
$$\frac{\partial^{l}}{\partial \varphi^{l}} \left\{ e^{\frac{\cos(\varphi - \phi)}{2\lambda}} \tilde{H}_{l}(\varphi, \phi; \lambda) \right\} = e^{\frac{\cos(\varphi - \phi)}{2\lambda}}$$

6. Explicit formulas for Hadamard coefficients

In this section we derive explicit formulas for both the Hadamard coefficients and the asymptotics of the resolvent kernel of (2.12). A number of papers have been written giving formulas for the Hadamard coefficients of the one-dimensional Schrödinger operator \mathcal{L} , i.e. solutions $U_k(x,\xi)$ of the one-dimensional transport equation

$$(x - \xi)\partial_x U_k + k U_k = \mathfrak{L}[U_{k-1}(\cdot, \xi)](x)$$

which are bounded as $x \to \xi$. These have largely been motivated by the connection between the Hadamard coefficients and the KdV hierarchy. Since [15] it has been known that the asymptotics of the resolvent kernel are related to the KdV hierarchy via the identity

(6.1)
$$K_n(u) := \left[(L^{\frac{2n-1}{2}})_+, L \right] = 2\partial_x \hat{\sigma}_{2n}(x, x)$$

Similarly, it has been known since [22] that the Hadamard coefficients U_n of the one-dimensional Schrödinger operator are related to the KdV hierarchy by

(6.2)
$$K_n(u) := \left[\left(L^{\frac{2n-1}{2}} \right)_+, L \right] = \frac{(2n-1)!!}{2^{n-1}} \partial_x U_n(x, x)$$

Even in the case of the one-dimensional Schrödinger operator, however, these formulas have had an unwiedly combinatorial structure (see e.g., [25]). In the case that the Schrödinger operator is known to admit a finite heat kernel expansion one can give more explicit formulas for its Hadamard coefficients. For one-dimensional operators, such formulas were given in [18]. To prove Theorem 1 we will use a different approach based on results of [4, 6]. We now prove a slight modification of Theorem 1:

Proposition 3. The Hadamard coefficients of (2.12) are exactly

$$\sigma_0 = 1$$

(6.3)
$$\sigma_{\nu} = \frac{(-2)^{\nu}}{\mathcal{W}(\varphi)\mathcal{W}(\phi)} \sum_{i=1}^{m} c_{i} \mathcal{W}_{i}(\varphi)\mathcal{W}_{i}(\phi) T_{k_{i}}^{(\nu)}(\cos(\varphi - \phi)) , \quad \nu \geq 1 ,$$

where c_i and W_i are defined are defined as in Theorem 1.

Proof. We prove this by induction on m and ν . For m=1, the operator (3.19) corresponding to (2.12) is obtained from $-\left(\frac{\partial}{\partial \varphi}\right)^2$ by the Darboux transformation (3.6)-(3.7) where

$$A = \frac{\partial}{\partial \varphi} + k_1 \tan(k_1 \varphi + \varphi_1)$$

and

$$A^* = -\frac{\partial}{\partial \varphi} + k_1 \tan(k_1 \varphi + \varphi_1).$$

So, applying Proposition 2, by a straightforward calculation we obtain

$$\sigma_1(\varphi,\phi) = -\frac{2T'_{k_1}(\cos(\varphi - \phi))}{\cos(k_1\varphi + \varphi_1)\cos(k_1\phi + \varphi_1)}$$

and for $\nu > 1$ we have

$$\sigma_{\nu}(\varphi,\phi) = -\frac{2}{\sin(\varphi - \phi)} A_0^* [\sigma_{\nu}^1(\cdot,\phi)](\varphi).$$

It can be directly verified that this is satisfied by

$$\sigma_{\nu}(\varphi,\phi) = \frac{(-2)^{\nu} T_{k_1}^{(\nu)}(\cos(\varphi - \phi))}{\cos(k_1 \varphi + \varphi_1) \cos(k_1 \phi + \varphi_1)}$$

From Theorem 3, it is also possible to obtain (6.3) for $\nu = 1$ and arbitrary m. Now we consider the general case. Let (σ_{ν}^{N}) be the Hadamard coefficients of an operator \mathfrak{L} of the form (2.12) with m = N and let (σ_{ν}^{N+1}) be the Hadamard coefficients of an operator $\tilde{\mathfrak{L}}$ obtained from \mathfrak{L} by adding $\chi_{m+1}(\varphi)$ to the sequence of functions (2.11). This implies that the operator (3.19) corresponding to $\tilde{\mathfrak{L}}$ can be obtained from the operator (3.19) corresponding to \mathfrak{L} by a single Darboux transformation, with

$$A = \frac{\partial}{\partial \varphi} - \frac{\partial}{\partial \varphi} \log \frac{\mathcal{W}(\varphi)}{\mathcal{W}_{N+1}(\varphi)} = \frac{\partial}{\partial \varphi} + \frac{\mathcal{W}'(\varphi)}{\mathcal{W}(\varphi)} - \frac{\mathcal{W}'_{N+1}(\varphi)}{\mathcal{W}_{N+1}(\varphi)}$$

and

$$A^* = -\frac{\partial}{\partial \varphi} - \frac{\partial}{\partial \varphi} \log \frac{W(\varphi)}{W_{N+1}(\varphi)} = -\frac{\partial}{\partial \varphi} + \frac{\mathcal{W}'(\varphi)}{\mathcal{W}(\varphi)} - \frac{\mathcal{W}'_{N+1}(\varphi)}{\mathcal{W}_{N+1}(\varphi)}$$

where $W = W[\chi_1, \dots, \chi_{N+1}]$ and $W_{N+1} = W[\chi_1, \dots, \chi_N]$. From Proposition 2, we therefore have for $\nu \geq 1$

$$\sigma_{\nu+1}^{N+1} = \sigma_{\nu+1}^{N} + \frac{2}{\sin(\varphi - \phi)} \left(\frac{\partial}{\partial \phi} + \frac{\mathcal{W}'(\phi)}{\mathcal{W}(\phi)} - \frac{\mathcal{W}'_{N+1}(\phi)}{\mathcal{W}_{N+1}(\phi)} \right) \sigma_{\nu}^{N} + \frac{2}{\sin(\varphi - \phi)} \left(\frac{\partial}{\partial \varphi} - \frac{\mathcal{W}'(\varphi)}{\mathcal{W}(\varphi)} + \frac{\mathcal{W}'_{N+1}(\varphi)}{\mathcal{W}_{N+1}(\varphi)} \right) \sigma_{\nu}^{N+1}$$

We wish to show that if (6.3) is valid for σ_{ν}^{N+1} , $\sigma_{\nu+1}^{N}$ and σ_{ν}^{N} , then it also holds for $\sigma_{\nu+1}^{N+1}$. So, we set

$$\sigma_{\nu}^{N+1} = \frac{(-2)^{\nu}}{\mathcal{W}(\varphi)\mathcal{W}(\phi)} \sum_{i=1}^{N+1} c_i^{(N+1)} \mathcal{W}_i(\varphi) \mathcal{W}_i(\phi) T_{k_i}^{(\nu)}(\cos(\varphi - \phi))
\sigma_{\nu+1}^{N} = \frac{(-2)^{\nu+1}}{\mathcal{W}_{N+1}(\varphi)\mathcal{W}_{N+1}(\phi)} \sum_{i=1}^{N} c_i^{(N)} \mathcal{W}_{i,N+1}(\varphi) \mathcal{W}_{i,N+1}(\phi) T_{k_i}^{(\nu+1)}(\cos(\varphi - \phi))
\sigma_{\nu}^{N} = \frac{(-2)^{\nu}}{\mathcal{W}_{N+1}(\varphi)\mathcal{W}_{N+1}(\phi)} \sum_{i=1}^{N} c_i^{(N)} \mathcal{W}_{i,N+1}(\varphi) \mathcal{W}_{i,N+1}(\phi) T_{k_i}^{(\nu)}(\cos(\varphi - \phi))$$

Here $c_i^{(N)}$ and $c_i^{(N+1)}$ are defined as in Theorem 1, with m=N and m=N+1, respectively. Because

$$\frac{2}{\sin(\varphi - \phi)} \frac{\partial}{\partial \varphi} T_k^{\nu}(\cos(\varphi - \phi)) = -2T_k^{\nu+1}(\cos(\varphi - \phi))$$

and

$$\frac{2}{\sin(\varphi - \phi)} \frac{\partial}{\partial \phi} T_k^{\nu}(\cos(\varphi - \phi)) = 2T_k^{\nu + 1}(\cos(\varphi - \phi)),$$

we get

$$\sigma_{\nu+1}^{N+1} = \frac{(-2)^{\nu+1}}{\mathcal{W}(\varphi)\mathcal{W}(\phi)} \sum_{i=1}^{N+1} c_i^{(N+1)} \, \mathcal{W}_i(\varphi) \mathcal{W}_i(\phi) T_{k_i}^{(\nu+1)}(\cos(\varphi - \phi))$$

provided that the following two equations hold:

(6.5)
$$\mathcal{W}_{i}'(\varphi)\mathcal{W}_{N+1}(\varphi) - \mathcal{W}_{i}(\varphi)\mathcal{W}_{N+1}(\varphi) = \mathcal{W}(\varphi)\mathcal{W}_{i,N+1}(\varphi)$$

(6.6)
$$\mathcal{W}'_{i,N+1}(\phi)\mathcal{W}(\phi) - \mathcal{W}_{i,N+1}(\phi)\mathcal{W}'(\phi) = (k_{N+1}^2 - k_i^2)\mathcal{W}_i(\phi)\mathcal{W}_{N+1}(\phi)$$

We will prove the first equation (6.5) and (6.6) can be proved in a similar way. First, we rewrite (6.5):

(6.7)
$$\frac{\partial}{\partial \varphi} \left(\frac{\mathcal{W}_i(\varphi)}{\mathcal{W}_{N+1}(\varphi)} \right) = \frac{\mathcal{W}(\varphi)\mathcal{W}_{i,N+1}(\varphi)}{\mathcal{W}_{N+1}(\varphi)^2}$$

By Cramer's rule, the functions $y_i := (-1)^{N+i} W_i / W_{N+1}$ satisfy the system of equations

$$\sum_{i=1}^{N} \chi_i^{(k)} y_i = \chi_{N+1}^{(k)} \text{ for } k = 0, 1, \dots, N-1.$$

By taking the derivative from both sides of this equation with respect to φ we obtain $\sum_{i=1}^N \chi_i^{(k)} y_i' = 0$ for $k = 0, 1, \dots, m-2$. For k = m-1, we have

$$\begin{split} \sum_{i=1}^{N} \chi_{i}^{(N-1)} y_{i}' &= \sum_{i=1}^{N} (-1)^{N+i} \chi_{i}^{(N-1)} \left(\frac{\mathcal{W}i}{\mathcal{W}_{N+1}} \right)' \\ &= \frac{1}{\mathcal{W}_{N+1}} \sum_{i=1}^{N} (-1)^{N+i} \chi_{i}^{(N-1)} \mathcal{W}_{i}' - \frac{\mathcal{W}_{N+1}'}{\mathcal{W}_{N+1}^{2}} \sum_{i=1}^{N} (-1)^{N+i} \chi_{i}^{(N-1)} \mathcal{W}_{i} \\ &= \frac{\mathcal{W}}{\mathcal{W}_{N+1}} - 0 = \frac{\mathcal{W}}{\mathcal{W}_{N+1}} \,. \end{split}$$

Solving the latter system of equations for y_i' we obtain $y_i' = (-1)^{N+i} \mathcal{W}_{N+1} \mathcal{W}_{i,N+1} / \mathcal{W}_{N+1}^2$, which is equivalent to (6.7).

The following result is an immediate consequences of (6.3):

Corollary 1. For the Hadamard coefficients U_{ν} of \mathcal{L} we have

$$U_{\nu} \equiv 0 \text{ for all } \nu > k_m$$
.

One can also prove from Theorem 3 the following explicit expression for the asymptotics of the resolvent kernel

Lemma 4. For the coefficients $\hat{\sigma}_{\nu}$ of the Schrödinger operator L with the potential $v(\varphi)$ defined in (3.19), we have

(6.8)
$$\hat{\sigma}_{\nu} = \frac{1}{\mathcal{W}_{m}(\varphi)\mathcal{W}_{m}(\phi)} \sum_{i=1}^{m} c_{i} \mathcal{W}_{m,i}(\varphi) \mathcal{W}_{m,i}(\phi) \frac{\partial^{\nu}}{\partial \varphi^{\nu}} \left[T_{k_{i}}(\cos(\varphi - \phi)) \right], \quad \nu \geq 1.$$

Proof. First, we recall that

$$\hat{\sigma}_{\nu}(\varphi,\phi) := \sum_{l=0}^{\nu} f_{l,\nu}(\varphi,\phi) \, \sigma_l(\varphi,\phi) \,,$$

where functions $f_{l,\nu}$ are determined by recurrence relations (2.2) and (2.3). Using now (2.14), we get

$$\hat{\sigma}_{\nu}(\varphi,\phi) = \sum_{l=0}^{\nu} \frac{(-2)^{\nu} f_{l,\nu}(\varphi,\phi)}{\mathcal{W}_{m}(\varphi) \mathcal{W}_{m}(\phi)} \sum_{i=1}^{m} c_{i} \mathcal{W}_{m,i}(\varphi) \mathcal{W}_{m,i}(\phi) T_{k_{i}}^{(l)}(\cos(\varphi-\phi)) = \frac{1}{\mathcal{W}_{m}(\varphi) \mathcal{W}_{m}(\phi)} \sum_{i=1}^{m} c_{i} \mathcal{W}_{m,i}(\varphi) \mathcal{W}_{m,i}(\phi) \sum_{l=0}^{\nu} (-2)^{\nu} f_{l,\nu}(\varphi,\phi) T_{k_{i}}^{(l)}(\cos(\varphi-\phi)).$$

Hence, in order to complete the proof it suffices to verify that

$$\frac{\partial^{\nu}}{\partial \varphi^{\nu}} \left[T_{k_i} (\cos(\varphi - \phi)) \right] = \sum_{l=0}^{\nu} (-2)^{\nu} f_{l,\nu}(\varphi, \phi) T_{k_i}^{(l)} (\cos(\varphi - \phi)).$$

Such verification can be easily done by induction in ν using relations (2.2) and (2.3).

We conclude the paper with explicit formulas for the Hadamard coefficients of specific operators (2.12).

Take $(k_1, k_2) = (2, 3)$ and $(\varphi_1, \varphi_2) = (\pi/2, 0)$. Then \mathfrak{L} takes the form

$$\mathfrak{L} = \Box_{n+1} + \frac{10(x_1^2 + x_2^2)(15x_2^2 - x_1^2)}{(5x_2^2 + x_1^2)x_1^2}$$

and the non-zero Hadamard coefficients are

$$U_0 = 1$$

$$U_{1} = \frac{10(8x_{2}\xi_{1}\xi_{2}x_{1} + 3\xi_{1}^{2}x_{2}^{2} + 15\xi_{2}^{2}x_{2}^{2} + 3\xi_{2}^{2}x_{1}^{2} - \xi_{1}^{2}x_{1}^{2})}{\xi_{1}x_{1}(5x_{2}^{2} + x_{1}^{2})(5\xi_{2}^{2} + \xi_{1}^{2})}$$

$$U_{2} = \frac{20(24x_{2}\xi_{1}\xi_{2}x_{1} + 3\xi_{2}^{2}x_{1}^{2} - \xi_{1}^{2}x_{1}^{2} + 3\xi_{1}^{2}x_{2}^{2} + 15\xi_{2}^{2}x_{2}^{2})}{\xi_{1}^{2}x_{1}^{2}(5x_{2}^{2} + x_{1}^{2})(5\xi_{2}^{2} + \xi_{1}^{2})}$$

$$U_{2} = \frac{960x_{2}\xi_{2}}{\xi_{1}^{2}x_{1}^{2}(5x_{2}^{2} + x_{1}^{2})(5\xi_{2}^{2} + \xi_{1}^{2})}$$

$$U_3 = -\frac{960x_2\xi_2}{\xi_2^2 x_1^2 (5x_2^2 + x_1^2)(5\xi_2^2 + \xi_1^2)}$$

Next, take $(k_1, k_2, k_3) = (1, 2, 3)$ and $(\varphi_1, \varphi_2, \varphi_3) = (\pi/2, \pi/2, \pi/2)$. Then

$$\mathfrak{L} = \square_{n+1} + \frac{12}{x_2^2}$$

and the non-zero Hadamard coefficients are

$$U_0 = 1$$

$$U_1 = \frac{12}{x_2 \xi_2}$$

$$U_2 = \frac{30(2x_1 \xi_1 + x_2 \xi_2)}{x_2^3 \xi_2^3}$$

$$U_3 = \frac{15}{x_2^3 \xi_2^3}$$

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