Reduced equations for models of laminated materials in thin domains. II.

R. E. Lee DeVille

Courant Institute of Mathematical Sciences, New York University, New York, NY 10012

February 28, 2005

Abstract

In a companion paper, we considered a scalar wave equation on a thin, laminated, three-dimensional plate. We showed that if the plate was sufficiently thin, then there exists a hierarchy of two-dimensional equations whose dynamics model the dynamics of the full plate, each of which successively lengthens the time interval over which the approximation is valid. In certain cases, these approximating equations may formally be ill-posed. In this paper, we consider modifications of the approximating equations which are themselves well-posed, and which qualitatively afford the same approximation. We also present an algorithm to compute the coefficients in the approximating equations in closed form, and show numerical evidence that the estimates on the efficacy of the approximating equations are sharp.

1 Introduction

In [3], a dynamic model for a scalar wave equation in a laminated thin plate was studied, based on static models considered in [1] and [4]. In [3], we began a study of the dynamics of those models and their approximation by "reduced equations" – that is, by equations defined on lower-dimensional spatial domains. The main theorem of [3] can be summarized as saying that for a solution to a full three-dimensional boundary-value problem which modeled the dynamics of a thin laminated plate, there are a sequence of two-dimensional boundary-value problems, each of which afford a successively better approximation to the full problem. These two-dimensional problems can be thought of as capturing the dynamics of the full three-dimensional model projected down onto the two thick dimensions in the problem. For more references and discussion of the history and applications of this problem, see [3].

In this paper, we extend [3] in two ways: First, in [3], a formal expression for each two-dimensional problem was written down, but in each case these equations contained a number of constants whose value was only implicitly defined. Here we will write down a formula for these constants. Second, it turns out that many of the two-dimensional models derived in [3] are given by PDE which look ill-posed. This is a seemingly paradoxical result where we have ill-posed PDE affording good approximations to well-posed PDE. Here we resolve this paradox and show a way to suitably modify the approximating PDE to both make them look well-posed and preserve the fact that they are good approximating models.

To be more precise, in [3] we considered the following boundary-value problem: Define $\omega \subset \mathbb{R}^2$ to be be bounded with $\mathcal{C}^1$ smooth boundary γ. Given ω and a positive thickness parameter d we define the three-dimensional domain $\Omega = \omega \times (0, \pi d)$, its lateral boundary $\Gamma = \gamma \times (0, \pi d)$, and the faces

$$\begin{aligned} R_- &= \{(x_1, x_2, y) | (x_1, x_2) \in \omega, y = 0\}, \\ R_+ &= \{(x_1, x_2, y) | (x_1, x_2) \in \omega, y = \pi d\}. \end{aligned}$$

In Ω we consider the hyperbolic problem with zero forcing terms on the faces, i.e.

$$\begin{aligned} u_{tt} &= Lu \text{ in } \Omega \times \mathbb{R}, \\ u &= 0 \text{ on } \Gamma \times \mathbb{R}, \\ \partial_n u &= 0 \text{ on } R_\pm \times \mathbb{R}, \end{aligned} \tag{1}$$

where the operator L is given by

$$Lu = \frac{\partial}{\partial y}\left(a(y/d)\frac{\partial u}{\partial y}\right) + b(y/d)\nabla_x \cdot (C(x)\nabla_x u),$$

where $\nabla_x = (\partial/(\partial x_1), \partial/(\partial x_2))^T$, and $x = (x_1, x_2)$, and we have an initial condition $(u^0, u_t^0) \in H^2(\Omega) \times H^1(\Omega)$.

The standard state space to consider when posing this equation is $H^s(\Omega) \times H^{s-1}(\Omega)$ for some s, and in fact we would like to consider this state space with $s = 1$, as that is the norm in which the estimates are done in the companion paper.

In [3], the two eigenproblems

$$L_x \phi = \hat{b}(0)(C(x)\nabla_x \phi)_x = -\mu\phi, \tag{2}$$

$$L_\eta \psi = (a(\eta)\psi_\eta)_\eta = -\lambda\psi, \tag{3}$$

were defined. It was then shown that the approximating two-dimensional equations were always of the form

$$u_{tt} = L_x u + \sum_{q=2}^{\infty} C^{(q)} d^{2(q-1)} L_x^q u, \tag{4}$$

for some constants $C^{(2)}, C^{(3)}, \ldots$, independent of d.

To restate the aims of this paper, we remind the reader that the equation given by (4) may in fact be ill-posed on $H^1(\omega) \times L^2(\omega)$, and that we have not given a formula for the constants $C^{(q)}$ which appear above.

In Section 2, we show that there are several situations in which the reduced equations give rise to PDE which are ill-posed on $H^1(\omega) \times L^2(\omega)$, and we show that there is a reasonable way to make these PDE well-posed without qualitatively affecting the approximation. In Section 3 we give an inductive algorithm for determining the constants $C^{(q)}$ exactly. In Section 4 we discuss the numerical efficiency of using the reduced models versus simulating the full model, and show some numerical evidence that shows that the dependence of the bounds in [3] on d are sharp up to powers of d.

2 Well-posedness of the reduced equation

In this section, we recall what it means for an equation to be well-posed, and show that the approximating equations obtained in [3] may not be well-posed.

Recall that the reduced PDE was always of the form

$$u_{tt} = L_x u + \sum_{q=2}^{n} C^{(q)} d^{2(q-1)} L_x^q u. \tag{4}$$

Definition 1. *Consider a PDE of the form*

$$u_{tt} = \sum_{q=1}^{n} A_q L_x^q u,$$

defined on a region ω, with

$$L_x^i u\big|_{\partial\omega} = 0 \text{ for all } i < n.$$

We say that this PDE is well-posed on $H^s(\omega) \times H^{s-1}(\omega)$ if, for any initial condition $(u^0, u_t^0) \in H^s(\omega) \times H^{s-1}(\omega)$, there exists a unique solution $u(x,t)$ for all t, and, for any t, there exists a $C(t)$ with the property that if we choose two differing initial conditions (u^0, u_t^0) and $(\tilde{u}^0, \tilde{u}_t^0)$, then

$$\|\tilde{u}(x,t) - u(x,t)\|_{H^s \times H^{s-1}} \leq C(t) \left\|(u^0, u_t^0) - (\tilde{u}^0, \tilde{u}_t^0)\right\|_{H^s \times H^{s-1}}. \tag{5}$$

For convenience, we are using a stronger notion of well-posed than is standard. Typically, one only requires that the solution at time t be continuous with respect to the initial data, and we have further required that it be Lipschitz.

It turns out that there are problems (1) which, when dimensionally reduced, give rise to an approximating equation as in (4) which is ill-posed on $H^1(\omega) \times L^2(\omega)$. This seems paradoxical, in that our original equation (1) is well-posed on $H^1(\Omega) \times L^2(\Omega)$, and we would not expect a well-posed equation to be well approximated by an ill-posed one. But, as was shown in [3], an equation of the form (4) effectively approximates (1) in general.

The reason that there is no contradiction is that we take our initial conditions in the space $H^1_\alpha(\omega) \times L^2_\alpha(\omega)$ for some $\alpha \in (-1/2, 0)$, as defined in [3]. Furthermore, it was shown that the solution to (4) lies in $H^1_\alpha(\omega) \times L^2_\alpha(\omega)$ for all time, and the PDE is well-posed on this space.

We will make two arguments in this section. The first is that the PDE (4) is well-posed on $H^1_\alpha(\omega) \times L^2_\alpha(\omega)$, and the second is that we can modify (4) so that we lose nothing in its efficacy in approximating (1), but that it is now well posed on $H^1(\omega) \times L^2(\omega)$.

Assume that we have a solution $u(x,t)$ of (4). Recall the sequence of functions ϕ_k defined in (2). For any t, we write u in a Fourier series in ϕ_k, and thus we have

$$u(x,t) = \sum_{k=0}^{\infty} a_k(t)\phi_k(x). \tag{6}$$

The eigenfunctions ϕ_k were chosen to satisfy $L_x\phi_k = -\mu_k\phi_k$, and thus

$$L_x^q \phi_k = (-1)^q \mu_k^q \phi_k.$$

Putting (6) into (4) gives us

$$\sum_k \ddot{a}_k \phi_k = \sum_{q=1}^{n} (-1)^q C^{(q)} d^{2(q-1)} \sum_k \mu_k^q a_k \phi_k,$$

and equating coefficients of the ϕ_k gives

$$\ddot{a}_k(t) = \beta_k^2 a_k(t),$$

where

$$\beta_k^2 = \sum_{q=1}^{n} (-1)^q C^{(q)} d^{2(q-1)} \mu_k^q.$$

From the asymptotic behavior of (2), we know that $\mu_k = \mathcal{O}(k)$, so that

$$\beta_k^2 \sim \sum_{q=1}^{n} (-1)^q C^{(q)} d^{2(q-1)} k^q.$$

If $(-1)^n C^{(n)} > 0$, or, equivalently, if $\operatorname{sgn}(C^{(n)}) = (-1)^n$, then the leading order term of this expression is positive, and thus as $k \to \infty$, we know that $\beta_k^2 \to \infty$. On the other hand, if $(-1)^n C^{(n)} < 0$, then this expression is uniformly bounded from above, i.e. there is a C such that $\beta_k^2 \le C$ for all k.

Clearly, if the wavenumbers grow without bound, an estimate such as (5) cannot hold. This argument gives us

Lemma 1. *Equation (4) satisfies (5) if and only if* $\operatorname{sgn}(C^{(n)}) = (-1)^{n-1}$. *Thus (4) is well-posed in* $H^1(\omega) \times L^2(\omega)$ *if and only if* $\operatorname{sgn}(C^{(n)}) = (-1)^{n-1}$.

Now, every equation whose solution lies in $H^1_\alpha(\omega) \times L^2_\alpha(\omega)$ for all time is well-posed in that space, because this is a finite-dimensional space. The well-posedness follows from continuity arguments for the theory of ODEs. But one can also calculate the frequencies β_k^2 directly here, where we only have contributions from modes where $\beta_k < d^\alpha$. Then β_k^2 can be bounded uniformly by

$$\sum_{q=1}^{n} (-1)^q C^{(q)} d^{(2+\alpha)q-2}.$$

If $\alpha < 0$ is chosen appropriately, this is bounded above.

Since all of the equations we study are linear hyperbolic equations, existence and uniqueness results are standard. Lemma 1 is a simple way to check whether or not (4) is well-posed on $H^1(\omega) \times L^2(\omega)$.

If our equation given by (4) is ill-posed, then we will make the equation well-posed by introducing perturbations which are small on our phase space. Some of the corrections that we add to our equations will be singular perturbations, so it is not a priori clear that this will not dramatically change the quality of our approximation. We will show below that it does not.

We will modify (4) only if it is ill-posed. If (4) is already well-posed, we will leave it as is. Thus we assume that $\operatorname{sgn}(C^{(n)}) = (-1)^n$.

Observe that the original equation

$$u_{tt} = L_x u + \sum_{q=2}^{n} C^{(q)} d^{2(q-1)} L_x^q u \tag{4}$$

looks formally like an equation of the form

$$u_{tt} = L_x u + (\text{small}),$$

or

$$L_x u = u_{tt} - (\text{small}).$$

Following this, we will replace one power of L_x in the last term of (4) by ∂^2_{tt}. We then get

$$u_{tt} = L_x u + \sum_{q=2}^{n-1} C^{(q)} d^{2(q-1)} L_x^q u + C^{(n)} d^{2(n-1)} \partial^2_{tt} L_x^{n-1} u, \tag{7}$$

and we want to demonstrate that it is well-posed on $H^1(\omega) \times L^2(\omega)$. Since it is not of the form mentioned in Lemma 1, we need to calculate the frequencies directly.

We expand

$$u(x,t) = \sum_{k \geq 0} a_k(t) \phi_k(x),$$

and if we insert this into (7), we have

$$\ddot{a}_k \phi_k = -\mu_k a_k \phi_k + \sum_{q=2}^{n-1} C^{(q)} d^{2(q-1)} (-1)^q \mu_k^q a_k \phi_k + (-1)^{n-1} C^{(n)} d^{2(n-1)} \mu_k^{n-1} \ddot{a}_k \phi_k,$$

or

$$\left(1+(-1)^n C^{(n)} d^{2(n-1)} \mu_k^{n-1}\right) \ddot{a}_k = \left(-\mu_k + \sum_{q=2}^{n-1} (-1)^q C^{(q)} d^{2(q-1)} \mu_k^q\right) a_k.$$

Stated differently, we have

$$\ddot{a}_k(t) = \beta_k^2 a_k(t),$$

where we now have

$$\beta_k^2 = \frac{\mu_k + \sum_{q=2}^{n-1} (-1)^q C^{(q)} d^{2(q-1)} \mu_k^q}{1+(-1)^n C^{(n)} d^{2(n-1)} \mu_k^{n-1}}. \tag{8}$$

Since we have assumed that $\operatorname{sgn}(C^{(n)}) = (-1)^n$, the denominator is never zero. We see that β_k is uniformly bounded above for non-negative k since

$$\lim_{k\to\infty} \beta_k^2 = -\frac{C^{n-1}}{d^2 C^{(n)}}.$$

Thus (7) is well-posed. Note also that in the expression (8), the numerator is the original frequency less the higher order term, and the denominator is of the form $1 + \mathcal{O}(d^{2(n-1)(1+\alpha)})$. Thus we have

Proposition 2. *If, instead of using (4) to approximate the dynamics of (1), we instead use (7) to approximate the dynamics of (1), then Theorem 1 of [3] still holds. Specifically, if we say that $u(x, y, t)$ satisfies (1) and $u_n^{\mathbf{r}}(x, t)$ satisfies (7), each with appropriate initial conditions as chosen in [3], then the energy of the error between the two approximations,*

$$\|u(x, y, t) - u_n^{\mathbf{r}}(x, t)\mathbf{1}(y)\|_{H^1(\omega)\times L^2(\omega)}$$

satisfies the same estimates as in Theorem 1 of [3].

Proof. If, instead of making the approximation $L_x u = u_{tt}$, we make the exact substitution

$$L_x u = u_{tt} - \sum_{q=2}^{n} C^{(q)} d^{2(q-1)} L_x^q u,$$

then

$$\begin{aligned} L_x^n u &= L_x^{n-1}(L_x u) \\ &= L_x^{n-1}\left(u_{tt} - \sum_{q=2}^{n} C^{(q)} d^{2(q-1)} L_x^q u\right) \\ &= \partial_t^2 L_x^{n-1} u - \sum_{q=2}^{n} C^{(q)} d^{2(q-1)} L_x^{q+n-1} u. \end{aligned}$$

This makes

$$C^{(n)}d^{2(n-1)}L_x^n u = C^{(n)}d^{2(n-1)}\partial_t^2 L_x^{n-1}u - \sum_{q=2}^{n} C^{(n)}C^{(q)}d^{2(n+q-2)}L_x^{q+n-1}u.$$

So our full equation is

$$\begin{aligned} u_{tt} = L_x u + C^{(n)}d^{2(n-1)}\partial_t^2 L_x^{n-1}u + \sum_{q=2}^{n-1} C^{(q)}d^{2(q-1)}L_x^q u \\ - \sum_{q=2}^{n} C^{(n)}C^{(q)}d^{2(n+q-2)}L_x^{q+n-1}u. \end{aligned} \tag{9}$$

The highest order term in this expression is

$$-(C^{(n)})^2 d^{4(n-1)}L_x^{2n-1}u.$$

Now the only difference between (7) and (9) is that the terms

$$\sum_{q=2}^{n} C^{(n)}C^{(q)}d^{2(n+q-2)}L_x^{q+n-1}u,$$

where $q \geq 2$, are dropped from (9) to obtain (7). These terms are, at worst, of order $d^{2n}L_x^{n+1}$ in $H^1(\omega) \times L^2(\omega)$. By Lemma 22 of [3], this does not appreciably affect the approximation. This is because the term we have thrown away is, by inspection, $\mathcal{O}(d^{2n+\alpha(2n+1)})$ and this is the same as the error we already had in the approximation of (1) by (4).

□

3 The coefficients of the reduced PDE

In this section, we will derive a formula for the constants $C^{(q)}$ which appear in (4). In [3] (cf. Equation (25)), it was shown that the full model could be written in certain variables as

$$\dot{z} = J\nabla H(z).$$

After some analysis, it was shown that the dynamics for z were well approximated by the flow (cf. Theorem 3 of [3])

$$\dot{\zeta} = J\nabla(H^0_{\text{diag}} + H^n_0)(\zeta), \tag{10}$$

where

$$H_0^n = \sum_{I \in \mathcal{M}_{n-1}} \Theta_{0+2}(I)L_I(G)_0,$$

and

$$L_I(G)_0 = C_I d^{p(I)}\omega_{k0}^{p(I)+1}.$$

(Here we are using notation from [3]. See the beginning of Section 3.2 to recall the definitions of $\Theta(I)$, C_I, L_I, and $p(I)$.)

We showed that we could write this as a reduced PDE in the form (4). We grouped the coefficients by the powers of L_x, and we obtained a PDE of the form

$$u_{tt} = L_x u + \sum_{q=2}^{N} C^{(q)} L_x^q u, \tag{4}$$

where

$$C^{(q)} = \sum_{\substack{I \in \mathcal{I}_{0+2}^q \\ p(I)=2(q-1)}} (-1)^q 4 \Theta_{0+2}(I) C_I. \tag{11}$$

Recall that the H^0_{diag} term in (10) is what generates the L_x term in (4), and the H_0^n term in (10) generates the higher-order terms in (4).

If we examine (11), it is clear that if we can write down a formula for every C_I and $\Theta_{0+2}(I)$, then we can generate from that a formula for any $C^{(q)}$. At this point, we have a working solution to the problem of finding the coefficients. In principle, one could compute C_I and $\Theta_{0+2}(I)$, at least numerically, for any I, since we have a recursive formula in Lemma 3 below, which comes straight from calculations in [3].

The drawback of this formulation is twofold. First, the formula for C_I is only in a recursive form. Second, and more importantly, the formula for C_I is expressed in terms of the Fourier coefficients of b and the eigenvalues of the operator L_η. We will not explicitly know these in practice, and would have to approximate them numerically. The formula we exhibit below will have neither of these drawbacks.

In Section 3.1, we examine the expressions in Fourier variables that we will encounter, and see what their continuous analogs are. In Section 3.2, we write down several inductive formulas for C_I, $Q_I(l)$, $f_I(l)$, and $g_I(l)$. In Section 3.3, we derive a non-recursive formula for the C_I which, for $I \in \mathcal{M}_n$, depends only n functions $b_0, \dots b_{n-1}$. In Section 3.4 we derive a non-recursive formula for these b_i. Finally, in Section 3.5, we write down a formula for $\Theta_1(I)$ and $\Theta_{0+2}(I)$. Armed with all of these formulas, we see from (11) that we can now calculate $C^{(q)}$ for any q. Finally, in Section 3.6, we carry out the procedure fully to compute $C^{(2)}$ and $C^{(3)}$.

3.1 Taking Fourier series

Recall from the eigenvalue problem (3) for η that the ψ_l are an orthonormal basis for L^2 with the property that

$$L_\eta \psi_l = -\lambda_l \psi_l.$$

We define the operator $\mathcal{F} \colon L^2 \to \ell^2$ as

$$\mathcal{F}(f)(l) = \int_0^\pi f(\eta) \psi_l(\eta) \, d\eta.$$

Given a function $f \in L^2([0,\pi])$, this integral is defined for all $l \geq 0$, and, furthermore, we know

$$\langle \mathcal{F}(f), \mathcal{F}(g) \rangle_{\ell^2} = \langle f, g \rangle_{L^2}, \quad \|\mathcal{F}(f)\|_{\ell^2} = \|f\|_{L^2}.$$

The operator $\mathcal{F}$ applied to a function f gives us the Fourier series of f with respect to the basis $\{\psi_l\}$. If we define

$$D(L_\eta) = \left\{ u \in H^2([0,\pi]) \mid u'(0) = u'(\pi) = 0 \right\},$$

then it is easy to see that L_η is symmetric on this domain, and that the image of L_η is

$$D(L_\eta^{-1}) := \left\{ u \in L^2([0,\pi]) \mid \int_0^\pi u(\eta)\, d\eta = 0 \right\}.$$

For any $l > 0$, $\psi_l \in D(L_\eta^{-1})$, and it makes sense for us to write the equation

$$L_\eta^{-1} \psi_l = -\frac{\psi_l}{\lambda_l}. \tag{12}$$

Another way of saying this is that for any function $f \in D(L_\eta^{-1})$, we are guaranteed that $\mathcal{F}(f)(0) = 0$, and thus we can define how L_η^{-1} acts on Fourier series as

$$\mathcal{F}(L_\eta^{-1}(f))(l) = -\frac{\mathcal{F}(f)(l)}{\lambda_l}. \tag{13}$$

Where convenient, we also use the notation that

$$\hat{f} = \mathcal{F}(f), \quad \check{g} = \mathcal{F}^{-1}(g).$$

Also, if we have two functions $f, g \in D(L_\eta^{-1})$, then Parseval's Equality can be written as

$$\int_0^\pi f(\eta) g(\eta)\, d\eta = \sum_{l>0} \mathcal{F}(f)(l) \mathcal{F}(g)(l). \tag{14}$$

Combining (13) and (14) gives us

$$\sum_{l>0} \frac{\mathcal{F}(f)(l)\mathcal{F}(g)(l)}{\lambda_l} = -\int_0^\pi L_\eta^{-1}(f) \cdot g\, d\eta = -\int_0^\pi f \cdot L_\eta^{-1}(g)\, d\eta, \tag{15}$$

$$\sum_{l>0} \frac{\mathcal{F}(f)(l)\mathcal{F}(g)(l)}{\lambda_l^2} = \int_0^\pi L_\eta^{-1}(f) \cdot L_\eta^{-1}(g)\, d\eta. \tag{16}$$

Also, we consider the expression $\beta_{l,l'}$ which was defined in [3] to be

$$\beta_{l,l'} = \frac{\hat{b}(l,l')}{\hat{b}(0)} - \delta_{l,l'}, \quad \hat{b}(l,l') = \int_0^\pi b(\eta)\psi_l(\eta)\psi_{l'}(\eta)\, d\eta, \quad \hat{b}(0) = \frac{1}{\pi}\int_0^\pi b(\eta)\, d\eta.$$

If we further define the function

$$\tilde{b}(\eta) = \frac{1}{\hat{b}(0)} \left(b(\eta) - \hat{b}(0) \right), \tag{17}$$

and note that $\psi_0 = 1/\sqrt{\pi}$, then we have

$$\beta_{l,l'} = \int_0^\pi \tilde{b}\psi_l\psi_{l'}, \tag{18}$$

$$\frac{1}{\sqrt{\pi}}\int_0^\pi \tilde{b}f = \sum_{l>0}\mathcal{F}(f)(l)\beta_{l,0}, \tag{19}$$

$$\tilde{b}f = \mathcal{F}^{-1}\left(\sum_{l'>0}\mathcal{F}(f)(l')\beta_{l,l'}\right), \tag{20}$$

for any $f \in D(L_\eta^{-1})$.

3.2 The inductive step

In this subsection, we will derive two inductive formulas. In Lemma 8 of [3], it was shown that all of the terms in our expansions led to a certain form, with unspecified coefficient functions. Lemma 3 below gives an inductive formula for these coefficient functions, using the calculations from [3].

We recall some notation from [3]. There are three types of terms, Type 0, 1, and 2. Type 0 terms were terms which coupled $l = 0$ modes to $l = 0$ modes, Type 1 terms were terms which coupled $l = 0$ modes to $l > 0$ modes, and Type 2 terms were terms which coupled $l > 0$ modes to $l > 0$ modes. In Lemma 3 of [3], it was shown that taking Poisson brackets with the functions denoted by χ_n sent Type 1 terms to Type $0+2$ terms, and sent Type $0+2$ terms to Type 1 terms. Of course, applying two of these Poisson brackets sends Type $0+2$ terms to Type $0+2$ terms, and Type 1 terms to Type 1 terms.

Also, we denoted in [3] the map

$$L_i(H) = \{\chi_i, H\},$$

and

$$L_I(H) = L_{i_1}\circ\cdots\circ L_{i_n}(H)$$

if $I = i_1 \dots i_n$. Recall that we also defined C_I, $Q_I(l)$ and $K^n(l)$ so that

$$L_I(G)_{0,k00} = C_I d^{p(I)}\omega_{k0}^{p(I)+1},$$

$$L_I(G)_{1,kl0} = Q_I(l)d^{p(I)}\omega_{k0}^{p(I)+1}\frac{\omega_{k0}^{1/2}}{\omega_{kl}^{1/2}},$$

$$S_{n,kl} = K^n(l)d^{2n+2}\omega_{k0}^{2n+2}\frac{\omega_{k0}^{1/2}}{\omega_{kl}^{1/2}}\frac{1}{\lambda_l}.$$

We first state inductive formulas for the C_I, f_I, q_I, Q_I:

Lemma 3. *We have the following formulas:*

$$
\begin{aligned}
C_{iI} &= -2\sum_{l>0}\frac{Q_I(l)K^i(l)}{\lambda_l}, \quad f_{iI}(l) = \frac{K^i(l)}{\lambda_l}, \quad g_{iI}(l) = Q_I(l),\\
Q_{iI}(l) &= C_I\frac{K^i(l)}{\lambda_l} - f_I(l)\sum_{l_2>0}\frac{K^i(l_2)g_I(l_2)}{\lambda_{l_2}} - g_I(l)\sum_{l_2>0}\frac{K^i(l_2)f_I(l_2)}{\lambda_{l_2}}.
\end{aligned}
$$

Proof. The calculation is straightforward, and was done in the proof of Lemma 9 in Appendix A of [3]. For a more detailed derivation, see Appendix H of [2].

□

Lemma 4 will be Lemma 3 iterated twice, but we state the formulas explicitly for convenience. Since taking two Poisson brackets sends Type 0+2 to Type 0+2 and Type 1 to Type 1, it is possible to derive a formula for Q_{ijI} which depends only on Q_I, and a formula for C_{ijI}, f_{ijI}, and g_{ijI} which depends only on C_I, f_I, and g_I.

Lemma 4. *We have the following two-step formulas:*

$$
\begin{aligned}
C_{ijI} &= -2\ C_I\sum_{l>0}\frac{K^i(l)K^j(l)}{\lambda_l^2} - 2\sum_{l>0}\frac{K^j(l)g_I(l)}{\lambda_l}\times\sum_{l>0}\frac{K^i(l)f_I(l)}{\lambda_l}\\
&\quad - 2\sum_{l>0}\frac{K^j(l)f_I(l)}{\lambda_l}\times\sum_{l>0}\frac{K^i(l)g_I(l)}{\lambda_l},\\
Q_{ijI}(l) &= 2\frac{K^i(l)}{\lambda_l}\sum_{l'>0}\frac{Q_I(l')K^j(l')}{\lambda_{l'}}\\
&\quad - \frac{K^j(l)}{\lambda_l}\sum_{l_1>0}\frac{Q_I(l_1)K^i(l_1)}{\lambda_{l_1}} - Q_I(l)\sum_{l'>0}\frac{K^i(l_1)K^j(l_1)}{\lambda_{l_1}^2},\\
f_{ijI}(l) &= \frac{K^i(l)}{\lambda_l},\\
g_{ijI}(l) &= C_I\frac{K^j(l)}{\lambda_l} - f_I(l)\sum_{l_1>0}\frac{K^j(l_1)g_I(l_1)}{\lambda_{l_1}} - g_I(l)\sum_{l_1>0}\frac{K^j(l_1)f_I(l_1)}{\lambda_{l_1}}.
\end{aligned}
$$

We consider the various sums in the above expressions. For example, consider the very first sum,

$$\sum_{l>0}\frac{K^i(l)K^j(l)}{\lambda_l^2}. \tag{21}$$

Let's say that for any $i \geq 0$, we had a function b_i such that $\mathcal{F}(b_i(\eta))(l) = K^i(l)$ for $l > 0$, i.e. the function K^i represents the Fourier coefficients of the function b_i. Then the sum in (21) would be

$$\int_0^\pi L_\eta^{-1}(b_i)\, L_\eta^{-1}(b_j)\ d\eta,$$

using the formula given in (16).

We will show below in (33) that for any $i \geq 0$, there is a function b_i such that $\mathcal{F}(b_i(\eta))(l) = K^i(l)$ for $l > 0$. Furthermore, we will exhibit a iterative formula for b_i. In the meantime, we need only be concerned with the fact that such b_i exist. Then, using (15), (16), and (19), we can rewrite Lemma 4 as

Lemma 5. *We have the following two-step formulas:*

$$\begin{aligned}
C_{ijI} &= -2\ C_I \int_0^\pi L_\eta^{-1}(b_i)\, L_\eta^{-1}(b_j) - 2\int_0^\pi L_\eta^{-1}(b_j)\, \check{g}_I \times \int_0^\pi L_\eta^{-1}(b_i)\, \check{f}_I \\
&\qquad - 2\int_0^\pi L_\eta^{-1}(b_j)\, \check{f}_I \times \int_0^\pi L_\eta^{-1}(b_i)\, \check{g}_I, \\
\check{Q}_{ijI} &= 2L_\eta^{-1}(b_i) \int_0^\pi L_\eta^{-1}(b_j)\, \check{Q}_I - L_\eta^{-1}(b_j) \times \\
&\qquad \times \int_0^\pi L_\eta^{-1}(b_i)\, \check{Q}_I - \check{Q}_I \int_0^\pi L_\eta^{-1}(b_i)\, L_\eta^{-1}(b_j), \\
\check{f}_{ijI} &= L_\eta^{-1}(b_i), \\
\check{g}_{ijI} &= C_I L_\eta^{-1}(b_j) - \check{f}_I \int_0^\pi L_\eta^{-1}(b_j)\, \check{g}_I - \check{g}_I \int_0^\pi L_\eta^{-1}(b_j)\, \check{f}_I.
\end{aligned}$$

3.3 A formula for C_I

Although Lemma 5 is good as an inductive lemma, we need a little more. In the next two sections, we turn the inductive lemma given by Lemma 5 into a closed-form formula for C_I and Q_I. In this section, we derive a formula for C_I using Lemma 5, and in the next, we do a similar analysis to derive a formula for Q_I. Thus we will use the first, third, and fourth equations in Lemma 5 in this section, and the second equation of Lemma 5 in the next section.

When deriving these formulas, we find that a notational complication arises because the process described in Lemma 5 generates many terms, especially if I is long. For example, if C_I and $\check{g}_I$ are both sums of n terms, then C_{ijI} and $\check{g}_{ijI}$ will have $3n$ terms. After a cursory inspection of the inductive formulas, we see that every term in C_I involves combinations of terms of the form $L_\eta^{-1}(b_{I_k})$. The complication is that at each stage they are combined in various ways, and we need to compute how they are organized.

Definition 2. *Given a set S, we define $P(S)$ to be the set of pairings of S. We say that a set of sets s is a pairing of S, or that $s \in P(S)$, if*

- *every element of s (except possibly one) is a two-element set,*
- *if there is an element of s which is not a two-element set, it is a singleton, and*
- *the elements of S are completely represented, i.e. every element of S appears exactly once in the elements of s.*

Remarks:

1. It follows from the definition that if $\#(S)$ is even, then the elements of s will only be two-element sets, but it $\#(S)$ is odd, then one of the elements of s will be a singleton.
2. For example, the set $P(\{1,2,3\})$ consists of the pairings

$$\{\{1,2\},\{3\}\},\{\{1,3\},\{2\}\},\{\{2,3\},\{1\}\}.$$

3. For the purposes of notational simplicity, we will write the pairing

$$\{\{1,2\},\{3\}\} \text{ as } [1\ 2][3].$$

Let I be a multiindex of length n, where n is odd. Let $s \in P(\{1,\dots,n,*\})$, and $t \in P(\{2,\dots,n,*\})$, where

$$s = [s_{11}s_{12}][s_{21}s_{22}]\cdots[s_{m1}s_{m2}],$$

and

$$t = [t_{11}t_{12}][t_{21}t_{22}]\cdots[t_m].$$

If n is even, we choose $s \in P(\{1,\dots,n-1,*\})$ and $t \in P(\{2,\dots,n-1,*\})$. Here we are thinking of $*$ as a special place marker. Note that in either case, whether n is even or odd, we have chosen s to be a pairing from a set with an even number of elements, and t to be a pairing from a set with an odd number of elements.

We then define

$$C_{I,s} = \prod_{i=1}^{m} \int L_\eta^{-1}\left(b_{I_{s_{i1}}}\right) L_\eta^{-1}\left(b_{I_{s_{i2}}}\right),$$

$$\check{g}_{I,t} = L_\eta^{-1}\left(b_{I_{t_m}}\right) \prod_{i=1}^{m-1} \int L_\eta^{-1}\left(b_{I_{t_{i1}}}\right) L_\eta^{-1}\left(b_{I_{t_{i2}}}\right),$$

where, if x is an integer and $b_x \in D(L_\eta^{-1})$, then $L_\eta^{-1}(b_x)$ is given by (12), and if $x = *$,

$$L_\eta^{-1}(b_*) = \begin{cases} \frac{1}{\sqrt{\pi}}\tilde{b} & \text{if } n \text{ is odd,} \\ \tilde{b} L_\eta^{-1}(b_n) & \text{if } n \text{ is even,} \end{cases}$$

where we define $\tilde{b}$ to be

$$\tilde{b}(\eta) = \frac{1}{\hat{b}(0)}\left(b(\eta) - \hat{b}(0)\right).$$

For simplicity of notation below, we say that $* + 2 = *$.

Let us calculate some examples explicitly. Choose $n = 3$, and $I = 7,5,4$, i.e. C_I will be the coefficient of the Type 0 piece of the term $L_7 \circ L_5 \circ L_4(H_1^0)$. Let's say that we choose the pairing $s = [13][2*] \in P(\{1,2,3,*\})$. Then

$$C_{I,s} = \frac{1}{\sqrt{\pi}} \int L_\eta^{-1}(b_7) \cdot L_\eta^{-1}(b_4)\, d\eta \times \int L_\eta^{-1}(b_5) \cdot \tilde{b}\, d\eta.$$

On the other hand, if we were to choose the pairing $s = [12][3*]$, then

$$C_{I,s} = \frac{1}{\sqrt{\pi}} \int L_\eta^{-1}(b_7) \cdot L_\eta^{-1}(b_5)\, d\eta \times \int L_\eta^{-1}(b_4) \cdot \tilde{b}\, d\eta.$$

Now, choose $n = 4$ and $I = 12, 9, 7, 6$, so that C_I is the coefficient of the Type 0 piece of the term $L_{12} \circ L_9 \circ L_7 \circ L_6(H_2^0)$, but we again choose $s = [13][2*] \in P(\{1, 2, 3, *\})$ (recall that for n even we choose $s \in P(\{1, \ldots, n-1, *\})$). Then

$$C_{I,s} = \int L_\eta^{-1}(b_{12}) \cdot L_\eta^{-1}(b_7)\, d\eta \times \int \tilde{b} L_\eta^{-1}(b_9)\, L_\eta^{-1}(b_6)\, d\eta.$$

There are two special sets, $S_n \subset P(\{1, \ldots, n, *\})$ and $T_n \subset P(\{2, \ldots, n, *\})$ (if n is odd), or $S_n \subset P(\{1, \ldots, n-1, *\})$ and $T_n \subset P(\{2, \ldots, n-1, *\})$ (if n is even), so that

$$C_I = \sum_{s \in S_n} C_{I,s}, \quad \check{g}_I = \sum_{t \in T_n} \check{g}_{I,t}.$$

To start, assume that we have an $s \in S_n$ and a $t \in T_n$, where

$$\begin{aligned} s &= [s_{11}s_{12}][s_{21}s_{22}] \cdots [s_{m1}s_{m2}], \\ t &= [t_{11}t_{12}][t_{21}t_{22}] \cdots [t_m]. \end{aligned}$$

Further assume that C_I and $\check{g}_I$ have a simple form, namely that $C_I = C_{I,s}$ and $\check{g}_I = \check{g}_{I,t}$, and we will be able to extend the argument by linearity.

Denote $\tilde{I} = ijI$. Consider the second term in C_{ijI} in Lemma 5,

$$-2 \int L_\eta^{-1}(b_i)\, \check{f}_I \times \int L_\eta^{-1}(b_j)\, \check{g}_I.$$

By definition,

$$\check{g}_{I,t} = L_\eta^{-1}\left(b_{I_{t_m}}\right) \prod_{i=1}^{m-1} \int L_\eta^{-1}\left(b_{I_{t_{i1}}}\right) L_\eta^{-1}\left(b_{I_{t_{i2}}}\right)$$

and we know that

$$\check{f}_I = L_\eta^{-1}(b_{I_1}),$$

so the second term in C_{ijI} in Lemma 5 becomes

$$-2 \int L_\eta^{-1}(b_i)\, L_\eta^{-1}(b_{I_1}) \int L_\eta^{-1}(b_j)\, L_\eta^{-1}\left(b_{I_{t_m}}\right) \prod_{i=1}^{m-1} \int L_\eta^{-1}\left(b_{I_{t_{i1}}}\right) L_\eta^{-1}\left(b_{I_{t_{i2}}}\right).$$

Noting that $\tilde{I} = ijI$, and thus $\tilde{I}_{k+2} = I_k$, we can write this as

$$\begin{aligned} -2 \int L_\eta^{-1}\left(b_{\tilde{I}_1}\right) L_\eta^{-1}\left(b_{\tilde{I}_3}\right) \int L_\eta^{-1}\left(b_{\tilde{I}_2}\right) L_\eta^{-1}\left(b_{\tilde{I}_{t_m+2}}\right) \times \\ \times \prod_{i=1}^{m-1} \int L_\eta^{-1}\left(b_{\tilde{I}_{t_{i1}+2}}\right) L_\eta^{-1}\left(b_{\tilde{I}_{t_{i2}+2}}\right). \end{aligned} \tag{22}$$

Thus (22) is $-2C_{\tilde{I},\tilde{s}}$, where

$$\tilde{s} = [1\ 3][2\ t_m + 2][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2].$$

In this way, we say that t gives rise to $\tilde{s}$. Looking at the terms in Lemma 5, we see that given a pair (s, t), we give rise to six terms $(\tilde{s}_1, \tilde{s}_2, \tilde{s}_3, \tilde{t}_1, \tilde{t}_2, \tilde{t}_3)$, where

$$\begin{aligned}
\tilde{s}_1 &= [12][s_{11} + 2\ s_{12} + 2] \cdots [s_{m1} + 2\ s_{m2} + 2], \\
\tilde{s}_2 &= [13][2\ t_m + 2][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2], \\
\tilde{s}_3 &= [1\ t_m + 2][23][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2], \\
\tilde{t}_1 &= [2][s_{11} + 2\ s_{12} + 2] \cdots [s_{m1} + 2\ s_{m2} + 2], \\
\tilde{t}_2 &= [3][2\ t_m + 2][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2], \\
\tilde{t}_3 &= [t_m + 2][23][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2].
\end{aligned} \tag{23}$$

More specifically, if we start with the terms $C_{I,s}$ and $\check{g}_{I,t}$, then applying L_{ij} generates the two terms

$$-2 \left(C_{\tilde{I},\tilde{s}_1} + C_{\tilde{I},\tilde{s}_2} + C_{\tilde{I},\tilde{s}_3} \right), \text{ and } -\left(\check{g}_{\tilde{I},\tilde{t}_1} + \check{g}_{\tilde{I},\tilde{t}_2} + \check{g}_{\tilde{I},\tilde{t}_3} \right),$$

where $\tilde{s}_i$ and $\tilde{t}_i$ are defined in (23).

Upon inspection, we see that if we take any $\tilde{t}$ above, and turn the odd singleton into a pair by inserting a 1, then we get one of the $\tilde{s}$'s above. So we define the map ϕ by

$$\phi([t_{11}t_{12}] \ldots [t_m]) = [t_{11}t_{12}] \ldots [1\ t_m].$$

Then if we start with $t \in T_n$ and $\phi(t) \in S_n$, then

$$\begin{aligned}
\tilde{s}_1 &= \phi(\tilde{t}_1), \\
\tilde{s}_2 &= \phi(\tilde{t}_2), \\
\tilde{s}_3 &= \phi(\tilde{t}_3), \\
\tilde{t}_1 &= [2][t_{11} + 2\ t_{12} + 2] \cdots [t_m + 2\ 3], \\
\tilde{t}_2 &= [3][2\ t_m + 2][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2], \\
\tilde{t}_3 &= [t_m + 2][23][t_{11} + 2\ t_{12} + 2] \cdots [t_{m-1,1} + 2\ t_{m-1,2} + 2].
\end{aligned} \tag{24}$$

If we have already defined the sets S_n and T_n, then this gives a method to define S_{n+2} and T_{n+2}. For example, we define the set of pairings T_{n+2} by saying that $\tilde{t} \in T_{n+2}$ iff it arises in one of the three ways in (24) from a pairing $t \in T_n$. Similarly, we define S_{n+2} as arising from one of the three ways in (23). It is then clear that if $S_n = \phi(T_n)$, then $S_{n+2} = \phi(T_{n+2})$. In particular, we have shown

Lemma 6. *Fix a multiindex $I = I_1 I_2 \ldots I_n$, and $\alpha \in \mathbb{R}$. We assume that we can write*

$$C_I = \alpha \sum_{s \in S_n} C_{I,s}, \quad \check{g}_I = \alpha \sum_{t \in T_n} \check{g}_{I,t},$$

where $S_n = \phi(T_n)$. Then if we define a new multiindex of length $n+2$ as $\tilde{I} = ijI$, then

$$C_{\tilde{I}} = -2\alpha \sum_{s \in S_{n+2}} C_{\tilde{I},s}, \quad \breve{g}_{\tilde{I}} = -\alpha \sum_{t \in T_{n+2}} \breve{g}_{\tilde{I},t},$$

where $S_{n+2} = \phi(T_{n+2})$, and T_{n+2} is related to T_n by (24).

The only thing left are the initial cases. Since Lemma 6 gives the formula for two steps in the process, we must have initial cases for $|I| = 1$ and $|I| = 2$.

First, we consider the case $L_i(G)_{0+2} = L_i(H_1^0)$. Using the formulas from Appendix A of [3], we have that

$$C_i = \frac{1}{2} \sum_{l_1 > 0} \frac{K^i(l_1)\beta_{l_1,0}}{\lambda_{l_1}}, \quad g_i(l) = -\frac{1}{2}\beta_{l,0},$$

and thus

$$C_i = -\frac{1}{2\sqrt{\pi}} \int \tilde{b} L_\eta^{-1}(b_i), \quad \breve{g}_i = -\frac{1}{2\sqrt{\pi}}\tilde{b}. \tag{25}$$

For the case $|I| = 1$, we see that C_i has one term, with $s = [1\ *]$, and $\breve{g}_i$ has one term, with $t = [*]$.

Next, we consider the initial case $L_{ij}(G)_{0+2} = L_{ij}(H_2^0)_{0+2}$. Using the formulas from Appendix A of [3],

$$C_{ij} = -\frac{1}{2} \sum_{l,l' > 0} \frac{K^i(l)K^j(l')\beta_{l,l'}}{\lambda_l \lambda_{l'}}, \qquad g_{ij} = \frac{1}{2} \sum_{l > 0} \frac{K^i(l)\beta_{l,l'}}{\lambda_{l'}},$$

or

$$C_{ij} = -\frac{1}{2} \int \tilde{b} L_\eta^{-1}(b_i) L_\eta^{-1}(b_j), \quad \breve{g}_{ij} = -\frac{1}{2}\tilde{b} L_\eta^{-1}(b_j). \tag{26}$$

For the case $|I| = 2$, we see that C_{ij} has one term, with $s = [1\ *]$, and $\breve{g}$ has one term, with $t = [*]$.

From the above we see that $S_2 = S_1 = \{[1\ *]\}$ and $T_2 = T_1 = \{[*]\}$. From this and Lemma 6 it is clear that for n even, $S_n = S_{n-1}$ and $T_n = T_{n-1}$. Note that functions we get in (25) and (26) are different, but the difference corresponds exactly to the difference in the definition of b_* for $|I|$ even and odd.

Theorem 1. *Given a multiindex $I = I_1 I_2 \dots I_n$, we define b_* so that*

$$L^{-1}(b_*) = \begin{cases} \dfrac{1}{\sqrt{\pi}}\tilde{b} & \text{if } |I| \text{ is odd,} \\ \tilde{b} L_\eta^{-1}(b_{I_n}) & \text{if } |I| \text{ is even.} \end{cases}$$

If we define

$$C_{I,s} = \prod_{i=1}^{m} \int L_\eta^{-1}\left(b_{I_{s_{i1}}}\right) L_\eta^{-1}\left(b_{I_{s_{i2}}}\right),$$

for

$$s = [s_{11}s_{12}][s_{21}s_{22}]\dots[s_{m1}s_{m2}],$$

then

$$C_I = (-2)^{\lfloor \frac{n-3}{2} \rfloor} \sum_{s \in S_n} C_{I,s}.$$

Proof. First consider $|I| = 1$. From the calculations above, we know that $C_i = -C_{i,s}/2$ with $s = [1\ *]$. Thus

$$C_i = -\frac{1}{2} \sum_{s \in S_1} C_{i,s},$$

and $-1/2 = (-2)^{-1}$. For $|I| = 2$, we know that $C_{ij} = -C_{ij,s}/2$ with $s = [1\ *]$, so that

$$C_{ij} = -\frac{1}{2} \sum_{s \in S_2} C_{ij,s},$$

and $-1/2 = (-2)^{-1}$. Our induction hypothesis is that

$$C_I = (-2)^{\lfloor \frac{n-3}{2} \rfloor} \sum_{s \in S_n} C_{I,s},$$

where $|I| = n$. We apply Lemma 6 and see that for $\tilde{I}$ with $|\tilde{I}| = n + 2$,

$$C_{\tilde{I}} = (-2)^{\lfloor \frac{n-1}{2} \rfloor} \sum_{\tilde{s} \in S_{n+2}} C_{\tilde{I},\tilde{s}}.$$

Noting that $|\tilde{I}| = n + 2$, we are done. □

Theorem 1 solves the problem fairly completely. It tells us that our coefficients are sums of terms which we can compute explicitly. We do not yet have an expression for S_n or T_n. We have what amounts to a recursive relationship between S_{n+2} and S_n, and we need to derive a non-recursive formula for S_n and T_n.

Let us fix n odd. Of course, if we know what T_n is for n odd, then we have $T_{n+1} = T_n$ and we know T_n for n even. There is a certain pairing $e_n \in P(\{2, 3, \dots, n, *\})$ which we will consider special, namely

$$e_n = [2\ 3][4\ 5]\dots[n-1\ n][*].$$

Given a permutation π of the set $\{2, \dots, n, *\}$, we can apply π to e_n and obtain another pairing $t \in P(\{2, \dots, n, *\})$. It is certainly true that every pairing $t \in P(\{2, \dots, n, *\})$ can be realized as a permutation of e_n. (In fact, since pairings ignore order, there are many permutations which will realize a given pairing as a permutation of e_n.) Characterizing the elements of T_n is equivalent to characterizing the set of permutations which gives rise to them. We will characterize T_n in such a manner, i.e. we will say that there is some set

Π_n of permutations of $\{2,\ldots,n,*\}$ such that $t \in T_n$ iff there is a permutation $\pi \in \Pi_n$ with $t = \pi(e_n)$.

We write the transposition which switches the elements a and b as $(a\ b)$. Given a pairing t, we define $(a\ b)t$ to be the pairing which switches the entries a and b in t. Of course, many transpositions will have no effect on a pairing, since order is irrelevant.

We note that we can always write

$$\pi = (*\ i_1)(*\ i_2)\cdots$$

for some collection of numbers $i_k \leq n$. This statement is not very strong. All we claim here is that every permutation can be realized as a product of transpositions with a given fixed element. This is true because every permutation can be written as a product of transpositions, and every transposition of the form $(a\ b)$ can be written as $(*\ a)(*\ b)(*\ a)$.

The unusual element here is that we will show that our permutations can be written in this fashion, with the i_k strictly decreasing.

Lemma 7. *Assume that every element of Π_n can be written as*

$$\pi = (*\ i_1)(*\ i_2)\ldots(*\ i_m) = \prod_{k=1}^{m}(*\ i_k). \tag{27}$$

with $i_1 > i_2 > \cdots > i_m$. Then

- *the same holds true for Π_{n+2},*
- *for every element $\pi \in \Pi_n$, there are three corresponding elements in Π_{n+2}, as follows. We define*

$$\tilde{\pi} = \prod_{k=1}^{m}(*\ i_k + 2)$$

and then

$$\begin{aligned}\tilde{\pi}_1 &= \tilde{\pi},\\ \tilde{\pi}_2 &= \tilde{\pi}(*\ 2),\\ \tilde{\pi}_3 &= \tilde{\pi}(*\ 3).\end{aligned}$$

Then $\pi \in \Pi_n$ iff the three elements $\tilde{\pi}_1, \tilde{\pi}_2, \tilde{\pi}_3$ are in Π_{n+2}.

Proof. Since the first conclusion follows directly from the second, we need only prove the second. Let us assume that $t = [t_{11}t_{12}][t_{21}t_{22}]\ldots[t_m] \in T_n$, and we denote by π the permutation which gives $t = \pi(e_n)$. Assume that π satisfies (27).

We recall that

$$\begin{aligned}\tilde{t}_3 &= [2\ 3][t_{11}+2\ t_{12}+2]\cdots[t_{m-1,1}+2\ t_{m-1,2}+2][t_m+2],\\ \tilde{t}_1 &= [3\ t_m+2][t_{11}+2\ t_{12}+2]\cdots[t_{m-1,1}+2\ t_{m-1,2}+2][2],\\ \tilde{t}_2 &= [2\ t_m+2][t_{11}+2\ t_{12}+2]\cdots[t_{m-1,1}+2\ t_{m-1,2}+2][3].\end{aligned}$$

Clearly, if $t = \pi(e_n)$ where $\pi = (*\ i_1)(*\ i_2)\cdots$, then $\tilde{t}_1 = \tilde{\pi}(e_{n+2})$ as defined above, so that $\tilde{\pi}_1 = \tilde{\pi}$. Also, we see that $\tilde{\pi}_2 = (2\ t_m+2)\tilde{\pi}_1$ and $\tilde{\pi}_3 = (3\ t_m+2)\tilde{\pi}_1$. So we will be done if we show that

$$(2\ t_m + 2)\tilde{\pi}_1 = \tilde{\pi}_1(*\ 2),$$

and similarly for $\tilde{\pi}_3$.

Before we continue with the proof, we make a couple of observations. Note that our special pairing e_n has a $*$ in the singleton. We are applying to this pairing a series of transpositions of the form $(*\ i)$. When we apply $(*\ i)$ to e_n, this will put the number i into the singleton. Furthermore, there is no way remove a number from the singleton once it is there, since all further transpositions will be of the form $(*\ j)$ with $j > i$. Thus, by inspecting $\pi(e_n)$, we know that the first (i.e., rightmost) transposition of π must be $(*\ i)$ where i is the number in the singleton of $\pi(e_n)$. By the same argument, if $*$ is in the singleton of $\pi(e_n)$, then π must be the identity.

Now, we prove that $(2\ t_m + 2)\tilde{\pi}_1 = \tilde{\pi}_1(*\ 2)$. There are two cases. Either $t_m + 2 = *$ or not. If $t_m + 2 = *$, it follows from above that π is the identity. But the identity commutes with everything, so that

$$(*\ 2)\mathrm{id} = \mathrm{id}(*\ 2),$$

and $\tilde{\pi}_2 = \tilde{\pi}(*\ 2)$.

So we assume that $t_m + 2 \neq *$. Since the number $t_m + 2$ is in the singleton, it follows from (27) that π is of the form

$$\pi = \left(\prod_{k=1}^{m-1} (*\ i_k)\right)(*\ t_m),$$

i.e. that the first permutation must have been $(*\ t_m)$. Then

$$\tilde{\pi}_1 = \left(\prod_{k=1}^{m-1} (*\ i_k + 2)\right)(*\ t_m + 2).$$

Note also that $i_k + 2 > t_m + 2$ for all k because of (27). And, of course, since $i_k + 2 \geq 4$ for all k, we know that the permutation $(2\ t_m + 2)$ will commute with all but the last. Then we have that

$$\begin{aligned}(2\ t_m + 2)\tilde{\pi}_1 &= (2\ t_m + 2)\left(\prod_{k=1}^{m-1} (*\ i_k + 2)\right)(*\ t_m + 2)\\ &= \left(\prod_{k=1}^{m-1} (*\ i_k + 2)\right)(2\ t_m + 2)(*\ t_m + 2),\end{aligned}$$

and it is a direct calculation that $(2\ t_m + 2)(*\ t_m + 2) = (*\ t_m + 2)(*\ 2)$, so that $\tilde{\pi}_2 = \tilde{\pi}(*\ 2)$. $\square$

Every permutation in Π_n gives rise to three in Π_{n+2}. Note that it follows from the proof that π will not contain both $(* \ 2)$ and $(* \ 3)$. It can have either one, or neither, but it cannot have both. From this it follows that no π has both $(* \ n)$ and $(* \ (n+1))$ for n even.

We know from direct calculation that Π_1 has one element, id. From this we can deduce that Π_3 has three permutations, $(* \ 2), (* \ 3)$, and id. Thus the three elements of T_3 (or T_4) are

$$[*][23], [3 \ *][2], [2 \ *][3].$$

Also, from this we know that the three elements of S_3 (or S_4) are

$$[1 \ *][23], [3 \ *][12], [2 \ *][13].$$

We know that Π_5 has nine elements. We can choose to do $(* \ 2)$, $(* \ 3)$, or do nothing at the first step, and we can then choose to do $(* \ 4), (* \ 5)$, or do nothing at the second step, giving a total of nine possibilities. We carry out this induction in the following theorem:

Theorem 2. *Let n be odd. Choose the $(n+1)/2$ permutations π_i, each of which has the property that $\pi_i = (* \ 2i), (* \ 2i+1)$, or the identity. Then Π_n is the set of all compositions*

$$\pi_{(n+1)/2} \circ \cdots \circ \pi_1.$$

If n is even, then $\Pi_n = \Pi_{n-1}$.

Proof. Choose n odd, and the proof is the same for even n. The theorem is certainly true for $n = 3$, since Π_3 is the set

$$(* \ 2), (* \ 3), \ \text{id}.$$

Let's assume that we have a $\pi = \pi_{(n+1)/2} \circ \cdots \circ \pi_1 \in \Pi_n$. Then in Lemma 7 we get $\tilde{\pi}$ by increasing each entry by 2. In this scheme, we can write

$$\tilde{\pi} = \pi_{(n+3)/2} \circ \cdots \circ \pi_3,$$

where $\pi_i = (* \ 2i), (* \ 2i+1)$, or the identity. Then we know the three permutations we get from this are

$$\begin{aligned} &\pi_{(n+3)/2} \circ \cdots \circ \pi_3, \\ &\pi_{(n+3)/2} \circ \cdots \circ \pi_3(* \ 2), \\ &\pi_{(n+3)/2} \circ \cdots \circ \pi_3(* \ 3), \end{aligned}$$

which can be written

$$\tilde{\pi} = \pi_{(n+3)/2} \circ \cdots \circ \pi_3 \circ \pi_1,$$

where $\pi_1 = (* \ 2), (* \ 3)$, or the identity. $\square$

This scheme says that at each step, the set of permutations (and thus the set of possible pairings) grows by a factor of 3. Since the increasing assumption means that there will be no repeats, we have that $|S_n| = 3^{\lfloor (n-1)/2 \rfloor}$.

3.4 A formula for K^n and b_n

At each step of the inductive process of [3], we chose χ_n to solve the equation $\left\{\chi_n, H^0_{\mathrm{diag}}\right\} = -H^n_{1,\mathrm{low}}$. It was shown that

$$H^n_{1,\mathrm{low}} = \sum_{\substack{I\in\mathcal{M}_{n-1}\\ p(I)=2n}} \Theta_1(I)L_I(G)_1.$$

We also recall that the function $Q_I(l)$ was defined in Lemma 9 of [3] to be the part of $L_I(G)_1$ which depended on l. With all of this in mind, it is not surprising that (for details, see the calculations leading to (109) in [3], or Appendix H in [2]) the function which encapsulates χ_n's dependence on l is given by

$$K^n(l) = \sum_{\substack{I\in\mathcal{M}_{n-1}\\ p(I)=2n}} 4Q_I(l). \tag{28}$$

We remind the reader that

$$p(I) = \sum_k 2(I_k+1),$$

where I_k are the entries of I.

At first glance, the reader might think that this formula has is circular, since the formulas for the Q_I depend on K^j themselves. The reason that this is not circular is that the function K^j enters the formula for Q_I only if j is one of the indices of I. If a multiindex I has an n as an entry, then by necessity, $p(I)\geq 2n+2$. It follows that the largest entry of any I with $p(I)=2n$ is $n-1$. Thus this formula for K^n might depend on K^j for all $j<n$, but the right hand side of (28) will not depend on any K^j with $j\geq n$.

To calculate K^n, we need a general algorithm to determine Q_I for any I. The calculation of Q_I is very similar to that of C_I. If we inspect Lemma 5, we see that the inductive two-step process which defines Q_I is very similar to the one which determines C_I. We will see that the main difference between the two formulas is the initial cases, but that the step-by-step process is almost exactly the same.

Let us fix a multiindex I. If $|I|$ is even, we choose $t\in P\left(\{1,\ldots,n,*\}\right)$, and if $|I|$ is odd, we choose $t\in P\left(\{1,\ldots,n-1,*\}\right)$. In contrast to the choice in the last section, here the set of elements includes a 1, for $|I|$ both even and odd. In either case, we are choosing from an odd number of elements, so that we can write

$$t = [t_{11}t_{12}]\ldots[t_m].$$

Then we define

$$\check{Q}_{I,t} = L_\eta^{-1}\left(b_{I_{t_m}}\right)\prod_{i=1}^{m-1}\int L_\eta^{-1}\left(b_{I_{t_{i1}}}\right)L_\eta^{-1}\left(b_{I_{t_{i2}}}\right),$$

where $L_\eta^{-1}(b_x)$ for x an integer is the same as defined in the previous section, and

$$L_\eta^{-1}(b_*) = \begin{cases} \frac{1}{\sqrt{\pi}}\tilde{b}, & \text{if } |I| \text{ is even,} \\ \tilde{b}L_\eta^{-1}(b_n), & \text{if } |I| \text{ is odd.} \end{cases}$$

There is a set $U_n \subset P(\{1,\dots,n,*\})$ or $U_n \subset P(\{1,\dots,n-1,*\})$ such that

$$\check{Q}_I = \sum_{t \in U_n} \check{Q}_{I,t}.$$

We see from Lemma 5 that if we choose a term of the form $\check{Q}_{I,t}$ and apply L_{ij} to it, we will get $-\check{Q}_{\tilde{I},\tilde{t}_1}$, $2\check{Q}_{\tilde{I},\tilde{t}_2}$, and $-\check{Q}_{\tilde{I},\tilde{t}_3}$, where

$$\begin{aligned} \tilde{t}_1 &= [1\ 2][t_{11} + 2t_{12} + 2]\dots[t_m + 2], \\ \tilde{t}_2 &= [2\ t_m + 2][t_{11} + 2t_{12} + 2]\dots[1], \\ \tilde{t}_3 &= [1\ t_m + 2][t_{11} + 2t_{12} + 2]\dots[2]. \end{aligned} \tag{29}$$

Just as before, we define U_{n+2} to be the set of pairings that arise in one of these ways from the set U_n.

Lemma 8. *Fix a multiindex I, and define $\tilde{I} = ijI$. If we can write*

$$\check{Q}_I = \sum_{t \in U_n} a(t)\check{Q}_{I,t},$$

then

$$\check{Q}_{\tilde{I}} = \sum_{t \in U_{n+2}} a(t)\check{Q}_{\tilde{I},t},$$

where a is some real number which depends on the pairing t.

Proof. The proof is exactly the same as in the case of Lemma 6, except that we have the coefficients $a(t)$. □

To determine the initial cases, we do something slightly different than in the previous lemma. Before, we chose $|I| = 1$ and $|I| = 2$ to be our initial cases. In this case we can simplify and choose $|I| = 0$ and $|I| = 1$ as the initial cases in the induction.

In this manner,

$$Q_\emptyset(l) = -\frac{1}{4}\beta_{l,0}, \tag{30}$$

or

$$\check{Q}_\emptyset = -\frac{1}{4\sqrt{\pi}}\tilde{b},$$

so that $\check{Q}_\emptyset$ has one term with $t = [*]$.

The calculations in Appendix A of [3] give

$$Q_i(l) = \frac{1}{4}\sum_{l'>0} \frac{K^i(l')\beta_{l,l'}}{\lambda_{l'}}, \tag{31}$$

or

$$\check{Q}_i = \frac{1}{4}\tilde{b}L_\eta^{-1}\left(b_i\right),$$

so that $\check{Q}_1$ has one term, with $t = [*]$. From this, we know that $U_0 = U_1$ and thus $U_n = U_{n+1}$ for n any even number. Moreover, the permutations corresponding to the Q_I are similar to those corresponding to the $\breve{g}_I$, in that $U_n = T_n$ for any odd n, and $U_n = T_{n-2}$ for any even n. Thus we have

Theorem 3. *Given a multiindex $I = I_1 I_2 \ldots I_n$, we define*

$$L_\eta^{-1}\left(b_*\right) = \begin{cases} \frac{1}{\sqrt{\pi}}\tilde{b}, & \text{if } |I| \text{ is even,} \\ \tilde{b}L_\eta^{-1}\left(b_n\right), & \text{if } |I| \text{ is odd.} \end{cases}$$

If we define

$$\check{Q}_{I,t} = L_\eta^{-1}\left(b_{I_{t_m}}\right)\prod_{i=1}^{m-1}\int L_\eta^{-1}\left(b_{I_{t_{i1}}}\right)L_\eta^{-1}\left(b_{I_{t_{i2}}}\right),$$

for

$$t = [t_{11}t_{12}]\ldots[t_m],$$

then there exists a set of pairings U_n and a function $a\colon U_n \to \mathbb{R}$ such that

$$\check{Q}_I = \sum_{t\in U_n} a(t)\check{Q}_{I,t}.$$

We need to determine the set U_n and the function $a(t)$. We do so in the following theorem. We should note that we will again characterize U_n as a set of permutations applied to a special element. Since the situation is so similar to that in the previous section, we compress this information in the following theorem.

Proposition 9. *Let n be even. Choose the $n/2$ permutations π_i, where $\pi_i = (*\ 2i)$, $(*\ 2i-1)$, or the identity, and let*

$$\pi = \pi_{n/2}\circ\cdots\circ\pi_1.$$

We define the special element $e_n \in P\left(\{1,\ldots,n,*\}\right)$ to be

$$e_n = [*][1\ 2][3\ 4]\cdots[n-1\ n].$$

Then $t \in U_n$ iff it can be written $\pi(e_n)$ for a permutation π in the form above.

Furthermore, let β be the number of transpositions in π of the form $(*\ i)$ with i odd. Then for $t \in U_n$ with $t = \pi(e_n)$,

$$a(t) = \frac{1}{4}(-1)^{\left\lfloor\frac{n-1}{2}\right\rfloor}(-2)^\beta.$$

If n is odd, then $U_n = U_{n-1}$.

Proof. The part of the proof which describes U_n is much like the proofs of the last section. Let us assume that we have $t \in U_n$, where $t = \pi(e_n)$. We define $\tilde{\pi}$ to be the permutation with all of the transpositions of π increased by 2. In other words, if

$$\pi = \prod_{k=1}^{n} (*\ i_k),$$

then

$$\tilde{\pi} = \prod_{k=1}^{n} (*\ i_k + 2).$$

Then referring to (29), we have that

$$\tilde{t}_1 = \tilde{\pi}_1(e_n), \quad \tilde{t}_2 = \tilde{\pi}_2(e_n), \quad \tilde{t}_3 = \tilde{\pi}_3(e_n),$$

where

$$\tilde{\pi}_1 = \tilde{\pi}, \quad \tilde{\pi}_2 = (1\ t_m + 2)\tilde{\pi}, \quad \tilde{\pi}_3 = (2\ t_m + 2)\tilde{\pi}.$$

An argument exactly like that in the proof of Lemma 7 gives us that

$$\tilde{\pi}_1 = \tilde{\pi}, \quad \tilde{\pi}_2 = \tilde{\pi}(*\ 1), \quad \tilde{\pi}_3 = \tilde{\pi}(*\ 2).$$

Now, we want to determine $a(t)$. We see from Lemma 5 that $\tilde{\pi}_2$ comes with a factor of 2, and $\tilde{\pi}_1$ and $\tilde{\pi}_3$ come with a factor of -1. This means that if we consider the formulation above where π is written as a product of transpositions, every time we use $(*\ 2i-1)$, we get a factor of 2, but if we choose $(*\ 2i)$, or the identity, then we add a factor of -1. Another way of writing this is that we choose a factor of -1 for every π_i, and then multiply an additional factor of -2 for any choice of $(*\ 2i-1)$. There are $\lfloor (n-1)/2 \rfloor + 1$ terms, so the permutation π comes with a prefactor of

$$(-1)^{\lfloor \frac{n-1}{2} \rfloor}(-2)^{\beta}, \tag{32}$$

where β is the number of transpositions of the form $(*\ 2i-1)$ (the number of transpositions of $*$ with an odd number). If we consider the equations (30) and (31), we see that $a([*]) = -1/4$. Combining this with (32) gives us the formula for $a(t)$. □

As we know, if we can calculate Q_I for any I, then to find K^n, we calculate the sum

$$K^n = 4 \sum_{\substack{I \in \mathcal{M}_{n-1} \\ p(I)=2n}} Q_I.$$

Recall that we define the function b_n so that $\mathcal{F}(b_n) = K^n$. If we want the function b_n, then we simply need to compute

$$b_n = 4 \sum_{\substack{I \in \mathcal{M}_{n-1} \\ p(I)=2n}} \check{Q}_I. \tag{33}$$

3.5 A formula for $\Theta_{0+2}(I)$ and $\Theta_1(I)$

We will show a recursive formula for $\Theta_{0+2}(I)$ and $\Theta_1(I)$. Not surprisingly, the formula for each function will depend recursively on the other. Let us fix a multiindex

$$I = n^{p_n}(n-1)^{p_{n-1}}\cdots 0^{p_0}, \text{ with } n > 0,$$

where we denote

$$\tilde{I} = (n-1)^{p_{n-1}}\cdots 0^{p_0},$$

and calculate $\Theta_{0+2}(I)$. First, consider the formula from [[3], Equation (46)]:

$$H^n_{0+2} = \sum_{i \text{ odd}} \frac{L^i_{n-1}(H^{n-1}_{1,\text{low}})}{\xi(i)} + \sum_{i \text{ odd}} \frac{L^i_{n-1}(\widehat{H^{n-1}_1})}{i!} + \sum_{i \text{ even}} \frac{L^i_{n-1}(H^{n-1}_{0+2})}{i!}, \qquad (34)$$

where we recall that $H^{n-1}_{1,\text{low}}$ are the terms of H^{n-1}_1 of order exactly $2n$ in d, and that we have defined $\xi(i) = (i+1)!/i$.

From this we see that

$$\Theta_{0+2}(I) = \begin{cases} \frac{1}{p_n!}\Theta_{0+2}(\tilde{I}), & \text{if } p_n \text{ is even,} \\ 0, & \text{if } p_n \text{ is odd, and } p(\tilde{I}) < 2n, \\ \frac{1}{\xi(p_n)}\Theta_1(\tilde{I}), & \text{if } p_n \text{ is odd, and } p(\tilde{I}) = 2n, \\ \frac{1}{p_n!}\Theta_1(\tilde{I}), & \text{if } p_n \text{ is odd, and } p(\tilde{I}) > 2n. \end{cases}$$

If we choose $I = 0^{p_0}$, then (34) gives us that

$$\Theta_{0+2}(0^{p_0}) = \begin{cases} \frac{1}{p_0!}, & \text{if } p_0 \text{ is even,} \\ \frac{1}{\xi(p_0)}, & \text{if } p_0 \text{ is odd.} \end{cases}$$

To calculate $\Theta_1(I)$, we consider [[3],Equation (47)]

$$H^{n+1}_1 = \sum_{i \text{ odd}} \frac{L^i_n(H^n_{0+2})}{i!} + \sum_{\substack{i \text{ even} \\ i>0}} \frac{L^i_n(H^n_{1,\text{low}})}{\xi(i)} + \sum_{i \text{ even}} \frac{L^i_n(\widehat{H^n_1})}{i!}, \qquad (35)$$

and thus

$$\Theta_1(I) = \begin{cases} \frac{1}{p_n!}\Theta_{0+2}(\tilde{I}), & \text{if } p_n \text{ is odd,} \\ 0, & \text{if } p_n \text{ is even and } p(\tilde{I}) < 2n, \\ \frac{1}{\xi(p_n)}\Theta_1(\tilde{I}), & \text{if } p_n \text{ is even and } p(\tilde{I}) = 2n, \\ \frac{1}{p_n!}\Theta_1(\tilde{I}), & \text{if } p_n \text{ is even and } p(\tilde{I}) > 2n. \end{cases}$$

If we have a sequence of the form $I = 0^{p_0}$, then (35) from [3] gives us that

$$\Theta_1(0^{p_0}) = \begin{cases} \dfrac{1}{p_0!}, & \text{if } p_0 \text{ is odd,} \\ \dfrac{1}{\xi(p_0)}, & \text{if } p_0 \text{ is even and positive,} \\ 0, & \text{if } p_0 = 0. \end{cases}$$

For example, let's say that we have $I = 2, 2, 2, 2, 1, 0$, i.e. we are considering the terms $L_{2,2,2,2,1,0}(G)_{0+2}$ and $L_{2,2,2,2,1,0}(G)_1$, and we want to calculate $\Theta_{0+2}(I)$ and $\Theta_1(I)$.

From the formulas above,

$$\Theta_{0+2}(2,2,2,2,1,0) = \frac{1}{4!}\Theta_{0+2}(1,0) = \frac{1}{4!\xi(1)}\Theta_1(0) = \frac{1}{4!\xi(1)1!} = \frac{1}{48}.$$

On the other hand

$$\Theta_1(2,2,2,2,1,0) = \frac{1}{4!}\Theta_1(1,0) = \frac{1}{4!1!}\Theta_{0+2}(0) = \frac{1}{4!1!1!} = \frac{1}{24}.$$

(The first step above gives a $1/4!$ since, even though there are an even number of 2's, $p(1,0) = 6 > 2 \cdot 2$.)

3.6 The coefficients $C^{(2)}$ and $C^{(3)}$

In this section, we summarize the steps needed to compute $C^{(q)}$, and compute the coefficients $C^{(2)}, C^{(3)}$ explicitly. First, we reproduce (11), noting that we can simplify because we have chosen all $\Theta_{0+2}(I)$ to be 0 when $I \notin \mathcal{I}^q_{0+2}$, and so we get

$$C^{(q)} = \sum_{p(I)=2(q-1)} (-1)^q 4\Theta_{0+2}(I)C_I. \tag{36}$$

Now, to compute $C^{(q)}$ using (36), we first need to find all I such that $p(I) = 2(q-1)$. Recall that $p(I) = 2\sum_k (I_k + 1)$ where I_k are the entries of I. One this set of I has been found, we then compute C_I and $\Theta_{0+2}(I)$ for each I.

First, we compute $C^{(2)}$. The only I for which $p(I) = 2$ is $I = 0$, so the sum in (36) has only one term with $I = 0$, and we have

$$C^{(2)} = 4\Theta_{0+2}(0)C_0 = 2C_0.$$

Using (25) we calculate that

$$C_0 = \frac{-1}{2\sqrt{\pi}} \int_0^\pi \tilde{b} L_\eta^{-1}(b_0)\, d\eta.$$

To calculate b_0, recall that there is only one multiindex I with $p(I) = 0$, that is, $I = \emptyset$. So, using (33) and (30), we have that

$$b_0 = \mathcal{F}^{-1} 4Q_\emptyset = -\frac{1}{\sqrt{\pi}}\tilde{b},$$

and thus

$$C^{(2)} = -\frac{1}{\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b})\, d\eta.$$

We can also write this as

$$C^{(2)} = -\frac{1}{\pi \hat{b}(0)^2}\int_0^\pi (b(\eta) - \hat{b}(0)) L_\eta^{-1}(b(\eta) - \hat{b}(0))\, d\eta.$$

This will be positive for any $b(\eta)$, since L_η^{-1} is negative definite.

Now we compute $C^{(3)}$. We know that

$$C^{(3)} = \sum_{p(I)=4} -4\Theta_{0+2}(I) C_I,$$

and we only have two multiindices contributing to this sum, 00 and 1.

We know from the formulas that C_{00} is the coefficient which arises from the term $L_0^2(H_2^0)$, and C_1 is the coefficient that arises from $L_1(H_1^0)$. We claim that we can make our calculation simpler, because by a happy coincidence, $L_0^2(H_2^0) = L_1(H_1^0)$. This is because of the following: Since $D_{i,kl} = 4d^2\omega_{k0} H^i_{1,\mathrm{low},kl}/\lambda_l$, and

$$L_i(L_I(G)_1)_{0,k00} = \sum_{l>0} L_I(G)_{1,kl0} D_{i,kl},$$

it is clear from inspection that $L_j(H^i_{1,\mathrm{low}}) = L_i(H^j_{1,\mathrm{low}})$. We also note that $H^0_{1,\mathrm{low}} = H^0_1$ and $H^1_{1,\mathrm{low}} = L_0(H^0_2)$, and thus $L_1(H^0_{1,\mathrm{low}}) = L_0(H^0_{1,\mathrm{low}})$, or

$$L_{00}(H_2^0) = L_1(H_1^0).$$

Then we know that

$$C^{(3)} = -4\left(\Theta_{0+2}(00) C_{00} + \Theta_{0+2}(1) C_1\right).$$

Since $\Theta_{0+2}(00) = \Theta_{0+2}(1) = 1/2$, we have that $C^{(3)} = -4C_{00}$. Using (15), (31) and Appendix A of [3], we can calculate that

$$\begin{aligned} C_{00} &= \frac{1}{2}\int_0^\pi \tilde{b} L_\eta^{-1}(b_0)\, L_\eta^{-1}(b_0) \\ &= \frac{1}{2\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b}) L_\eta^{-1}(\tilde{b})\, d\eta, \end{aligned}$$

and thus

$$C^{(3)} = -\frac{2}{\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b}) L_\eta^{-1}(\tilde{b})\, d\eta.$$

4 Numerical Simulation of the PDE

4.1 Numerical efficiency

Here we compare the numerical efficiency of the two methods of computing a solution. Given an equation of the form (1), we can solve (1) directly, or solve its approximation (4). A reasonable question to ask is, how much more efficient is the algorithm that computes the reduced equation versus the full equation? This is not as clear as it first seems. Although the reduced equation is posed on a lower dimensional space, it is of higher order, and it could be true that needing to choose smaller timesteps for the purposes of stability could overwhelm the gains made by being on a lower-dimensional space.

We will consider this question for the simplest case consistent with the PDE posed in (1). We will assume that ω is a rectangle, and thus Ω is a thin rectangular prism. To compute the numerical approximation for (1), we have to choose $\Delta t = \mathcal{O}(\Delta y)$ to ensure numerical stability. Assume that we choose a grid which is uniform in the dimensionless variables, so that $\Delta x_1 = \Delta x_2 = \pi/N$, and $\Delta y = d\pi/N$. We can see that to compute any step in the numerical approximation, we need to do $\mathcal{O}(N^3)$ operations. Since we must choose $\Delta t = \mathcal{O}(\Delta y) = \mathcal{O}(d/N)$, to compute (1) until time T directly, we need to do $\mathcal{O}(N^4/d)$ operations.

On the other hand, if we want to compute (4) directly, we are given the n CFL conditions

$$\Delta t = \mathcal{O}\left(\max_{i=1,\ldots n} d^{1-i}\Delta x^i\right).$$

Now, as the solution is stated in [3], we chop off the modes with wavenumber greater than d^α (for some $-1/2 < \alpha < 0$) in the initial condition. Thus it is reasonable to consider grid-sizes in the x direction with $\Delta x > d^{-\alpha}$. Then, for each CFL condition we have

$$\begin{aligned} d^{1-i}(\Delta x)^i &\geq \Delta x(\Delta x/d)^{i-1} \geq \Delta x d^{-(1+\alpha)(i-1)} \\ &\geq \Delta x d^{-\frac{1}{2}(i-1)} \geq \Delta x. \end{aligned}$$

Thus we see that the most restrictive condition is $\Delta t = \mathcal{O}(\Delta x)$. If we want to compute until a fixed time T, the simulation of the reduced problem requires $\mathcal{O}(N^3)$ operations, and the simulation of the full problem requires $\mathcal{O}(N^4/d)$ operations.

Contrasting the two algorithms, we see, first of all, that the algorithm that approximates the reduced PDE is superior in that it is one order better in N. In fact, the difference is even more pronounced, since the full problem is stiff in the sense that as $d \to 0$, we need to resolve the grid more finely to get resolution in the thin direction, but there is no small parameter in the reduced equation, and simulating it is independent of d.

4.2 Some example reduced equations

In the problem described in [3], we were working on a domain of the form $\Omega = \omega \times [0, \pi d]$, where ω was a two-dimensional domain. We can work out an exactly analogous theory if we assume instead that ω is simply the one-dimensional interval $[0, \pi]$. It turns out that all of the estimates, and even all of the formulas, are exactly the same, as long as we redefine L_x appropriately, i.e. we define

$$L_x = \frac{\partial}{\partial x}\left(c(x)\frac{\partial}{\partial x}\right) \tag{37}$$

for some *scalar* function $c(x)$, and thus our full PDE is

$$u_{tt} = \frac{\partial}{\partial y}\left(a(y/d)\frac{\partial u}{\partial y}\right) + b(y/d)\frac{\partial}{\partial x}\left(c(x)\frac{\partial u}{\partial x}\right), \tag{38}$$

and the reduced PDE can still be written as

$$u_{tt} = L_x u + \sum_{q=2}^{n} C^{(q)} d^{2(q-1)} L_x^q u, \tag{39}$$

where we have redefined L_x as in (37).

In this section, we assume that we have chosen $a = 1, c = 1$ in (38). We will pick three different choices of the function b. In each case, we will derive the reduced equation up to the third (L_x^3) term.

We note here that the numerical evidence suggests even more than has been proved. Theorem 1 of [3] says that the successive approximating reduced equations will afford a good approximation for longer intervals of time, but the numerical evidence suggests that they also afford qualitatively better approximations over the intervals on which they are valid.

4.2.1 The case $b = 1$

In this case, the PDE (1) is in the form

$$u_{tt} = u_{yy} + L_x u,$$

which is simply the standard two-dimensional wave equation. There is no interaction between the x and y derivatives. We can see by inspection that there is no coupling when, using the notation of [3], we go to discrete variables, i.e. that $\Gamma_{k,l,l'} = 0$ for all $l, l' > 0$. In this case, we would expect that the reduced PDE

$$u_{tt} = L_x u$$

would afford as good an approximation as possible. This is because any energy we start with in the $l > 0$ modes will stay there for all time. We now compute the coefficients and show that this heuristic argument is true.

By inspection, we can see that $b_0 = b_1 = 0$, from the formulas in (30) and (31). From this it is clear that for any $I = 1^n 0^m$, we have that $Q_I = 0$. But since $Q_1, Q_{00} = 0$, we know that $b_2 = 0$. This implies that for all $I = 2^n 1^m 0^p$, $Q_I = 0$. Proceeding through this inductively, we can show that $b_i = 0$ for all i, and from the formula in Theorem 1, this means that $C_I = 0$ for all I, and thus $C^{(q)} = 0$ for all $q \geq 2$. This means that the reduced PDE affords a good approximation for any timescale that we would desire.

In Figure 1, we show some numerical evidence for this. What we did was numerically simulate the two equations

$$u_{tt} = u_{yy} + L_x u, \tag{40}$$

and

$$u_{tt} = L_x u. \tag{41}$$

We took the solution of (41) and multiplied by $\mathbf{1}(y)$, and compared the $H^1 \times L^2$ norm of the difference of the two solutions. Below, we will refer to this as the "energy of the error". Figure 1 is a time-series of this error. As we describe above, we analytically expect this to be 0 for all time, and up to numerical error, this is what we get.

4.2.2 The case $b = 1 + \cos(\eta)/10$

We use the formulas in Section 3.6. We know that

$$C^{(2)} = -\frac{1}{\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b})\, d\eta,$$

and

$$C^{(3)} = -\frac{2}{\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b}) L_\eta^{-1}(\tilde{b})\, d\eta.$$

From the definition of $\tilde{b}$, we have that

$$\tilde{b} = \frac{1}{10}\cos(\eta).$$

Thus

$$C^{(2)} = -\frac{1}{\pi}\int_0^\pi -\frac{1}{100}\cos^2(\eta)\, d\eta = \frac{1}{200},$$

and

$$C^{(3)} = -\frac{2}{\pi}\int_0^\pi \frac{1}{10}\cos(\eta)\frac{-1}{10}\cos(\eta)\frac{-1}{10}\cos(\eta)\, d\eta = 0.$$

Thus we expect that the reduced PDE

$$u_{tt} = L_x u + \frac{1}{200} d^2 L_x^2 u$$

affords a good approximation to (1) for timescales of $\mathcal{O}(d^{-6})$. This is because, since $C^{(3)} = 0$, the second approximating equation is really also the third.

For the numerical simulations, we simulated

$$u_{tt} = u_{yy} + b(\eta) L_x u, \tag{42}$$

and the two reduced equations

$$u_{tt} = L_x u, \tag{43}$$

and

$$u_{tt} = L_x u + C^{(2)} d^2 L_x^2 u. \tag{44}$$

As we stated above, we expect that (44) will afford a much better approximation to (42) than (43) would. The first figure, Figure 2, shows two time-series. The first is the energy of the error between the solutions to (42) and (43). The second is the energy of the error between the solutions to (42) and (44). In both cases, we fixed $d = 0.01$. As we expect, the error is much smaller in the second case. Note the scales on both graphs; the error in the second case is about 10^{-4} times that in the first.

The next figure, Figure 3, again shows the difference between the two approximations. Each picture shows the energy of the error at three selected times, and for four different values of d. In each picture, we compute the error at $T = 10^5$ (cross), $T = 5 * 10^5$ (circle), and $T = 10^6$ (star). We see that the error at any fixed time gets smaller as d does, and the line in each picture shows which power law the error follows. This is evidence that the error at fixed time goes to 0 like d^2 for the first approximating equation, and like d^6 for the second. The reason that we would expect the error to go like d^6 for the second approximation is, again, the second approximating equation is actually also the third approximating equation, since $C^{(3)} = 0$.

4.2.3 The case $b = 1 + (\eta - \pi/2)/10 + (\eta - \pi/2)^3/10$

As before, we use the formulas

$$\begin{aligned} C^{(2)} &= -\frac{1}{\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b})\, d\eta, \\ C^{(3)} &= -\frac{2}{\pi}\int_0^\pi \tilde{b} L_\eta^{-1}(\tilde{b}) L_\eta^{-1}(\tilde{b})\, d\eta, \end{aligned}$$

where $\tilde{b} = (\eta - \pi/2)/10 + (\eta - \pi/2)^3/10$. Numerically evaluating the integrals in these expressions one finds that $C^{(2)} = 0.0474808$ and $C^{(3)} = -0.0304309$.

For the numerical simulations, we simulated

$$u_{tt} = u_{yy} + b(\eta) L_x u, \tag{45}$$

and the three reduced equations

$$\begin{aligned} u_{tt} &= L_x u, && (46) \\ u_{tt} &= L_x u + C^{(2)} d^2 L_x^2 u, && (47) \\ u_{tt} &= L_x u + C^{(2)} d^2 L_x^2 u + C^{(3)} d^4 L_x^3 u. && (48) \end{aligned}$$

As we have proved, each successive approximating equation should afford a better approximation to the solution of (42). The next figures suggest that this is true.

In Figure 4, we have three time-series. Each is the energy of the error between (45) and one of the reduced equations. As predicted, when we add an additional term in the approximating equation, we get a much better approximation.

As we did before for Equation #2, we also compute the error at a selection of three different times, $T = 10^5$ (cross), $T = 5*10^5$ (circle), and $T = 10^6$ (star). This is shown in Figure 5. Again, we insert a line to show what power law the error observes. This is evidence that the error at fixed time goes like d^2 for the first approximation, like d^4 for the second, and like d^6 for the third.

Acknowledgments: Many of these results originally appeared in the author's Ph.D. thesis at Boston University. The research of the author was supported in part by the National Science Foundation through grant DMS-9803164 and also supported in the VIGRE program under National Science Foundation grant DMS-9983646.

References

[1] I. Babuška and C. Schwab. A posteriori error estimation for hierarchic models of elliptic boundary value problems on thin domains. *SIAM Journal on Numerical Analysis*, 33(1):221–246, 1996.

[2] R. E. Lee DeVille. *Reduced Equations for Hyperbolic Problems on Thin Domains*. PhD thesis, Boston University, May 2001.

[3] R. E. Lee DeVille and C. Eugene Wayne. Reduced equations for models of laminated materials in thin domains. I. To appear in *Asymptotic Analysis*.

[4] C. Schwab. A posteriori modeling error estimation for hierarchic plate models. *Numer. Math.*, 74(2):221–259, 1996.

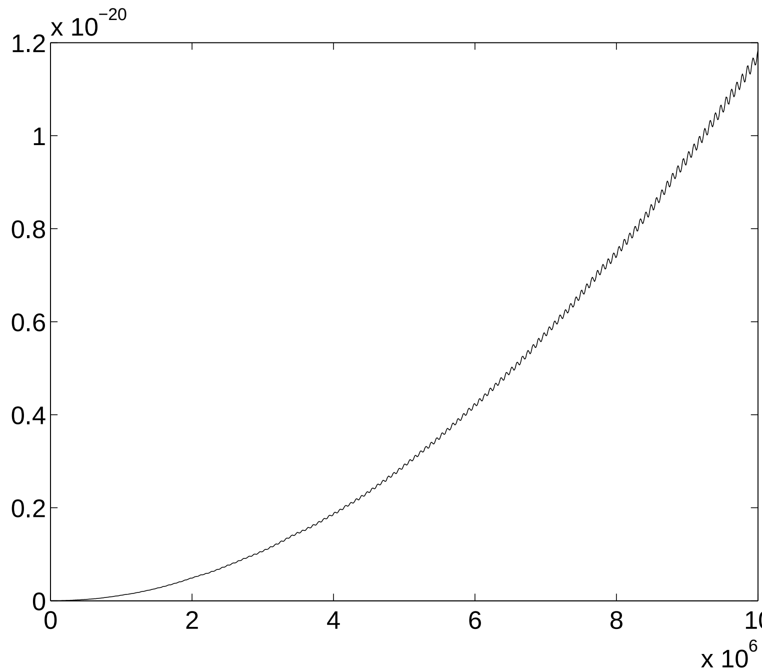

Figure 1: Energy of error vs. time for Equation #1

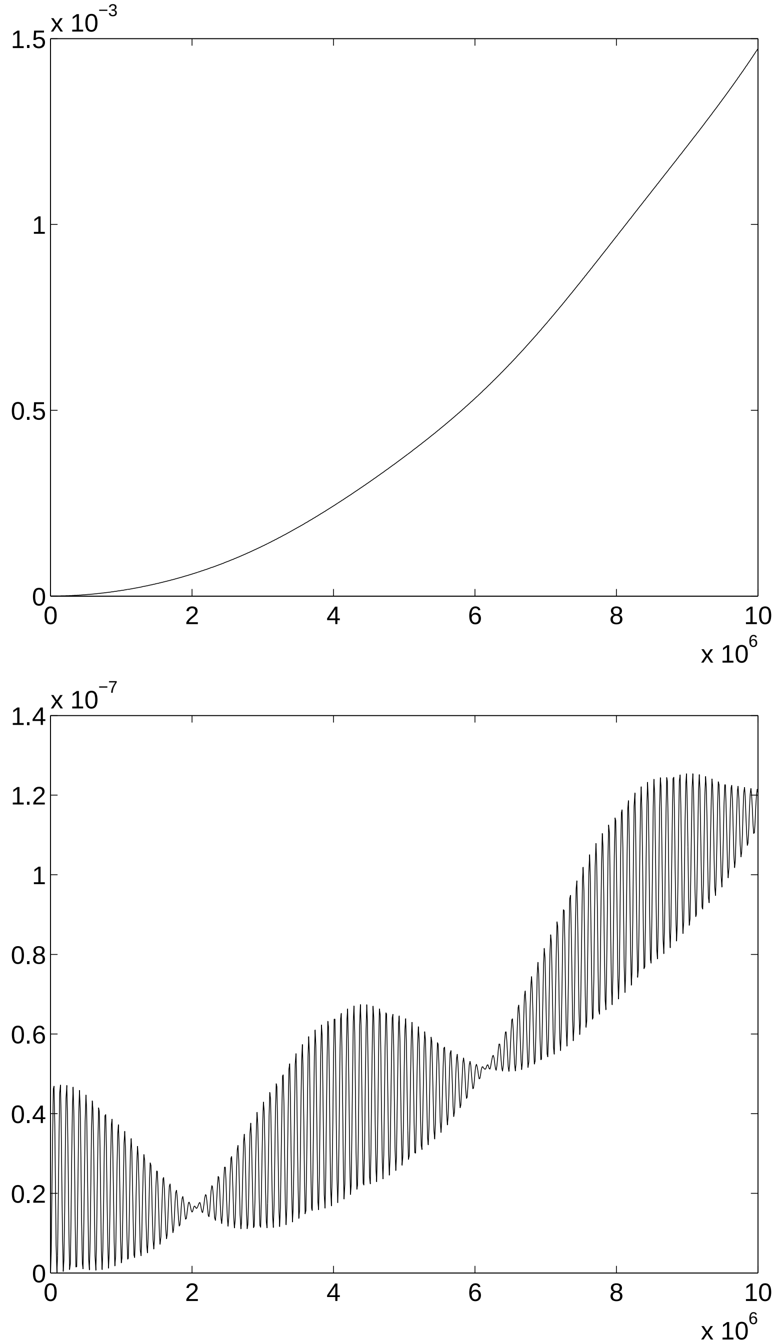

Figure 2: Energy of error vs. time for Equation #2, for two different approximating equations

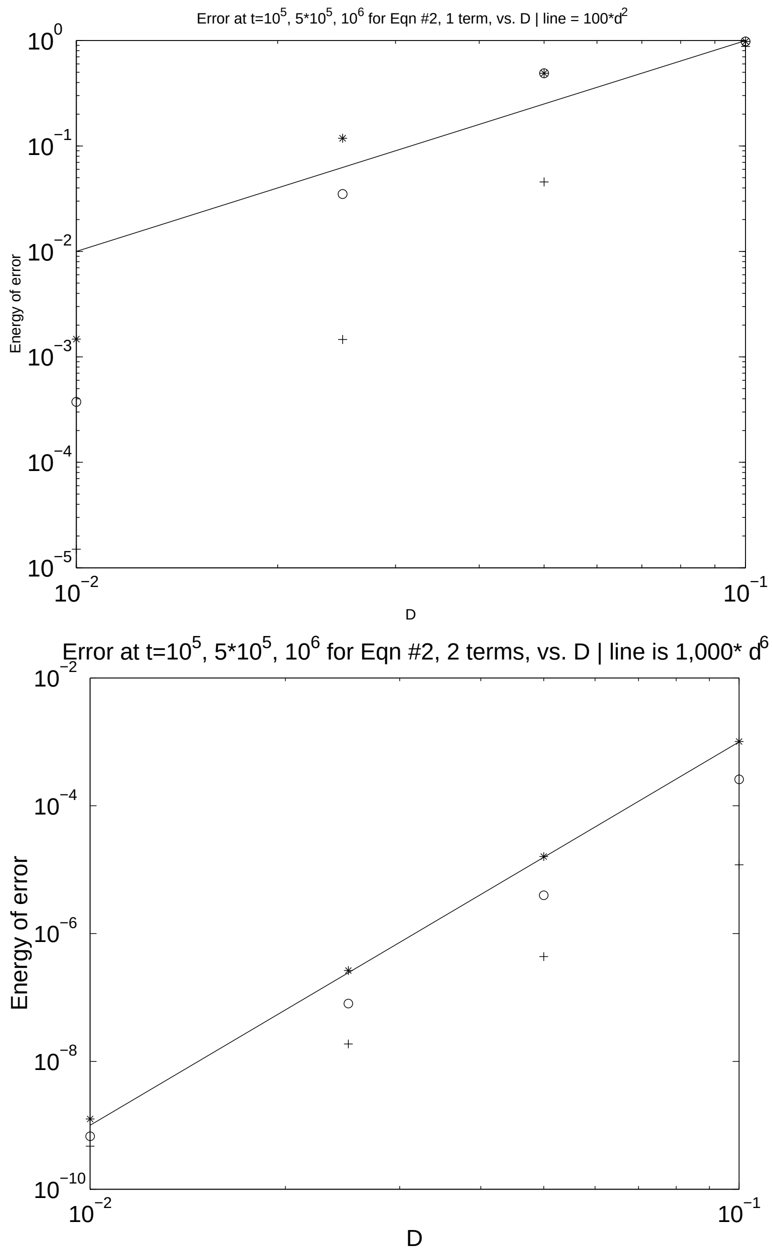

Figure 3: The power law of the error for Equation #2, for two different approximating equations

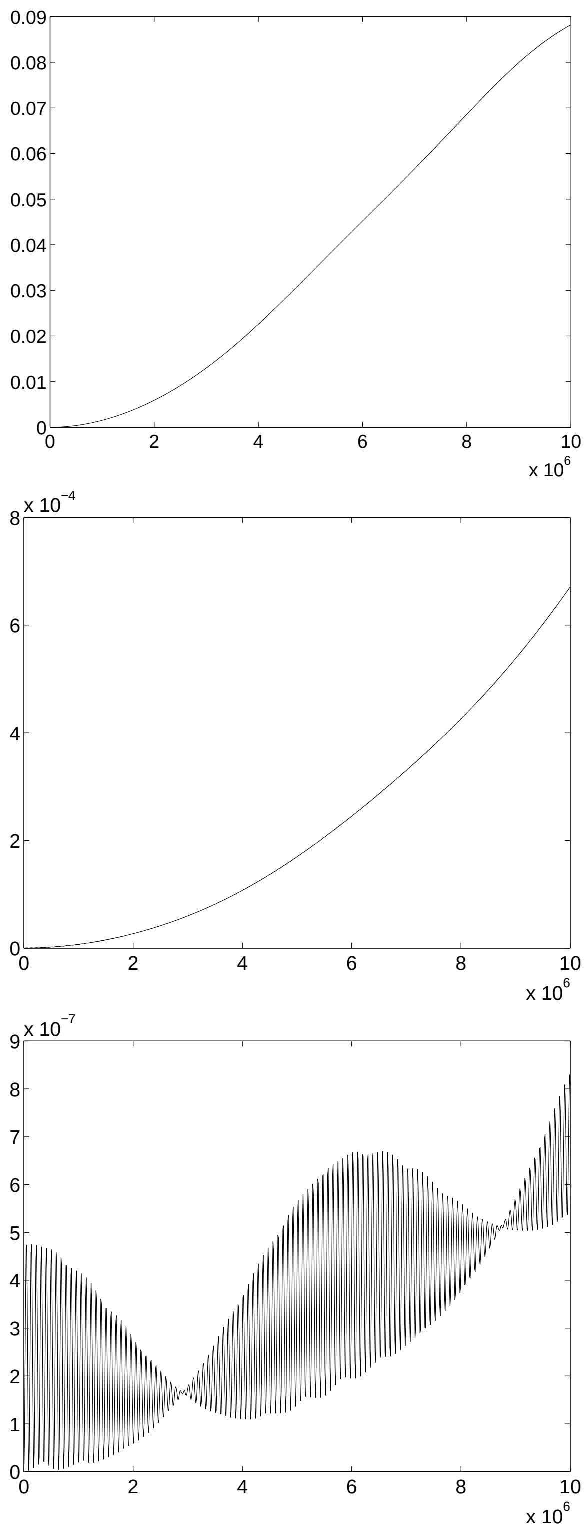

Figure 4: Energy of error vs. time for Equation #3, for three different approximating equations

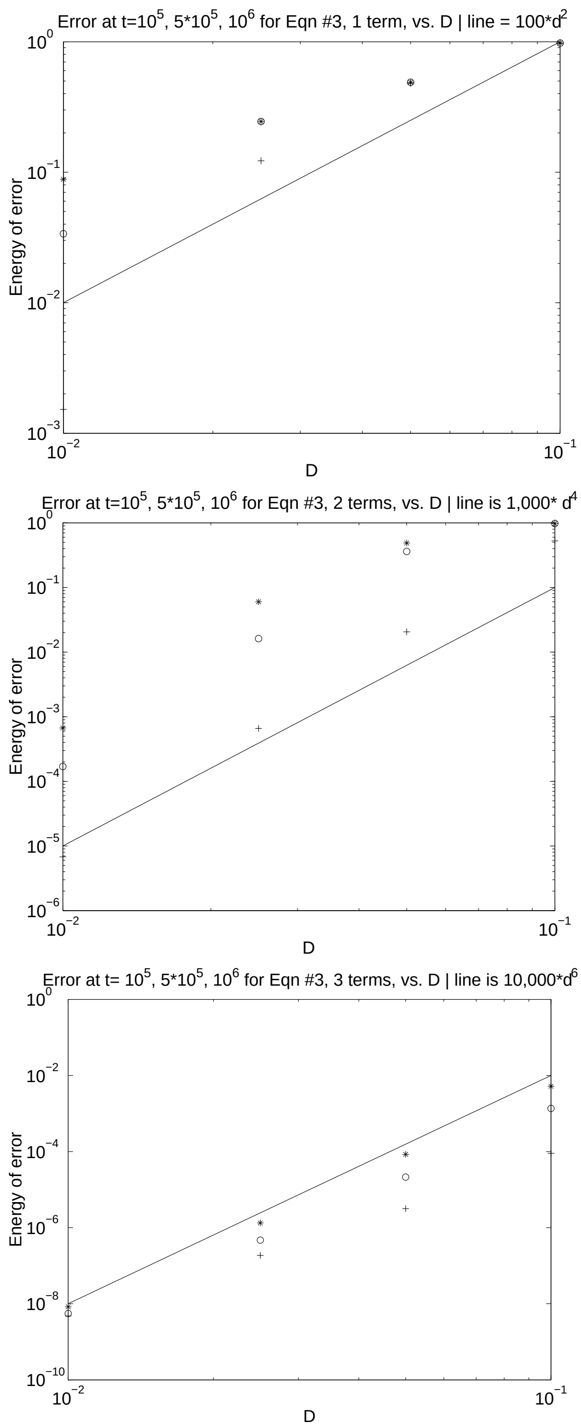

Figure 5: The power law of the error for Equation #3, for three different approximating equations