Numerical solutions to an inverse problem for a non-linear Helmholtz equation

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Abstract

In this work, we develop numerical methods to solve forward and inverse wave problems for a nonlinear Helmholtz equation defined in a spherical shell between two concentric spheres centred at the origin. A spectral method is developed to solve the forward problem while a combination of a finite difference approximation and the least squares method are derived for the inverse problem. Numerical examples are given to verify the method.

Contents

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1 Introduction

The nonlinear Helmholtz equation models the propagation of electromagnetic waves in Kerr media, and describes a range of important phenomena in nonlinear optics and in other areas [3, 4, 2]. In this article, we consider forward and inverse problems regarding the following nonlinear Helmholtz equation in $\mathbb{R}^3$:

$$\Delta U(\boldsymbol{x}) + k^2 \nu(\boldsymbol{x}) U(\boldsymbol{x}) = -\epsilon(\boldsymbol{x}) F(|U(\boldsymbol{x})|^2) U(\boldsymbol{x}) \,, \quad \boldsymbol{x} \in \Omega \subset \mathbb{R}^3 \,, \qquad (1)$$

where $\boldsymbol{x} = (x_1, x_2, x_3)$ are the spatial coordinates, $U = U(\boldsymbol{x})$ denotes the scalar electric field, $|\cdot|$ denotes the Euclidean norm, $\Delta = \partial^2_{x_1} + \partial^2_{x_2} + \partial^2_{x_3}$ is the Laplacian operator, and $\nu(\boldsymbol{x})$ and $\epsilon(\boldsymbol{x})$ are some functions.

For simplicity, we consider the case where Ω is a spherical shell between two concentric spheres of radii R_0 and R_1 centred at the origin; that is

$$\Omega := \{\boldsymbol{x} \in \mathbb{R}^3 : R_0 \leqslant |\boldsymbol{x}| \leqslant R_1\} \,.$$

We also assume that ν and ϵ are radially symmetric and that U satisfies the axially symmetric boundary conditions

$$U|_{r=R_0} = H(t) \,, \quad \left.\frac{\partial U}{\partial r}\right|_{r=R_0} = G(t) \,, \quad -1 \leqslant t \leqslant 1 \,, \qquad (2)$$

where $r = |\mathbf{x}|$ and $t = \cos\theta$, with θ being the polar angle measured from the north pole. The solution U is then axially symmetric as well. Equation (1) now takes the form

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(rU(r,t))+\frac{1}{r^2}\mathcal{L}U(r,t)+k^2\nu(r)U(r,t) = -\epsilon(r)F(|U(r,t))|^2)U(r,t)\,, \quad (3)$$

where $\mathcal{L}$ is the Legendre differential operator defined in equation (5).

In the forward problem, U is unknown, F is non-linear, for example $F(|U|^2) = |U|^{2p}$ with some integer p, or $F = \sin(|U|^2)$, and we find an approximation of U. In the inverse problem, the values of the solution $U(\mathbf{x}_q)$, for $q = 1, \ldots, Q$ are known, and the problem is to approximate the unknown nonlinear function F.

The article is organized as follows. In Section 3 we introduce a spectral method for the forward problem and a fast algorithm to evaluate the non-linear term. In Section 4 we describe an algorithm for the inverse problem to identify the nonlinearity of the function F via its Chebyshev coefficients. The article is concluded with some numerical experiments described in Section 5.

2 Background

The Legendre polynomial P_ℓ is a polynomial of degree ℓ with leading coefficients. We have the orthogonality relation

$$\int_{-1}^{1} P_\ell(t)P_{\ell'}(t)\,dt = \frac{2\ell+1}{2}\delta_{\ell,\ell'}\,. \quad (4)$$

The polynomials P_ℓ for $\ell = 0, 1, \ldots$ satisfy

$$\mathcal{L}P_\ell(t) = (1-t^2)P_\ell''(t) - 2tP_\ell'(t) = -\lambda_\ell P_\ell(t) \quad \text{where } \lambda_\ell = \ell(\ell+1)\,. \quad (5)$$

The Fourier–Legendre coefficients of an integrable function $g : [-1, 1] \to \mathbb{R}$ are defined by

$$\hat{g}(\ell) = \int_{-1}^{1} g(t)P_\ell(t)\,dt\,, \quad \ell \in \mathbb{Z}_+\,, \quad (6)$$

To compute the Fourier–Legendre coefficients of the product of two functions

$$\widehat{g_1 g_2}(\ell) = \int_{-1}^{1} g_1(t) g_2(t) P_\ell(t)\,dt\,, \quad \ell \in \mathbb{Z}_+\,, \tag{7}$$

we define

$$\Gamma(L;\ell,\ell') = \frac{2L+1}{2} \int_{-1}^{1} P_L(t) P_\ell(t) P_{\ell'}(t)\,dt\,. \tag{8}$$

It is known that $0 \leqslant \Gamma(L;\ell,\ell') \leqslant 1$ and $\sum_{L=0}^{\ell+\ell'} \Gamma(L;\ell,\ell') = 1$ [1, Chapter 5]. Then, the following formal equation holds:

$$\widehat{g_1 g_2}(L) = \sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} \Gamma(L;\ell,\ell') \hat{g}_1(\ell) \hat{g}_2(\ell')\,. \tag{9}$$

In terms of the sequences of Fourier–Legendre coefficients, we denote

$$(\hat{g}_1 \star \hat{g}_2)(L) = \sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} \Gamma(L;\ell,\ell') \hat{g}_1(\ell) \hat{g}_2(\ell')\,. \tag{10}$$

3 Spectral method for the forward problem

In this section, we discuss how to construct a numerical solution to (1). For this purpose, we first establish some notations.

The spectral method for the forward problem approximates the exact solution U by

$$U_N(r,t) = \sum_{\ell=0}^{N} u_\ell(r) P_\ell(t)\,, \quad u_\ell(r) = \widehat{u(r,\cdot)}(\ell)\,, \tag{11}$$

and finds the coefficients $u_\ell(r)$ so that U_N satisfies (3). By substituting U_N into (3), we deduce using (5) that

$$\frac{2}{2\ell+1}\left(\frac{1}{r}\frac{d^2}{dr^2}(r u_\ell) - \frac{\lambda_\ell}{r^2} u_\ell + k^2 \nu(r) u_\ell\right) = -\epsilon(r)\mathcal{F}_\ell\,, \tag{12}$$

where

$$\mathcal{F}_\ell = \mathcal{F}_\ell(r) = \int_{-1}^{1} U_N(r,t)F(|U_N(r,t)|^2)P_\ell(t)\,dt\,. \tag{13}$$

Equivalently,

$$\frac{d^2}{dr^2}(ru_\ell) = \frac{\lambda_\ell}{r}u_\ell - rk^2\nu u_\ell - r\epsilon(r)(\ell+1/2)\mathcal{F}_\ell\,. \tag{14}$$

Comparing (6) and (13) shows that $\mathcal{F}_\ell$ is the Fourier–Legendre coefficient of $U_N(r,t)F(|U_N(r,t)|^2)$. Clearly, there exist α and β such that $|U_N|^2 \in [\alpha, \beta]$. We assume α and β to be known. Our strategy is to approximate F using its Fourier–Chebyshev expansion:

$$F(|U_N|^2) \approx \mathcal{P}_d\left(\frac{2|U_N|^2-\alpha-\beta}{\beta-\alpha}\right) = \sum_{k=0}^{2^d-1} a_k T_k\left(\frac{2|U_N|^2-\alpha-\beta}{\beta-\alpha}\right), \tag{15}$$

where T_k is the Chebyshev polynomial defined by $T_k(\cos\phi) = \cos(k\phi)$. The use of Chebyshev polynomials facilitates the use of recurrence relations (22) leading to an algorithm with logarithmic complexity. We need to evaluate the Fourier–Legendre coefficients $\mathcal{F}_\ell$ of $U_N F(|U_N|^2)$ in terms of a_k. In Section 6, we describe a general procedure to accomplish this task efficiently.

Towards the goal of evaluating Fourier–Legendre coefficients, we note first using (9) that

$$\begin{aligned} |U_N|^2(t) &= \left(\sum_{\ell=0}^{N} u_\ell P_\ell(t)\right)^2 = \sum_{L=0}^{2N} d_L P_L(t)\,, \quad d_L = (\{u_\ell\} \star \{u_\ell\})(L)\,, \\ \frac{2|U_N(t)|^2-\alpha-\beta}{\beta-\alpha} &= \frac{1}{\beta-\alpha}\left\{(2d_0-\alpha-\beta)P_0(t) + 2\sum_{L=1}^{2N} d_L P_L(t)\right\}. \end{aligned} \tag{16}$$

Similarly,

$$|U_N|^2 U_N = \left(\sum_{\ell=0}^{2N} d_\ell P_\ell(t)\right)\left(\sum_{\ell'=0}^{N} u_{\ell'} P_{\ell'}(t)\right)$$

$$= \sum_{L=0}^{3N} c_L P_L(t)\,, \quad c_L = (\{d_\ell\} \star \{u_\ell\})(L)\,. \tag{17}$$

By comparing (17) with (13) we also have $c_L = \frac{2L+1}{2}\mathcal{F}_L$.

We convert the system of second order ODEs (14) to first order ODEs as follows. For $\ell = 0, \dots, N$ let $v_\ell = \frac{d(ru_\ell)}{dr}$, then the boundary conditions are

$$v_\ell(R_0) = u_\ell(R_0) + R_0 \left.\frac{du_\ell}{dr}\right|_{r=R_0} = h_\ell + R_0 g_\ell\,,$$

where $h_\ell := \widehat{H}(\ell)$ and $g_\ell := \widehat{G}(\ell)$ are the Fourier–Legendre coefficients of the boundary conditions given in (2).

Let

$$\vec{Z} = \begin{bmatrix} Z_1 & Z_2 & \cdots & Z_{2N+2} \end{bmatrix}^\top = \begin{bmatrix} ru_0 & ru_1 & \cdots & ru_N & v_0 & v_1 & \cdots & v_N \end{bmatrix}^\top$$

We re-write the above system into the form $d\vec{Z}/dr = \mathfrak{F}(r, \vec{Z})$ with

$$\mathfrak{F}(r, \vec{Z}) = \begin{bmatrix} Z_{N+2} \\ Z_{N+3} \\ \vdots \\ Z_{2N+2} \\ \frac{\lambda_0}{r^2} Z_1 - k^2 \nu(r) Z_1 - r\epsilon(r)(0 + 1/2)\mathcal{F}_0 \\ \frac{\lambda_1}{r^2} Z_2 - k^2 \nu(r) Z_2 - r\epsilon(r)(1 + 1/2)\mathcal{F}_1 \\ \vdots \\ \frac{\lambda_L}{r^2} Z_{N+1} - k^2 \nu(r) Z_{N+1} - r\epsilon(r)(L + 1/2)\mathcal{F}_N \end{bmatrix}$$

and initial condition

$$\begin{aligned} Z(R_0) &= \begin{bmatrix} ru_0(R_0) & ru_1(R_0) & \cdots & ru_N(R_0) & v_0(R_0) & v_1(R_0) & \cdots & v_N(R_0) \end{bmatrix} \\ &= \begin{bmatrix} R_0 h_0 & R_0 h_1 & \cdots & R_0 h_N & h_0 + R_0 g_0 & h_1 + R_0 g_1 & \cdots & h_N + R_0 g_N \end{bmatrix}. \end{aligned}$$

We may now use standard ODE solvers. In our experiments we used the adaptive solver `ode45` in Matlab.

4 The inverse problem

For the inverse problem, the values $U(r_i)$ are known on the collection of points $\mathcal{R} := \{r_i : i = 1, \ldots, M\}$ which might not be equally spaced on the interval $[R_0, R_1]$ since they might come from an adaptive ODE solver. The corresponding values $u_\ell(r_j)$ are computed using numerical integration. In our numerical experiments, we extract u_ℓ directly from the numerical solutions of the ODE solver.

Our approach is to evaluate $\mathcal{F}_\ell$ first using (12). In turn, this requires computing the second derivative of ru_ℓ at $r = r_j$ for non-equidistant values r_j. These are computed by

$$\frac{d^2}{dr^2}(ru_\ell(r))\bigg|_{r=r_j} \approx \frac{h_j^- r_{j+1} u_\ell(r_{j+1}) + h_j^+ r_{j-1} u_\ell(r_{j-1}) - (h_j^+ + h_j^-) r_j u_\ell(r_j)}{0.5 h_j^- h_j^+ (h_j^+ + h_j^-)},$$

with $h_j^+ = r_{j+1} - r_j$ and $h_j^- = r_j - r_{j-1}$. We then compute the approximated $\mathcal{F}_\ell$ at $r = r_j$ via

$$\mathcal{F}_\ell = \frac{-2}{(2\ell+1)\epsilon(r)} \left(\frac{1}{r} \frac{d^2}{dr^2}(ru_\ell) - \frac{\lambda_\ell}{r^2} u_\ell + k^2 \nu(r) u_\ell \right).$$

The next task is to approximate F from $\mathcal{F}_\ell$. Since we know $\mathcal{F}_\ell$, this leads to a (not necessarily square) system of linear equations. In turn, a_k in (15) is determined using a least squares computation. Thus, the problem reduces to computing a_k using the expansion (16).

5 Numerical experiments

The expansion of a plane wave is given by Morse and Ingard [5]

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell P_\ell(\widehat{\mathbf{k}} \cdot \widehat{\mathbf{r}}) j_\ell(kr), \tag{18}$$

where $\widehat{\mathbf{k}} = \mathbf{k}/\|\mathbf{k}\|$, $\widehat{\mathbf{r}} = \mathbf{r}/\|\mathbf{r}\|$, $P_\ell(t)$ is the Legendre polynomial of degree ℓ and $j_\ell(kr)$ is the ℓth spherical Bessel function of the first kind. Here $\mathbf{r}$ is the position vector of length r, $\mathbf{k}$ is the wave vector of length k. In the special case when $\mathbf{k}$ is aligned with the z-axis, we have

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell P_\ell(\cos\theta) j_\ell(kr) ,$$

where θ is the spherical polar angle of $\mathbf{r}$. With $t = \cos\theta$, we have $H(t) = e^{ikR_0 t}$ and

$$h_\ell = (2\ell+1) i^\ell j_\ell(kR_0) ,$$

and by using the identity $\frac{d}{dz} j_\ell(z) = j_{\ell-1}(z) - \frac{(\ell+1)}{z} j_\ell(z)$, we have

$$g_\ell = (2\ell+1) i^\ell \left. \frac{d j_\ell(kr)}{dr} \right|_{r=R_0} = (2\ell+1) i^\ell \frac{1}{k} \left(j_{\ell-1}(kR_0) - \frac{\ell+1}{kR_0} j_\ell(kR_0) \right) .$$

5.1 Experiment 1

We consider the forward problem

$$\Delta U(\mathbf{x}) + k^2 \nu U(\mathbf{x}) = -\epsilon |U(\mathbf{x})|^4 U(\mathbf{x}) , \tag{19}$$

where k, ν and ϵ are positive constants on the spherical shell Ω with inner radius $R_0 = 1$ and outer radius $R_1 = 2$. The boundary conditions on the inner sphere are

$$U(R_0) = e^{ikR_0 t} , \quad \frac{\partial U}{\partial r} = \frac{\partial}{\partial r} e^{ikrt}|_{r=R_0} , \quad t = \cos\theta .$$

The numerical solution $U(R_1)$ of the forward problem is given in the left panel of Figure 1.

We now consider the inverse problem. On the right-hand side, in our framework $F(|U|^2) = |U|^4$, so $F(t) = t^2$. In terms of a linear combination of Chebyshev polynomials T_0 and T_2:

$$F(t) = \frac{1}{2} T_0(t) + \frac{1}{2} T_2(t) .$$

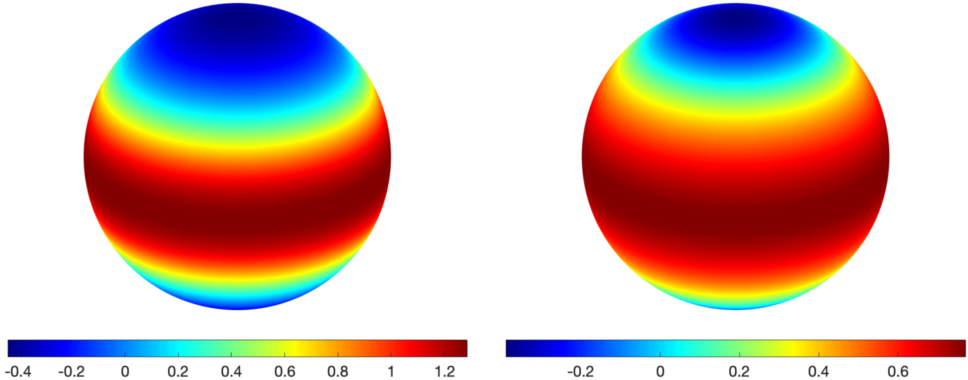

Figure 1: $U(r = R_1)$ with $R_1 = 2$ for $\epsilon = 2$, $\nu = 0.1$ and $k = 1$ for Experiment 1 (left) and Experiment 2 (right).

Table 1: Computed Chebyshev coefficients for $F(|U|^2) = |U|^4$.

r	$a_0\ (\times 10^{-1})$	a_1	$a_2\ (\times 10^{-1})$
1.0009	5.0000	-6.3171×10^{-6}	5.0000
1.0018	5.0000	-6.2524×10^{-6}	5.0000
1.0027	5.0000	-6.3744×10^{-6}	5.0000
1.0036	4.9591	-7.1347×10^{-3}	4.9815
1.0065	4.9995	-6.3584×10^{-5}	4.9997
1.0094	4.9996	-6.1446×10^{-5}	4.9997
1.0123	4.9995	-6.5269×10^{-5}	4.9997
1.0152	4.9992	-1.2534×10^{-4}	4.9995
1.0181	4.9995	-6.4420×10^{-5}	4.9997

So the exact coefficients are $a_0 = 0.5$, $a_1 = 0$ and $a_2 = 0.5$. The computed coefficients from the inverse problem a_0, a_1 and a_2 on each ring are shown in Table 1.

5.2 Experiment 2

Let $F(|U|^2) = \sin|U|^2$ and $|U|^2 \in [\alpha, \beta]$. Let

$$q_k(z) := \begin{cases} J_0(z)\,, & \text{if } k = 0\,, \\ 2J_k(z)\,, & \text{if } k \in \mathbb{N}\,, \end{cases}$$

where J_k is the Bessel function of order k. From Watson's book [6, page 22, (3)–(4)], we have for $t \in [-1, 1]$,

$$\begin{aligned} \sin(\gamma + zt) &= \sin\gamma\cos(zt) + \cos\gamma\sin(zt) \\ &= \sin\gamma\sum_{k=0}^{\infty}(-1)^k q_{2k}(z)T_{2k}(t) + \cos\gamma\sum_{k=0}^{\infty}(-1)^k q_{2k+1}(z)T_{2k+1}(t) \\ &= \sum_{k=0}^{\infty}\sin\left(\gamma + \frac{2k\pi}{2}\right)q_{2k}(z)T_{2k}(t) \\ &\quad + \sum_{k=0}^{\infty}\sin\left(\gamma + \frac{(2k+1)\pi}{2}\right)q_{2k+1}(z)T_{2k+1}(t) \\ &= \sum_{n=0}^{\infty}\sin\left(\gamma + \frac{n\pi}{2}\right)q_n(z)T_n(t)\,. \end{aligned}$$

So with $\gamma = (\alpha+\beta)/2$ and $z = (\beta-\alpha)/2$, $|U|^2 = \gamma + zt$ and

$$\sin(|U|^2) = \sum_{n=0}^{\infty}\sin\left(\frac{\alpha+\beta}{2} + \frac{n\pi}{2}\right)q_n\left(\frac{\beta-\alpha}{2}\right)T_n(t)\,, \quad t = \frac{2|U|^2 - \alpha - \beta}{\beta - \alpha}\,.$$

Let's assume $|U| \in [0, 1]$, that is, $\alpha = 0$ and $\beta = 1$, and we use only the first eight terms of the infinite series of $\sin(|U|^2)$ to define

$$F(|U|^2) = \sum_{n=0}^{7}\sin\left(\frac{1}{2} + \frac{n\pi}{2}\right)q_n\left(\frac{1}{2}\right)T_n(t)\,, \quad t = 2|U|^2 - 1\,. \qquad (20)$$

Table 2: Computed Chebyshev coefficients for $F(|U|^2)$ as in (20).

	$a_0\,(\times 10^{-1})$	$a_1\,(\times 10^{-1})$	$a_2\,(\times 10^{-2})$	$a_3\,(\times 10^{-3})$
exact	4.4993	4.2522	−2.9345	−4.4998
$r = 1.001634$	4.4993	4.2522	−2.9344	−4.4999
$r = 1.003268$	4.4993	4.2522	−2.9344	−4.4999
$r = 1.004902$	4.4993	4.2522	−2.9344	−4.4999
	$a_4\,(\times 10^{-4})$	$a_5\,(\times 10^{-5})$	$a_6\,(\times 10^{-7})$	$a_7\,(\times 10^{-8})$
exact	1.5412	1.4135	−3.2224	−2.1090
$r = 1.001634$	1.5409	1.4148	−3.2558	−2.0502
$r = 1.003268$	1.5408	1.4150	−3.2638	−2.0376
$r = 1.004902$	1.5408	1.4150	−3.2587	−2.0499

So the exact coefficients are $a_n = \sin(1/2 + n\pi/2) q_n(1/2)$ for $n = 0, \dots, 7$. The numerical solution of the forward problem $U(R_1)$ is given in right panel of Figure 1. For the inverse problem, the computed coefficients a_n for $n = 0, \dots, 7$ on each ring are shown in Table 2.

6 Computational issues

Let $f \in C([-1, 1]$,

$$\mathcal{P}_d(t) = \sum_{k=0}^{2^d - 1} a_k T_k(t), \quad \mathbb{P}_d(t) = \mathcal{P}_d(f(t)), \quad t \in [-1, 1].$$

Note that there are two distinct notations, $\mathbb{P}_d = \mathcal{P}_d \circ f$. We wish to compute the Fourier–Legendre coefficients $\{b_\ell\}$ of $\mathbb{P}_d$ explicitly and efficiently using the Fourier–Legendre coefficients of f and the coefficients a_k.

We proceed inductively. If $d = 1$, then we observe that

$$\begin{aligned} \langle T_0(f), P_0 \rangle = 1, &\quad \langle T_1(f), P_1 \rangle = \hat{f}(1), \\ \mathbb{P}_1(t) = \frac{1}{2} + \frac{3}{2}\hat{f}(1) P_1(t). & \end{aligned} \tag{21}$$

Next, we assume that the problem is solved in the case of polynomials of degree $\leqslant 2^{d-1}-1$. Using the recurrence relations

$$T_{2^j+k} = 2T_{2^j}T_k - T_{2^j-k}\,, \quad j=1,2,\ldots,k=1,\cdots 2^j\,, \tag{22}$$

it is not difficult to deduce that

$$\begin{aligned}\sum_{k=0}^{2^d-1} a_k T_k &= \sum_{k=0}^{2^{d-1}-1}(a_k - a_{2^d-k})T_k + 2T_{2^{d-1}}\sum_{k=0}^{2^{d-1}} a_{k+2^{d-1}}T_k \\ &= \mathcal{Q}_{d-1} + 2T_{2^{d-1}}\widetilde{\mathcal{R}}_{d-1}\,,\end{aligned} \tag{23}$$

for polynomials $\mathcal{Q}_{d-1}$ and $\widetilde{\mathcal{R}}_{d-1}$ of degree at most 2^{d-1}. We let $\mathbb{Q}_{d-1}(t) = \mathcal{Q}_{d-1}(f(t))$ and $\widetilde{\mathbb{R}}_{d-1}(t) = \widetilde{\mathcal{R}}_{d-1}(f(t))$. Given our induction hypothesis, we may now compute

$$\widehat{\mathbb{P}_d} = \widehat{\mathbb{Q}_{d-1}} + 2\widehat{(T_{2^{d-1}}\circ f)} \star \widehat{\widetilde{\mathbb{R}}_{d-1}}\,. \tag{24}$$

Using (21) and (24) one can compute $\widehat{\mathbb{P}_d} = \widehat{\mathcal{P}_d(f)}$ with $O(d)$ convolutions.

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