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Numerical Solution of the Lippmann–Schwinger Equation by Approximate Approximations

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ABSTRACT. A new method for the numerical solution of volume integral equations is proposed and applied to a Lippmann–Schwinger type equation in diffraction theory. The approximate solution is represented as a linear combination of the scaled and shifted Gaussian. We prove spectral convergence of the method up to some negligible saturation error. The theoretical results are confirmed by a numerical experiment.

1. Introduction

In this article we propose a new method for solving the integral equation of Lippmann–Schwinger type

$$u(x) + q(x) \int_{\Omega} \mathcal{E}_k(x-y)\, u(y) = f(x)\ ,\ \ \Omega \subset \mathbb{R}^d, \tag{1.1}$$

where the kernel $\mathcal{E}_k$ is the fundamental solution of the Helmholtz equation. Many scattering problems in inhomogeneous media can be transformed to integral equations of this form. Their numerical solution with standard cubature methods is very expensive due to the singularity of the kernel $\mathcal{E}_k$ and its fast oscillations (for large k), especially in the multi-dimensional case. In this article we study a collocation method with trial functions which provide efficient formulas for the computation of the integral operator. The approach is based on the method of *approximate approximations* introduced in [5]. More precisely,

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we choose as approximate solution u_h to (1.1) a linear combination of scaled Gaussians centered on a uniform grid covering Ω. Since the diffraction potential of the Gaussian can be expressed by special functions the computation time for the discrete system is significantly smaller than in other approaches. The convolutional structure of the discretization matrices allows to apply fast solution methods as FFT and multigrid techniques, studied in a recent article by Vainikko [11], which treats simple cubature methods and trigonometric collocation for the Lippmann–Schwinger equation. Here we focus on the convergence analysis of the Gaussian collocation and prove spectral convergence of the method. To be more precise, under the assumption that the solution u satisfies the smoothness condition

$$\int_{\mathbb{R}^d} |\mathcal{F}u(\lambda)|\,(1+|\lambda|)^N\,d\lambda < \infty \ ,$$

($\mathcal{F}u$ is its Fourier transform), we show that

$$|u(x) - u_h(x)| \le c_u\, h^N + c_1 \varepsilon h^2$$

with small ε, negligible in numerical computations. This estimate does not depend on the wave number k, which is confirmed in numerical tests.

2. Problem

Consider for example, the scattering problem

$$\Delta w + \big(k^2 - q\big) w = g\ ,\ \ x \in \mathbb{R}^d\ , \tag{2.1}$$

where $k > 0$ is constant, the potential $q(x)$ and the right-hand side $g(x)$ are compactly supported and possibly complex-valued functions. The radiated field w has to satisfy Sommerfeld's radiation condition

$$\lim_{|x|\to\infty} |x|^{(d-1)/2}\left(\left(\frac{x}{|x|}, \nabla w(x)\right) - ik\, w(x)\right) = 0\ . \tag{2.2}$$

The fundamental solution of the Helmholtz equation is given by

$$\mathcal{E}_k(x) = \frac{i}{4}\left(\frac{k}{2\pi|x|}\right)^{d/2-1} H^{(1)}_{d/2-1}(k|x|)\ ,$$

$H^{(1)}_n = J_n + iY_n$ is the n^{th} order Hankel function of the first kind. The application of the diffraction potential

$$\mathcal{K}u(x) = \int_{\mathbb{R}^d} \mathcal{E}_k(x-y)\, u(y)\, dy\ , \tag{2.3}$$

leads to the integral equation for the radiated field

$$w(x) + \mathcal{K}(qw)(x) = -\mathcal{K}g(x)\ . \tag{2.4}$$

In the special case that an incident field w^i, i.e., a given entire solution of the Helmholtz equation $\Delta w^i + k^2 w^i = 0$, is scattered by the potential $q(x)$, the right-hand side of (2.1) is given by $g = qw^i$, and Equation (2.4) leads to the well-known Lippmann–Schwinger equation for the total field $w^{\text{tot}} = w + w^i$

$$w^{\text{tot}}(x) + \mathcal{K}\big(q\, w^{\text{tot}}\big)(x) = w^i(x)\ ,\ x \in \mathbb{R}^d\ . \tag{2.5}$$

We refer to [3] for more details concerning this equation.

In the following we consider the Equation (2.4). Multiplying both sides with the potential q we derive at the integral equation of the form

$$u(x) + q(x)\,\mathcal{K}u(x) = -q(x)\mathcal{K}g(x) \tag{2.6}$$

for the function $u = qw$. If a solution u of (2.6) is found, then from (2.4) one obtains the solution w of the original problem by the formula

$$w(x) = -\int\limits_{\mathbb{R}^d} \mathcal{E}_k(x-y)\,(g(y)+u(y))\,dy\ . \tag{2.7}$$

So the partial differential Equation (2.1), given on the whole space $\mathbb{R}^d$, is transformed into an integral equation over a bounded domain Ω containing $\operatorname{supp} q$.

In [11] Vainikko studied two approximation methods for solving integral equations of the form (1.1). The first one is a simple cubature method of second order, which can be applied in the case of piecewise smooth potentials. The second method is a sophisticated trigonometric collocation applied to periodized versions of integral equations of the form (1.1). The values of the periodized diffraction operator on the trigonometric polynomials are computed via Fourier techniques and it is shown that this method provides optimal convergence orders if $q(x)$ is smooth on $\mathbb{R}^d$. Utilizing the convolution structure of the problems Vainikko showed that by using FFT and two grid iterations the discrete problems can be solved in $\mathcal{O}(N^d \log N)$ operations.

In the present article we propose a collocation method for solving (1.1) with similar properties, which does not use Fourier series techniques, but is based on the direct computation of integrals of the basis functions. A major problem for the efficient solution of multi-dimensional integral equations consists in the efficient and accurate computation of the integrals. In our example this is even more complicated due to the singularity of the kernel $\mathcal{E}_k(x-y)$ and its fast oscillations (for large k). The cubature of those integrals is the main application of a new approximation method introduced in [5]. This method uses approximating functions having the property, that the action of many important integral operators of mathematical physics on Gaussians can be computed efficiently.

To solve (1.1) we choose as basis functions the elements of the set

$$X_h := \left\{ \exp\left(-\frac{|x-mh|^2}{\mathcal{D}h^2}\right),\ mh \in \Omega_h, m \in \mathbb{Z}^d \right\}, \tag{2.8}$$

where Ω_h is some domain containing the support of the potential q, $\Omega \subset \Omega_h$, the parameter $\mathcal{D}$ is a fixed positive number and h is the discretization parameter. Thus, the approximating functions are linear combinations of scaled Gaussians centered at the grid points $\{mh \in \Omega_h\}$.

The action of many important integral operators of mathematical physics on Gaussians can computed very efficiently. For example, if the integral operator of interest has a radial kernel function, then this integral transforms to a one-dimensional one. In some cases one gets even analytic formulas for these integrals. This concerns also the diffraction operator at least in the one- and three-dimensional case, where the kernel is given by

$$\mathcal{E}_k(x) = \begin{cases} \dfrac{\exp(ik|x|)}{2ik}\,, & d = 1\,, \\ \dfrac{\exp(ik|x|)}{4\pi|x|}\,, & d = 3\,. \end{cases}$$

The one-dimensional diffraction operator applied to the Gaussian gives

$$\begin{aligned} \frac{1}{2ik}\int_{-\infty}^{\infty} e^{ik|x-y|}e^{-y^2}\,dy &= \frac{\sqrt{\pi}e^{-x^2}}{4ik}\left(W\left(\frac{k}{2}+ix\right)+W\left(\frac{k}{2}-ix\right)\right) \\ &= \frac{\sqrt{\pi}e^{-k^2/4}}{2ik}e^{ik|x|}+\frac{\sqrt{\pi}e^{-x^2}}{2k}\ \mathrm{Im}\ W\left(\frac{k}{2}+i|x|\right). \end{aligned} \tag{2.9}$$

Here W denotes the scaled complementary error function

$$W(z) := e^{-z^2}\ \mathrm{erfc}(-iz) = e^{-z^2}\frac{2}{\sqrt{\pi}}\int_{-iz}^{\infty} e^{-t^2}\,dt = \frac{2}{\sqrt{\pi}}\int_{0}^{\infty} e^{-t^2}e^{2izt}\,dt\,, \tag{2.10}$$

which is also known as Faddeeva function and which has the properties

$$W(-\overline{z}) = \overline{W(z)} \quad \text{and} \quad W(-z) = 2e^{-z^2} - W(z)\,.$$

From (2.10) it is clear, that numerical computations with the Faddeeva function can lead to overflow problems if Im $z < 0$. This does not concern the case Im $z \geq 0$, where reliable and efficient implementations for computing $W(z)$ with double precision are available. Therefore one should use the second equation in formula (2.9) for numerical computations.

In the three-dimensional case one can easily check that

$$\begin{aligned} \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{e^{ik|x-y|}}{|x-y|}e^{-|y|^2}\,dy &= \frac{\sqrt{\pi}e^{-|x|^2}}{8|x|}\left(W\left(\frac{k}{2}-i|x|\right)-W\left(\frac{k}{2}+i|x|\right)\right) \\ &= \frac{\sqrt{\pi}e^{-k^2/4}}{4|x|}e^{ik|x|}+\frac{\sqrt{\pi}e^{-|x|^2}}{4|x|}\ \mathrm{Re}\ W\left(\frac{k}{2}+i|x|\right)\,. \end{aligned} \tag{2.11}$$

If $x = 0$, then

$$\frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{e^{ik|y|}}{|y|}e^{-|y|^2}\,dy = \frac{1}{2}+\frac{ik\sqrt{\pi}}{4}W\left(\frac{k}{2}\right).$$

Other basis functions commonly used for solving three-dimensional problems, finite elements for example, do not give such simple formulas, here special cubature formulas have to be utilized. The use of the Gaussian reduces the numerical expenses to discretize the integral equation significantly. Moreover, since any point value of the integral operator applied the approximating functions can be computed exactly (of course within the computer precision) no cubature errors occur.

The integral Equation (2.6) is solved by collocation: Find $u_h \in X_h$ such that

$$u_h(mh) + q(mh)\,\mathcal{K}u_h(mh) = -q(mh) \int\limits_{\mathbb{R}^d} \mathcal{E}_k(mh - y)\, g(y)\, dy \tag{2.12}$$

for all grid points $mh \in \Omega_h$. Hence, the coefficients $\{u_m\}$ of the discrete solution

$$u_h(x) = \sum_{mh \in \Omega_h} u_m e^{-(x-mh)^2/\mathcal{D}h^2}$$

are determined from the linear system

$$u_m + q(mh) \sum_{jh \in \Omega_h} a_{m-j} u_j = -q(mh) \int\limits_{\mathbb{R}^d} \mathcal{E}_k(mh - y)\, g(y)\, dy\,, \tag{2.13}$$

for $mh \in \Omega_h$, where

$$a_j = \chi(jh) \quad \text{with} \quad \chi(x) = \int\limits_{\mathbb{R}^d} \mathcal{E}_k(x - y)\, e^{-y^2/\mathcal{D}h^2}\, dy\,. \tag{2.14}$$

In the one-dimensional case (2.9) gives for $j \in \mathbb{Z}$

$$a_j = \frac{\sqrt{\pi \mathcal{D}} h e^{-k^2 \mathcal{D} h^2/4}}{2ik} e^{ikh|j|} + \frac{\sqrt{\pi \mathcal{D}} h e^{-j^2/\mathcal{D}}}{2k} \ \mathrm{Im}\ W\!\left(\frac{kh\sqrt{\mathcal{D}}}{2} + i\frac{|j|}{\sqrt{\mathcal{D}}}\right),$$

whereas in $\mathbb{R}^3$ formula (2.11) leads to the coefficients

$$a_j = \frac{\sqrt{\pi \mathcal{D}^3} h^2 e^{-k^2 \mathcal{D} h^2/4}}{4|j|} e^{ikh|j|} - \frac{\sqrt{\pi \mathcal{D}^3} h^2 e^{-|j|^2/\mathcal{D}}}{4|j|} \ \mathrm{Re}\ W\!\left(\frac{kh\sqrt{\mathcal{D}}}{2} + i\frac{|j|}{\sqrt{\mathcal{D}}}\right)$$

$$a_{(0,0,0)} = \frac{\mathcal{D}h^2}{2} + \frac{ik\sqrt{\pi \mathcal{D}^3} h^3}{4} W\!\left(\frac{kh\sqrt{\mathcal{D}}}{2}\right),$$

here $|j|$ denotes the Euclidean norm of $j \in \mathbb{Z}^3$.

3. Approximation Properties of Gaussians and Cubature Formulas

Here we describe high order semi-analytic cubature formulas for the integrals on the right-hand side of (2.13). The formulas are based on a new class of quasi-interpolation formulas and a general method to construct cubature formulas for multi-dimensional integral operators with singular kernel functions which was studied in [8]. It was shown that these formulas can provide arbitrary approximation orders up to any prescribed accuracy. The method uses quasi-interpolation formulas of the type

$$\mathcal{M}_{\mathcal{D},h} u(x) = \mathcal{D}^{-d/2} \sum_{m \in \mathbb{Z}^d} u(mh)\, \eta\!\left(\frac{x - mh}{\sqrt{\mathcal{D}}h}\right) \tag{3.1}$$

where η is a sufficiently smooth and rapidly decaying function. For simplicity we suppose that η belongs the Schwartz class $\mathcal{S}(\mathbb{R}^d)$. Under the assumption that

$$\int_{\mathbb{R}^d} \eta(x)\,dx = 1\,,\ \int_{\mathbb{R}^d} x^\alpha \eta(x)\,dx = 0, \quad \forall \alpha\,,\ 1 \le |\alpha| < N\,, \tag{3.2}$$

the following assertion was proved in [7].

Theorem 1.
If $u \in W_\infty^N(\mathbb{R}^d)$, then

$$|\mathcal{M}_{\mathcal{D},h}u(x) - u(x)| \le c\left(\sqrt{\mathcal{D}}h\right)^N \sum_{|\alpha|=N} \frac{\|\partial^\alpha u\|_{L_\infty(\mathbb{R}^d)}}{\alpha!} + \sum_{|\alpha|=0}^{N-1} \varepsilon_\alpha \left(\sqrt{\mathcal{D}}h\right)^{|\alpha|} \frac{|\partial^\alpha u(x)|}{\alpha!}\,,$$

where the constant c depends only on η and the numbers ε_α are given by

$$\varepsilon_\alpha = \max_{\mathbb{R}^d} \left| \sum_{\nu \in \mathbb{Z}^d \setminus \{0\}} \partial^\alpha \mathcal{F}\eta\left(\sqrt{\mathcal{D}}\nu\right) e^{-2\pi i(\nu,x)} \right|,$$

($\{0\}$ *denotes the null vector in* $\mathbb{Z}^d$). *For any* $\varepsilon > 0$ *there exists* $\mathcal{D} > 0$ *such that the error of the quasi-interpolation can be estimated by*

$$|\mathcal{M}_{\mathcal{D},h}u(x) - u(x)| \le c\left(\sqrt{\mathcal{D}}h\right)^N \sum_{|\alpha|=N} \frac{\|\partial^\alpha u\|_{L_\infty(\mathbb{R}^d)}}{\alpha!} + \varepsilon |\nabla_{N-1}u(x)|\,. \tag{3.3}$$

Here we use standard multi-index notations for $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{Z}^d_{\ge 0}$ and $\mathcal{F}$ denotes the Fourier transform

$$\mathcal{F}\varphi(\lambda) = \int_{\mathbb{R}^d} \varphi(x)\, e^{-2\pi i(\lambda,x)}\,dx\ .$$

Due to Theorem 1 the sum (3.1) approximates the function u with the order $\mathcal{O}(\sqrt{\mathcal{D}}h)^N$ up to a saturation error, which does not tend to zero and is mainly determined by $\varepsilon_0|u(x)|$. But one can choose the parameter $\mathcal{D}$ so that this error can be neglected in numerical computations. For example, the Gaussian $\eta = \pi^{-d/2}\exp(-x^2)$ satisfies (3.2) with $N = 2$ and the saturation term $\varepsilon_0 \approx 2d\exp(-\pi^2\mathcal{D})$. Since $\exp(-\pi^2) = 0.51723\ldots \cdot 10^{-4}$ this error is already below rounding errors in single precision arithmetics if $\mathcal{D} = 2$. The idea to use numerical algorithms which provide good approximations only up to some prescribed error level, but do not converge in rigorous mathematical sense, was proposed by the second author in [5]. In [6], which describes several applications, this approach was called *Approximate Approximations.*

Applied to the cubature of diffraction potentials this method gives the following. We approximate the right-hand side g in the original Equation (2.1) by

$$\mathcal{M}_{\mathcal{D},h}g(x) = (\pi\mathcal{D})^{-d/2} \sum_{m \in \mathbb{Z}^d} g(mh)\, \exp\left(-\frac{|x-mh|^2}{\mathcal{D}h^2}\right).$$

Using (2.14) we can approximate $\mathcal{K}g$ by the sum

$$\mathcal{K}_h g(x) := \mathcal{K}(\mathcal{M}_{\mathcal{D},h}f)(x) = (\pi\mathcal{D})^{-d/2} \sum_{m \in \mathbb{Z}^d} g(mh)\, \chi(x-mh)\,, \tag{3.4}$$

which represents, a second order cubature formula up to some prescribed accuracy. This follows immediately from the boundedness of $\mathcal{K} : C(\Omega) \to C(\Omega)$ for any bounded domain Ω. Additionally, it is easy to find approximations, for example, of derivatives of $\mathcal{K}f$ since χ can be analytically expressed.

The interesting feature of this approach consists in the possibility to construct higher order semi-analytic cubature formulas if an appropriate basis function η with nonzero moment has been found. We mention here two methods which we apply directly to the Gaussian function. A more detailed discussion is given in [7, 9].

Lemma 1.

The function

$$\eta_{2M}(x) = \pi^{-d/2}\, L_M^{(d/2)}\big(|x|^2\big)\, e^{-|x|^2} \tag{3.5}$$

with the generalized Laguerre polynomial

$$L_n^{(\gamma)}(y) = \frac{e^y y^{-\gamma}}{n!}\left(\frac{d}{dy}\right)^n \left(e^{-y} y^{n+\gamma}\right)\,,$$

satisfies the moment condition (3.2) *for* $N = 2M + 2$. *It has the Fourier transform*

$$\mathcal{F}\eta_{2M}(\lambda) = e^{-\pi^2|\lambda|^2} \sum_{j=0}^{M} \frac{\big(\pi^2|\lambda|^2\big)^j}{j!}\,.$$

The function η_{2M} is derived from the application of a general analytic formula for radial functions $\eta(x) = \eta(|x|)$

$$\Gamma\!\left(\frac{d}{2}\right) \sum_{j=0}^{M} \frac{(-1)^j\ \Delta^j (\mathcal{F}\eta)^{-1}(0)}{j!\,(4\pi)^{2j}\,\Gamma\!\left(j+\frac{d}{2}\right)}\,\Delta^j \eta(x) \tag{3.6}$$

to the Gaussian. Here $\Delta^j(\mathcal{F}\eta)^{-1}(0) := \Delta^j(1/\mathcal{F}\eta(\lambda))|_{\lambda=0}$. Hence, to get an analytic formula for $\mathcal{K}\eta_{2M}$ one has only to perform the differentiation in (3.6) with $\eta(x)$ replaced by $\mathcal{K}(e^{-|\cdot|^2})$. Since $\mathcal{K} = (k^2+\Delta)^{-1}$ we have

$$(-\Delta)^j \mathcal{K} = k^{2j}\mathcal{K} - \sum_{p=0}^{j-1} k^{2(j-p-1)}(-\Delta)^p$$

and from the relation

$$\Delta^j e^{\pi^2|\lambda|^2}\Big|_{\lambda=0} = \frac{\big(4\pi^2\big)^j\,\Gamma\big(j+\frac{d}{2}\big)}{\Gamma\big(\frac{d}{2}\big)}$$

we derive

$$\begin{aligned}\mathcal{K}\eta_{2M} &= \mathcal{K}\left(e^{-|\cdot|^2}\right)\sum_{j=0}^{M}\frac{k^{2j}}{4^j\,j!} - \sum_{j=0}^{M}\sum_{p=0}^{j-1}\frac{(-1)^{j-p}k^{2(j-p-1)}}{4^j\,j!}\,\Delta^p\left(e^{-|\cdot|^2}\right)\\ &= \mathcal{K}\left(e^{-|\cdot|^2}\right)\sum_{j=0}^{M}\frac{k^{2j}}{4^j\,j!} - \sum_{p=0}^{M-1}\Delta^p\left(e^{-|\cdot|^2}\right)\sum_{j=p+1}^{M}\frac{(-1)^{j-p}k^{2(j-p-1)}}{4^j\,j!}\,.\end{aligned}$$

Note that (cf. [1])

$$\Delta^p e^{-|x|^2} = (-1)^p \, p! \, 4^p L_p^{(d/2-1)}\big(|x|^2\big) e^{-|x|^2} = \begin{cases} H_{2p}(x)\, e^{-x^2}, & d=1\,, \\ \dfrac{H_{2p+1}(|x|)}{2|x|}\, e^{-|x|^2}, & d=3\,, \end{cases}$$

with the Hermite polynomials H_j. Thus, in the one-dimensional case

$$\begin{aligned} \mathcal{K}\eta_{2M}(x) = &\left(\frac{\sqrt{\pi} e^{-k^2/4}}{2ik} e^{ik|x|} + \frac{\sqrt{\pi} e^{-x^2}}{2k} \ \mathrm{Im} \ W\left(\frac{k}{2} + i|x|\right)\right) \sum_{j=0}^{M} \frac{k^{2j}}{4^j j!} \\ &- e^{-x^2} \sum_{p=0}^{M-1} H_{2p}(x) \sum_{j=1}^{M-p} \frac{(-1)^j k^{2(j-1)}}{4^{j+p}(j+p)!} \,. \end{aligned} \tag{3.7}$$

Similarly, for the three-dimensional case

$$\begin{aligned} \mathcal{K}\eta_{2M}(x) = &\left(\frac{\sqrt{\pi} e^{-|x|^2}}{8|x|} \left(W\left(\frac{k}{2} - i|x|\right) - W\left(\frac{k}{2} + i|x|\right)\right)\right) \sum_{j=0}^{M} \frac{k^{2j}}{4^j j!} \\ &- e^{-|x|^2} \sum_{p=0}^{M-1} \frac{H_{2p+1}(|x|)}{2|x|} \sum_{j=1}^{M-p} \frac{(-1)^j k^{2(j-1)}}{4^{j+p}(j+p)!} \,. \end{aligned} \tag{3.8}$$

The second kind of generating functions is a linear combination of translates of Gaussians so that the moment condition holds for large N. In order to describe their construction we introduce the multi-index $\xi(j) = (|j_1|, \dots, |j_d|)$, $j \in \mathbb{Z}^d$, with the length $|\xi(j)| = |j_1| + \dots + |j_d|$.

Lemma 2.

For any $M > 0$ there exist uniquely determined coefficients c_j such that the generating function

$$\widetilde{\eta}_{2M}(x) = \sum_{|\xi(j)| \le M} c_j \ \exp\left(- \left| x - \frac{j}{\sqrt{\mathcal{D}}} \right|^2 \right) \tag{3.9}$$

satisfies the moment condition (3.2) *with $N = 2M+2$. These coefficients are given by $c_j = 2^{-\kappa(j)} a_{\xi(j)}$, where the vector $(a_{\xi(j)})$ is the solution of the linear system*

$$\sum_{|\beta| \le M} a_\beta \beta^{2\alpha} = \pi^{-d/2} \frac{(-\mathcal{D})^{|\alpha|} \, (2\alpha)!}{2^{2|\alpha|} \, \alpha!} \quad , \ 0 \le |\alpha| \le M \,, \tag{3.10}$$

and $\kappa(j)$ is the number of nonzero components of $j \in \mathbb{Z}^d$. Moreover,

$$\partial^\alpha \mathcal{F}\widetilde{\eta}_{2M}\big(\sqrt{\mathcal{D}}\nu\big) = \left(- \frac{\sqrt{\mathcal{D}}}{2} \right)^{|\alpha|} \nu^\alpha e^{-\pi^2 \mathcal{D} |\nu|^2} \,.$$

Note that the quasi-interpolation formula (3.1) with the basis function $\widetilde{\eta}_{2M}$ can be transformed to the sum

$$\sum_{m \in \mathbb{Z}^d} u(hm) \, \widetilde{\eta}_{2M}\left(\frac{x - mh}{\sqrt{\mathcal{D}} h} \right) = \sum_{m \in \mathbb{Z}^d} u_m \ \exp\left(- \frac{|x - mh|^2}{\mathcal{D} h^2} \right) \tag{3.11}$$

with the coefficients

$$u_m = \sum_{|\xi(j)|\le M} c_j\, u((m-j)h)\,. \tag{3.12}$$

From Theorem 1 and Lemma 2 it follows immediately.

Corollary 1.

For any sufficiently smooth function u with compact support, any $\varepsilon > 0$ and integer n there exists $\mathcal{D} > 0$ and elements of

$$S_h := \operatorname{span}\left\{ \exp\left(-\frac{|x-mh|^2}{\mathcal{D}h^2} \right),\ m \in \mathbb{Z}^d \right\} \tag{3.13}$$

approximating u with the order $\mathcal{O}(h^n)$ up to the prescribed accuracy ε.

To obtain a high order semi-analytic cubature for $\mathcal{K}g$, which is based on the basis function $\widetilde{\eta}_{2M}$, in view of (3.11) one has only to solve system (3.10), to determine the coefficients g_m from (3.12) and to sum up

$$\mathcal{K}_h g(x) = \mathcal{D}^{-d/2} \sum_{m\in\mathbb{Z}^d} g_m \chi(x-mh)$$

using the analytic formulas for the function $\chi(x)$; cf. (2.14).

For example, the coefficients c_j for the 8-th order quadrature in the one-dimensional case are

$$c_0 = \frac{1}{\sqrt{\pi}}\left(1 + \frac{49\mathcal{D}}{72} + \frac{7\mathcal{D}^2}{24} + \frac{5\mathcal{D}^3}{96}\right),\quad c_{\pm1} = -\frac{\mathcal{D}}{\sqrt{\pi}}\left(\frac{3}{8} + \frac{13\mathcal{D}}{64} + \frac{5\mathcal{D}^2}{128}\right),$$
$$c_{\pm2} = \frac{\mathcal{D}}{\sqrt{\pi}}\left(\frac{3}{80} + \frac{\mathcal{D}}{16} + \frac{\mathcal{D}^2}{64}\right),\qquad c_{\pm3} = -\frac{\mathcal{D}}{\sqrt{\pi}}\left(\frac{1}{360} + \frac{\mathcal{D}}{192} + \frac{\mathcal{D}^2}{384}\right).$$

The construction of the sixth order cubature for the three-dimensional case leads to the linear system (3.10) with 10 unknowns. Its solution determines 25 coefficients c_j with $|\xi(j)| \le 2$, which provide the numbers g_m via (3.12). These coefficients are given by the relations

$$c_{(0,0,0)} = \frac{1}{\pi^{3/2}}\left(1 + \frac{15\mathcal{D}}{8} + \frac{21\mathcal{D}^2}{16}\right),$$
$$c_j = \begin{cases} -\dfrac{\mathcal{D}}{\pi^{3/2}}\left(\dfrac{1}{3} + \dfrac{3\mathcal{D}}{8}\right), & |\xi(j)| = 1\,, \\ \dfrac{\mathcal{D}}{\pi^{3/2}}\left(\dfrac{1}{48} + \dfrac{\mathcal{D}}{32}\right), & |\xi(j)| = 2,\ \kappa(j) = 1\,, \\ \dfrac{\mathcal{D}^2}{\pi^{3/2}16}, & |\xi(j)| = 2,\ \kappa(j) = 2\,. \end{cases}$$

At the end of this section we show that the cubature error of the described formulas converge to zero as $h \to 0$.

Theorem 2.
Assume that $u \in C^N(\mathbb{R}^d)$ has compact support and let the mesh width satisfy $hk \le C < 2\pi$ with k the wavenumber in (2.1). *Then for any $\varepsilon > 0$ there exists $\mathcal{D} > 0$ such that the cubature formulas generated by the functions η_{2M} or $\widetilde{\eta}_{2M}$ provide the error estimate*

$$|\mathcal{K}_h u(x) - \mathcal{K}u(x)| \le c\left(\sqrt{\mathcal{D}}h\right)^N \sum_{|\alpha|=N} \frac{\|\partial^\alpha u\|_C}{\alpha!} + h^2 \varepsilon \|u\|_{C^{N-1}} ,$$

with $N = 2M + 2$.

Proof. To prove Theorem 1 the difference $\mathcal{M}_{\mathcal{D},h}u(x) - u(x)$ is decomposed into a function $R_N(x)$ with $\|R_N\|_C = \mathcal{O}((\sqrt{\mathcal{D}}h)^N)$ and sums of the form

$$\left(\sqrt{\mathcal{D}}h\right)^\alpha \frac{\partial^\alpha u(x)}{\alpha!} \sum_{\nu \in \mathbb{Z}^d \setminus \{0\}} \partial^\alpha \mathcal{F}\eta\left(\sqrt{\mathcal{D}}\nu\right) e^{2\pi i (\nu, x)/h} , \; |\alpha| < N .$$

Since obviously $\|\mathcal{K}R_N\|_C \le c(\sqrt{\mathcal{D}}h)^N$ and the sums converge absolutely it remains to estimate the value of the diffraction operator applied to fast oscillating functions of the form $v(x)\, e^{-2\pi i (\nu,x)/h}$, $\nu \in \mathbb{Z}^d \setminus \{0\}$, with a compactly supported and sufficiently smooth function v. The pseudodifferential operator $\mathcal{K}$ has the symbol $(k^2 - 4\pi^2|\lambda|^2)^{-1}$. Let us introduce the set

$$B = \left\{\lambda \in \mathbb{R}^d : \left|4\pi^2 |\lambda|^2 - k^2\right| \le \rho\right\} \text{ with } \rho = \frac{\left(4\pi^2 - C^2\right)k^2}{C^2} ,$$

and a smooth function $a(\lambda)$ satisfying $a(\lambda) = (k^2 - 4\pi^2|\lambda|^2)^{-1}$ for $\lambda \notin B$. Then

$$\begin{aligned}
\mathcal{K}\left(v\, e^{2\pi i (\cdot,\nu)/h}\right)(x) &= \iint\limits_{\mathbb{R}^d \mathbb{R}^d} e^{2\pi i (x-y,\lambda)} a(\lambda)\, v(y) e^{-2\pi i (y,\nu)/h}\, d\lambda\, dy \\
&\quad + \iint\limits_{\mathbb{R}^d B} \left(\frac{1}{k^2 - 4\pi^2|\lambda|^2} - a(\lambda)\right) e^{2\pi i (x,\lambda)} e^{-2\pi i (y, \nu/h - \lambda)} v(y)\, d\lambda\, dy \\
&= \iint\limits_{\mathbb{R}^d \mathbb{R}^d} e^{2\pi i (x-y,\lambda)} a(\lambda)\, v(y)\, e^{-2\pi i (y,\nu)/h}\, d\lambda\, dy \\
&\quad + \int\limits_B \left(\frac{1}{k^2 - 4\pi^2|\lambda|^2} - a(\lambda)\right) e^{2\pi i (x,\lambda)}\, \mathcal{F}v(\lambda - \nu/h)\, d\lambda .
\end{aligned}$$

The integral

$$I_1 := \iint\limits_{\mathbb{R}^d \mathbb{R}^d} e^{2\pi i (x-y,\lambda)} a(\lambda)\, v(y)\, e^{-2\pi i (y,\nu)/h}\, d\lambda\, dy$$

is a pseudodifferential operator with smooth symbol $a \in S^{-2}(\Omega)$, hence, the expansion

$$I_1 = e^{2\pi i (x,\nu)/h} \sum_{|\alpha|<N} \frac{\partial^\alpha a(\nu/h) \partial^\alpha v(y)}{i^{|\alpha|} \alpha!} + R_N(x,h)$$

holds (see [4, Section 3.3.4]), where

$$|R_N(x,h)| \le C_{N,\Omega} h^{2+N} .$$

Since the number ρ is chosen such that $\nu/h \notin B$ for all $\nu \in \mathbb{Z}^d \setminus \{0\}$ we obtain

$$\partial^\alpha a(\nu/h) = \partial_\lambda^\alpha \frac{1}{k^2 - 4\pi^2|\lambda|^2}\bigg|_{\lambda=\nu/h} = h^{2+|\alpha|}\partial_\nu^\alpha \frac{1}{h^2k^2 - 4\pi^2|\nu|^2},$$

which leads to the asymptotics

$$I_1 = e^{2\pi i(x,\nu)/h} h^2 \sum_{|\alpha|<N} \frac{h^{|\alpha|}\,\partial^\alpha v(y)}{i^{|\alpha|}\alpha!}\,\partial_\nu^\alpha \frac{1}{h^2k^2 - 4\pi^2|\nu|^2} + R_N(x,h).$$

To estimate the second integral we note that $|\lambda|^N|\mathcal{F}v(\lambda)| \to 0$ as $|\lambda| \to \infty$. Using spherical coordinates one easily sees that the integral is a principal value integral of a compactly supported smooth function, therefore

$$\left|\int_B \left(\frac{1}{k^2 - 4\pi^2|\lambda|^2} - a(\lambda)\right) e^{2\pi i(x,\lambda)}\,\mathcal{F}v(\lambda - \nu/h)\,d\lambda\right| \le c_v h^N. \qquad \square$$

4. Error Analysis for the Collocation Method

To estimate the asymptotic error of the collocation method we introduce an interpolation projection Q_h satisfying $Q_h f(mh) = f(mh)$ for all $mh \in \Omega_h$. Then the discretization (2.12) of the integral Equation (2.4), which has the form

$$u + q\,\mathcal{K}u = -q\mathcal{K}g, \tag{4.1}$$

can be written as

$$Q_h u_h + Q_h q\,\mathcal{K}u_h = -Q_h q\mathcal{K}_h g, \tag{4.2}$$

where $\mathcal{K}_h$ is an appropriately chosen cubature for $\mathcal{K}$. The linear systems (4.2) are uniquely solvable for all sufficiently small h. This follows from the fact that $\mathcal{K}$ is a compact operator in any reasonable function space over bounded domains. Hence, under certain smoothness assumptions on q the operator $q\,\mathcal{K}$ remains compact if the domain under consideration contains the support of q.

Furthermore, the interpolation problem with Gaussian functions is uniquely solvable (see [10]). Moreover, the proof of [10, Lemma 3.1] shows that in our situation the interpolation matrix $A = \|\exp(-(j-k)^2/\mathcal{D})\|_{jh,kh\in\Omega_h}$ has the property

$$(Av, v) = (\pi\mathcal{D})^{d/2} \int_{\mathbb{R}^d} e^{-\pi^2\mathcal{D}|x|^2} \left|\sum_{jh\in\Omega_h} v_j e^{2\pi i(j,x)}\right|^2 dx,$$

for any vector $v \in \mathbb{C}^n$ with $n = \#\{jh \in \Omega_h\}$, the number of knots jh lying in Ω_h. Therefore we obtain the inequality

$$e^{-\pi^2\mathcal{D}d/4}\,\|v\|_{\ell^2}^2 < \frac{(Av, v)}{(\pi\mathcal{D})^{d/2}} < \max_{\mathbb{R}^d}\left|\sum_{m\in\mathbb{Z}^d} e^{-\pi^2\mathcal{D}|x-m|^2}\right| \|v\|_{\ell^2}^2$$

with bounds not depending on the mesh size h and the number of unknowns of the interpolating sum of scaled and shifted Gaussians. Hence, the condition number of A can be estimated by $(\pi\mathcal{D})^{-d/2}\,e^{\pi^2\mathcal{D}\,d/4}$. This means, for large $\mathcal{D}$ the numerical solution of the interpolation problem can cause stability problems. However, since the scaling of the trial functions coincides with the mesh width h, the condition number of A does not depend on the number of grid points and does not become worse for finer meshes. In practical calculations for three-dimensional problems direct solvers from LAPACK are stable up to the parameter $\mathcal{D} = 4$.

Since the Equations (4.2) are compact perturbations of the uniquely solvable interpolation problems standard results for projection methods imply that these equations are solvable provided that (4.1) or equivalently the original problem (2.1) are uniquely solvable. The approximate solution w_h to (2.1) is then obtained from the relation

$$w_h(x) = -\mathcal{K}_h g(x) - \mathcal{K} u_h(x)\,,\ \ x \in \mathbb{R}^d\,, \tag{4.3}$$

where again the analytic formulas for the diffraction operator can be used. Hence, from (4.2) one has

$$Q_h u_h - Q_h q(\mathcal{K}_h g + w_h) = -Q_h q \mathcal{K}_h g\,,$$

and therefore

$$Q_h q w_h = Q_h u_h\,.$$

On the other hand, putting

$$\mathcal{K} u_h = \mathcal{K} Q_h u_h + \mathcal{K}(I - Q_h) u_h$$

into (4.3) we see that w_h solves the integral equation

$$w_h + \mathcal{K} Q_h q w_h = -\mathcal{K}_h g - \mathcal{K}(I - Q_h) u_h\,. \tag{4.4}$$

Since from (2.4)

$$w + \mathcal{K}(qw) = -\mathcal{K} g\,,$$

we obtain the relation

$$\begin{aligned} w_h - w &= -(I + \mathcal{K} Q_h q)^{-1}\big(\mathcal{K}_h g + \mathcal{K}(I - Q_h) u_h\big) - w \\ &= -(I + \mathcal{K} Q_h q)^{-1}\big(\mathcal{K}_h g + w + \mathcal{K} Q_h q w + \mathcal{K}(I - Q_h) u_h\big) \\ &= (I + \mathcal{K} Q_h q)^{-1}\big((\mathcal{K} - \mathcal{K}_h) g + \mathcal{K}(I - Q_h) q w - \mathcal{K}(I - Q_h) u_h\big)\,. \end{aligned} \tag{4.5}$$

To estimate the error we have therefore to show that the operators $(I + \mathcal{K} Q_h q)^{-1}$ exist and are uniformly bounded as well as to find upper bounds for the three terms inside the brackets. The first term $(\mathcal{K} - \mathcal{K}_h) g$ does not depend on the choice of the interpolation operator Q_h and has been estimated already in Theorem 2. The term $\mathcal{K}(I - Q_h) u_h$ vanishes if we choose Q_h to be the interpolation projection onto the space of Gaussians X_h, defined in (2.8).

Before dealing with the second term and the operators $(I + \mathcal{K} Q_h q)^{-1}$ we recall some properties of the interpolants from the set S_h, cf. (3.13), at the lattice $\{mh\,,\ m \in \mathbb{Z}^d\}$, which have been stated in [7]. Roughly speaking, the interpolant approximates continuous functions with optimal order up to some saturation error. To estimate this error we introduce the function

$$\vartheta(z) := \prod_{j=1}^{d} \vartheta_3(z_j | i\pi\mathcal{D}) \,, \tag{4.6}$$

where ϑ_3 is the Jacobi's Theta-function (see e.g., [12])

$$\vartheta_3(z|i\pi\mathcal{D}) = \sum_{k=-\infty}^{+\infty} e^{-\pi^2\mathcal{D}k^2} e^{2ikz} \,.$$

This is an entire function and for real z and large $\mathcal{D}$ very close to 1.

Lemma 3.

Suppose that the continuous function u is such that

$$\|u\|'_{N+\delta} := \int\limits_{\mathbb{R}^d} |\mathcal{F}u(\lambda)| \, (1+|\lambda|)^{N+\delta} \, d\lambda < \infty$$

for some $\delta : O < \delta \leq 1$. Then the interpolation error can be estimated in the form

$$|u(x) - Q_h u(x)| \leq c\,(2h)^{N+\delta} \, \|u\|'_{N+\delta} + \sum_{|\alpha|=0}^{N} |a_\alpha(x)| \left(\frac{\pi\mathcal{D}h}{2}\right)^{|\alpha|} \frac{|\partial^\alpha u(x)|}{\alpha!} \,,$$

with some constant c not depending on u. The saturation error is determined by N and the functions

$$a_\alpha(x) = \partial_z^\alpha \left(1 - \frac{\vartheta\left(z + \frac{\pi x}{h}\right)}{\vartheta(z)}\right)\Bigg|_{z=0} \,. \tag{4.7}$$

These properties obviously remain valid if we restrict the interpolation knots to the set $\{mh \in \Omega_h, m \in \mathbb{Z}^d\}$, where $\Omega_h \supset \Omega \supset \operatorname{supp} q$ is chosen such that the basis functions with centers at Ω are smaller than the saturation error outside Ω_h,

$$\exp\left(-\frac{|x-mh|^2}{\mathcal{D}h^2}\right) < \varepsilon \quad \text{for } x \notin \Omega_h \quad \text{and} \quad mh \in \Omega \,.$$

Now we are in the position to treat the remaining terms in (4.5). First we show that the operators $I + \mathcal{K}Q_h q$ have uniformly bounded inverses for all sufficiently small h. Since the set $\|Q_h q\|$ is bounded and $\mathcal{K}$ is compact, the operators $\mathcal{K}Q_h q$ are collectively compact, cf. [2]. It can be easily seen, that the functions a_α defined by (4.7) are rapidly oscillating with the period π/h. Hence, as in the proof of Theorem 2 we conclude that even the saturation errors tend to zero, i.e.,

$$\|\mathcal{K}(I - Q_h)qu\| \to 0 \quad \text{as} \quad h \to 0$$

for the dense subset of functions u with $\|u\|'_{N+\delta} < \infty$. Therefore all conditions of the collectively compact operator theory are satisfied and we obtain, under the assumption that

$I+\mathcal{K}q$ is invertible, that for sufficiently small h the inverse operators $(I+\mathcal{K}Q_h q)^{-1}$ exist and are uniformly bounded. On the other hand, if the solution w satisfies the condition

$$\|qw\|'_N = \int_{\mathbb{R}^d} |\mathcal{F}(qw)(\lambda)|\,(1+|\lambda|)^N\,d\lambda < \infty \tag{4.8}$$

then the same arguments lead to the estimate

$$|\mathcal{K}(I-Q_h)q(x)w(x)| \le c\left(\sqrt{\mathcal{D}}h\right)^N \|qw\|'_N + c_1\,h^2\varepsilon\|qw\|_{C^{N-1}}\,,$$

which bounds the second term inside the brackets in (4.5).

Summarizing all arguments we obtain the following convergence result:

Theorem 3.

Suppose that the solution w of Equation (2.1) *satisfies the smoothness condition* (4.8) *with $N=2M+2$ and the cubature formula for the right-hand side of* (2.6) *is generated by the functions η_{2M} or $\widetilde{\eta}_{2M}$. Then the difference between w and the solutions w_h of the system* (2.13) *can be estimated as follows*

$$|w(x)-w_h(x)| \le c_u\left(\sqrt{\mathcal{D}}h\right)^N + c_1\varepsilon h^2\,.$$

5. Numerical Example

As a simple test case we consider the following one-dimensional problem:

$$w'' + \left(k^2+\mu\,q(x)\right)w = -\delta(x)\,,\ x\in\mathbb{R}\,. \tag{5.1}$$

Here μ is some constant parameter and the potential q is given as

$$q(x) = \frac{v(x)}{\mu\,\mathcal{K}v(x)+e^{ik|x|}/2ik}$$

with some function $v(x)$, $|x|\le 1$, which is obviously a solution of the integral equation

$$u(x) - \frac{\mu\,q(x)}{2ik}\int_{-1}^{1} e^{ik|x-y|}\,u(y)\,dy = \frac{q(x)\,e^{ik|x|}}{2ik}\,. \tag{5.2}$$

Then (5.1) has the solution

$$w(x) = \mu\,\mathcal{K}v(x) + \frac{e^{ik|x|}}{2ik}\,.$$

The following tables give convergence rates for the difference $\max|w-w_h|$, where

$$w_h(x) = \mu\,\mathcal{K}u_h(x) + \frac{e^{ik|x|}}{2ik}\,,$$

with the approximate solution u_h of (5.2). The obtained convergence rates should correspond to the smoothness of v.

We tried different values of the parameter μ and the wavenumber k. Convergence rates for $v \in C^1$ are shown on the following table.

h^{-1}	$k = 1$	$k = 10$	$k = 20$	$k = 50$
20	5.1519	6.5723	8.1984	7.8392
30	1.1945	1.0650	0.8227	2.2741
40	1.0463	1.0665	0.9640	0.6128
50	1.0244	1.0482	0.9853	1.1107
60	1.0186	1.0462	0.9894	0.9759
70	1.0155	1.0417	0.9912	1.0305
80	1.0134	1.0292	0.9925	0.9321
90	1.0118	1.0303	0.9934	0.9793
100	1.0106	1.0263	0.9941	1.0000

For a function $v \in C_0^4[-1, 1]$ we obtained the following rates of $\max |w - w_h|$

h^{-1}	$k = 1$	$k = 10$	$k = 20$	$k = 50$
20	16.5432	17.1947	21.2600	17.3789
30	4.4344	3.8187	3.3097	2.9959
40	4.0306	3.9816	6.3844	3.2325
50	4.0015	3.9991	4.1470	4.0169
60	3.9999	4.0020	3.4357	3.6604
70	3.9998	4.0029	4.7079	3.8351
80	3.9998	4.0033	4.0115	3.9777
90	3.9999	4.0000	4.0088	4.1684
100	3.9999	3.9982	4.0069	4.0862

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