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Analysis and Application of the Super-Potential Method to the
Screened Poisson Equation

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Abstract

This work develops two super-potential methods for solving the screened Poisson equation $(-\Delta + \kappa^2)u = \rho$ in free space with compactly supported, smooth source density. Both methods replace the convolution with the Yukawa kernel, which is singular at the origin, by the convolution with a more regular surrogate kernel that is bounded at the origin. The Mixed-Screened approach obtains the solution by applying the Laplace operator to a super-potential, the Double-Screened approach by applying the screened operator. The evaluation is based on separable Gaussian-sum approximations of the kernels and an FFT-based convolution followed by spectral operator application, where a one-time precomputation is separated from the actual solution phase.

For both approaches, an a priori error estimate is derived whose kernel approximation component contains a near-field contribution of order $\mathcal{O}(\varepsilon^3)$ and which additionally contains a discretization term that decays with the grid size for smooth densities. In the Double-Screened approach, the transformed integrand is analytic and double exponentially decaying on both sides, so that a standard sinc quadrature error bound is directly applicable and a more favorable number-of-terms asymptotics results. In the Mixed-Screened approach, the double exponential decay at the left boundary is absent, which is why a manual error decomposition is required.

The methods are examined on test problems with known exact solution, including Gaussian, anisotropic, compactly supported, and oscillating sources as well as a variation of the screening parameter. At the finest grid size examined, $N = 128$, both approaches achieve relative ℓ^∞ -errors near machine accuracy in most benchmark configurations, and nearly coinciding accuracy at identical configurations. In the considered variation of the screening parameter, the accuracy remains stable. The Double-Screened approach requires fewer Gauss terms in the majority of cases and achieves shorter mean solve times for most configurations. This work thereby transfers the super-potential principle, formulated for the Poisson equation, to the screened operator and supplements it with two explicit kernel constructions together with the associated error theory depending on the screening parameter.

Kurzfassung

Diese Arbeit entwickelt zwei Super-Potential-Verfahren zur Lösung der abgeschirmten Poisson-Gleichung $(-\Delta + \kappa^2)u = \rho$ im freien Raum mit kompakt getragener, glatter Quelldichte. Beide Verfahren ersetzen die Faltung mit dem im Ursprung singulären Yukawa-Kern durch die Faltung mit einem reguläreren, im Ursprung beschränkten Ersatzkern. Der Mixed-Screened-Ansatz gewinnt die Lösung durch Anwendung des Laplace-Operators auf ein Super-Potential, der Double-Screened-Ansatz durch Anwendung des abgeschirmten Operators. Die Auswertung beruht auf separablen Gaußsummen-Approximationen der Kerne und einer FFT-basierten Faltung mit anschließender spektraler Operatoranwendung, wobei eine einmalige Vorberechnung von der eigentlichen Lösungsphase getrennt ist.

Für beide Ansätze wird eine a-priori-Fehlerabschätzung hergeleitet, deren Kernapproximationsanteil einen Nahfeldbeitrag der Ordnung $\mathcal{O}(\varepsilon^3)$ enthält und die zusätzlich einen für glatte Dichten mit der Gittergröße abklingenden Diskretisierungsterm enthält. Beim Double-Screened-Ansatz ist der transformierte Integrand analytisch und beidseitig doppelt-exponentiell abklingend, sodass eine Standard-Sinc-Quadraturfehlerschranke direkt anwendbar ist und sich eine günstigere Termzahlasymptotik ergibt. Beim Mixed-Screened-Ansatz fehlt der doppelt-exponentielle Abfall am linken Rand, weshalb eine manuelle Fehlerzerlegung erforderlich ist.

Die Verfahren werden an Testproblemen mit bekannter exakter Lösung untersucht, darunter Gauß-, anisotrope, kompakt getragene und oszillierende Quellen sowie eine Variation des Abschirmparameters. Bei der feinsten untersuchten Gittergröße $N = 128$ erreichen beide Ansätze in den meisten Benchmark-Konfigurationen relative ℓ^∞ -Fehler nahe der Maschinengenauigkeit und bei identischer Konfiguration nahezu übereinstimmende Genauigkeit. In der betrachteten Variation des Abschirmparameters bleibt die Genauigkeit stabil. Der Double-Screened-Ansatz benötigt dabei überwiegend weniger Gaußterme und erzielt für die Mehrzahl der Konfigurationen kürzere mittlere Löserzeiten. Die Arbeit überträgt damit das für die Poisson-Gleichung formulierte Super-Potential-Prinzip auf den abgeschirmten Operator und ergänzt es um zwei explizite Kernkonstruktionen samt zugehöriger, vom Abschirmparameter abhängiger Fehlertheorie.

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Declaration

The large language models *ChatGPT* [15] and *Claude* [2] were used as assistive tools during the preparation of this thesis for code development, drafting text, and language improvement, as English is not the author's first language. All AI-generated content was reviewed, verified, and adapted by the author, who assumes full responsibility for the final work.

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1. Introduction

1.1. Motivation and Application Context

Elliptic partial differential equations form one of the central classes of second-order partial differential equations [7]. In contrast to parabolic or hyperbolic equations, which describe time-dependent evolution problems, elliptic equations model stationary phenomena, in which the sought solution typically describes a physical quantity in equilibrium, such as a concentration or a potential.

One of the most important elliptic operators is the negative Laplace operator $-\Delta$. The associated Poisson equation

$$-\Delta u(x) = \rho(x), \quad x \in \mathbb{R}^3, \quad \lim_{|x| \rightarrow \infty} |u(x)| = 0, \quad (1)$$

serves as the standard model for stationary potential and field problems, where $\rho \in L^\infty(\mathbb{R}^3)$ denotes a compactly supported source density and u denotes the sought potential. Its fundamental solution is the free-space Green's function, also referred to as the Coulomb kernel, $U(r) = \frac{1}{4\pi r}$, $r = |x|$, and the solution can be represented as the convolution $u = U * \rho$. The Poisson equation (1) describes, for example, the electrostatic potential of a charge distribution as well as the gravitational potential of a mass density.

In numerous applications, however, screening effects arise that can be modelled by an additional linear term. A natural one-parameter extension of the Laplace operator is $(-\Delta + \kappa^2)$ with the screening parameter $\kappa > 0$, which reduces to $-\Delta$ in the limit $\kappa \rightarrow 0$. The subject of this work is the screened Poisson equation

$$(-\Delta + \kappa^2)u = \rho, \quad x \in \mathbb{R}^3, \quad \lim_{|x| \rightarrow \infty} |u(x)| = 0. \quad (2)$$

The associated fundamental solution is the Yukawa Green's function

$$G(r) = \frac{e^{-\kappa r}}{4\pi r}, \quad r = |x|,$$

and the solution can be represented as the convolution

$$u(x) = (G * \rho)(x) = \int_{\mathbb{R}^3} G(|y|) \rho(x - y) dy.$$

In contrast to the Coulomb kernel U , whose interactions decay algebraically as r^{-1} , the factor $e^{-\kappa r}$ causes an exponential decay on the length scale κ^{-1} .

Since G describes screened interactions, equation (2) arises in numerous applications in physics and chemistry, in particular in electrolyte solutions within the framework of Debye–Hückel theory [6], in complex plasmas [11], and in the modelling of interactions in Debye plasmas in quantum collision dynamics [14].

1. Introduction

1.2. Existing Approaches and Their Limitations

The kernel G has a non-removable singularity at $r = 0$, which complicates the numerical evaluation of the convolution $u = G * \rho$ and typically requires special regularization strategies. An analogous situation arises for the Coulomb kernel U of the Poisson equation (1), for which several common approaches have been developed, such as truncated-kernel methods, Ewald-type techniques, and direct Gauss-sum regularizations of the singular kernel. One such approach is based on the Gaussian-sum approximation of the kernel, applied to nonlocal potentials as in [9]. Without additional near-field treatment, this direct approximation typically leads to a truncation error of order $\mathcal{O}(\varepsilon^2)$, where $\varepsilon > 0$ denotes a near-field truncation parameter. To compensate for this error, local correction terms are usually introduced, which are based on a Taylor expansion of the density near the kernel and require a subsequent FFT evaluation. These near-field corrections increase the computational effort and complicate an FFT-based evaluation. This issue arises for the Coulomb kernel as well as for the Yukawa kernel, and motivates in both cases the development of an approach without near-field correction.

1.3. The Super-Potential Idea and Objective of the Work

Exl and Schaffer pursue the following approach in [10] for the Poisson case. Instead of evaluating the convolution with the singular kernel directly, they introduce a super-potential v satisfying the relation $u = \Delta v$. The solution then takes the form $v = V * \rho$ with the biharmonic kernel $V(y) = \frac{|y|}{8\pi}$, $y \in \mathbb{R}^3$. In contrast to the singular Coulomb kernel, V is bounded at the origin and satisfies $V(0) = 0$ with linear behaviour $V(y) = \mathcal{O}(|y|)$ as $|y| \rightarrow 0$. This improved regularity enables a Gaussian-sum approximation without near-field correction and contributes to the fact that a truncation error of order $\mathcal{O}(\varepsilon^4)$ can be achieved. The overall method achieves machine-accurate results at a computational complexity of $\mathcal{O}(N \log N)$.

The objective of this work is to transfer the super-potential method of Exl and Schaffer [10] to the screened Poisson equation. Building on this fundamental idea, two super-potential approaches for $(-\Delta + \kappa^2)u = \rho$ are constructed, analysed, and implemented. For both approaches, separable Gaussian-sum approximations of the respective kernels are derived, FFT-based algorithms are developed, and complete a priori error estimates are proved. The theoretical results are verified by numerical experiments that examine the accuracy, stability with respect to κ , and efficiency of the methods. Since the constructed kernels do not vanish at the origin, and the near-field contribution is therefore not suppressed by the kernel behaviour, a reduced near-field order $\mathcal{O}(\varepsilon^3)$ results compared to the Poisson case.

1.4. Overview of the Developed Methods

The W -approach (Mixed-Screened) obtains the solution by applying the Laplace operator to a super-potential, $u = -\Delta(W * \rho)$, where W is the fundamental solution of the operator

$(-\Delta)(-\Delta + \kappa^2)$. The H -approach (Double-Screened) uses the screened operator to recover u from a super-potential, $u = (-\Delta + \kappa^2)(H * \rho)$, where H is the fundamental solution of $(-\Delta + \kappa^2)^2$. Both kernels are bounded at the origin, in contrast to the non-removable singularity of the Yukawa kernel G . The structural difference between the two approaches lies in the integral representation: in the H -approach, the transformed integrand decays double exponentially, so that the sinc quadrature bound can be applied directly.

1.5. Structure of the Work

Chapter 2 presents the super-potential method for the Poisson equation following Exl and Schaffer [10] and thereby establishes the methodological foundation for the subsequent chapters. Chapter 3 develops the W -approach (Mixed-Screened) for the screened Poisson equation. The kernel construction and fundamental solution, the regularity analysis, the Gaussian-sum approximation, and the complete a priori error estimate are addressed. Chapter 4 treats the H -approach (Double-Screened) in a structurally analogous manner. Since the transformed integrand decays double exponentially, the direct application of the sinc quadrature bound leads to improved asymptotics of the number of terms. Chapter 5 presents the numerical results in two parts. First, the theoretical predictions of both approaches are verified numerically. Subsequently, both methods are compared by means of systematic benchmarks with respect to accuracy, number of terms, and runtime. Chapter 6 summarises the main results and discusses open questions.

2. The Super-Potential Method: Basic Principle in the Poisson Case

The application of the super-potential method to the Poisson equation presented in this chapter is based on the work of Exl and Schaffer [10]. In the following, the components of their approach that are relevant to this work are presented in consolidated form and used as the basis for the later transfer to the screened Poisson equation.

We consider a (rescaled) source density ρ and assume for simplicity that it is compactly supported in the unit cube $B_1 := [-1/2, 1/2]^3$. We study the Poisson equation (1). The classical representation of the solution is then given by

$$u(x) = (U * \rho)(x) = \int_{\mathbb{R}^3} U(y) \rho(x - y) dy, \quad x \in \mathbb{R}^3.$$

Although this classical representation is exact, its practical application is demanding and its direct evaluation requires $\mathcal{O}(N^2)$ operations for N grid points. As discussed in 1.2, the singularity of the kernel U at $y = 0$ furthermore leads to near-field problems, which in common methods require local correction terms.

2.1. Kernel Construction and Fundamental Solution

The method is based on a super-potential v satisfying the relation

$$u = \Delta v \tag{3}$$

(cf. 1.3). With this substitution, the Poisson equation (1) becomes the biharmonic equation $-\Delta^2 v = \rho$. Let V be the biharmonic Green's function in $\mathbb{R}^3$, which is related to the Green's function of the Laplace operator via $\Delta V = U$. For the three-dimensional case it is given by $V(y) = \frac{1}{8\pi}|y|$, $y \in \mathbb{R}^3$. Thus the super-potential possesses the Green's representation

$$v(x) = (V * \rho)(x) = \int_{\mathbb{R}^3} V(y) \rho(x - y) dy = \int_{\mathbb{R}^3} \frac{|y|}{8\pi} \rho(x - y) dy.$$

The solution to the original Poisson problem is then obtained by applying the Laplace operator,

$$u(x) = \Delta v(x) = \Delta(V * \rho)(x), \tag{4}$$

where this differentiation is later carried out spectrally in Fourier space.

2.2. Regularity of the Kernel and Near-Field Order

Since ρ is compactly supported in B_1 , the convolution representation for $x \in B_1$ can be restricted to the doubled cube $B_2 := 2 \cdot B_1 = [-1, 1]^3$. Indeed, for $x \in B_1$ and $y \notin B_2$, it holds that $x - y \notin B_1$. Since $\text{supp}(\rho) \subset B_1$, it follows that $\rho(x - y) = 0$, so that no contribution to the integral arises outside of B_2 . Thus for $x \in B_1$

$$u(x) = \Delta \int_{B_2} V(y) \rho(x - y) dy = \Delta \int_{B_2} \frac{|y|}{8\pi} \rho(x - y) dy.$$

2.2. Regularity of the Kernel and Near-Field Order

The biharmonic kernel V is bounded at the origin and satisfies $V(0) = 0$ with linear behavior $V(y) = \mathcal{O}(|y|)$ for $|y| \rightarrow 0$. This regularity forms the basis of the subsequent error analysis and in particular enables a Gaussian-sum approximation without near-field correction with a truncation error of order $\mathcal{O}(\varepsilon^4)$ (cf. 1.3).

For the numerical evaluation of the convolution (4), the density is first approximated by a truncated Fourier series. For an L -periodic function f we use the Fourier representation

$$f(x) = \sum_{k \in \mathbb{Z}^3} \hat{f}_k e^{2\pi i k \cdot x / L}, \quad \hat{f}_k = \frac{1}{L^3} \int_{B_L} f(x) e^{-2\pi i k \cdot x / L} dx.$$

By zero-padding we extend ρ from B_1 to the doubled domain $B_2 = [-1, 1]^3$ and consider its $L = 2$ -periodic continuation on $\mathbb{R}^3$. In the notation we do not distinguish between ρ and its periodic continuation. For $L = 2$ one obtains the Fourier representation

$$\rho(x) \approx \sum_{k \in \mathbb{Z}^3} \hat{\rho}_k e^{\pi i k \cdot x}, \quad \hat{\rho}_k = \frac{1}{8} \int_{B_2} \rho(x) e^{-\pi i k \cdot x} dx.$$

Since ρ vanishes outside of B_1 , a Fourier pseudospectral approximation on the doubled domain B_2 suffices [9]. The corresponding Fourier coefficients are computed by means of FFT-based trapezoidal quadratures.

The application of the Laplace operator appearing in (3) is then carried out by means of the Fourier symbol of Δ . For an L -periodic function f , by integration by parts, since the boundary terms vanish due to periodicity,

$$\widehat{\partial_{x_j}^2 f}(k) = -\left(\frac{2\pi k_j}{L}\right)^2 \hat{f}_k, \quad \text{and thus} \quad \widehat{\Delta f}(k) = -\left(\frac{2\pi}{L}\right)^2 |k|^2 \hat{f}_k.$$

With $v = V * \rho$, the convolution theorem yields $\hat{v}(k) = \hat{V}_k \hat{\rho}_k$, and therefore $\widehat{\Delta v}(k) = -\left(\frac{2\pi}{L}\right)^2 |k|^2 \hat{V}_k \hat{\rho}_k$. For $L = 2$ one thus obtains from (4) by spectral differentiation the representation

$$u(x) = \sum_k \widehat{\Delta v}(k) e^{\pi i k \cdot x} = -\pi^2 \sum_k |k|^2 \hat{V}_k \hat{\rho}_k e^{\pi i k \cdot x}, \quad (5)$$

with the kernel Fourier integrals

$$\hat{V}_k = \int_{B_2} \frac{|y|}{8\pi} e^{-\pi i k \cdot y} dy. \quad (6)$$

The sum (5) is evaluated by means of inverse FFT.

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2.3. Gaussian-Sum Approximation of the Kernel

The kernel Fourier coefficients (6) are both computationally expensive and numerically demanding. To make this step efficient and to shift a substantial part of the computational effort into a precomputation phase, we approximate the kernel $|y|$ by a separable Gaussian-sum. This reduces the computation of the three-dimensional coefficients to sums of tensor products of one-dimensional integrals.

The basis of the Gaussian-sum approximation is the following integral representation, which follows from the Gamma/Laplace transform:

$$\frac{1}{|y|} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-|y|^2 t^2} dt. \quad (7)$$

To approximate the integral (7) we use sinc quadrature [8, 9, 13]. Here the integral is approximated by the truncated quadrature rule

$$\int_{\mathbb{R}} f(x) dx \approx h \sum_{|k| \leq S} f(kh)$$

The associated error estimate is provided by the following proposition.

Proposition 1 ([13, Prop. 2.1], [9, Prop. 1]). *Let $f \in H^1(D_\lambda)$ with $\lambda < \pi/2$, where*

$$D_\lambda := \{z \in \mathbb{C} : |\Im z| < \lambda\}, \quad N(f, D_\lambda) := \int_{\mathbb{R}} (|f(u + i\lambda)| + |f(u - i\lambda)|) du < \infty.$$

If f satisfies the double exponential decay condition, i.e.,

$$|f(t)| \leq C \exp(-b e^{a|t|}) \quad \forall t \in \mathbb{R}, \quad a, b, C > 0,$$

then for the quadrature error with step size $h = \ln(2\pi a S/b)/(aS)$ the estimate

$$\left| \int_{\mathbb{R}} f(t) dt - h \sum_{|k| \leq S} f(kh) \right| \leq C N(f, D_\lambda) \exp\left(\frac{-2\pi\lambda a S}{\ln(2\pi a S/b)}\right)$$

holds.

After the variable substitution $t = \sinh(\omega)$ one obtains

$$\frac{1}{|y|} = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-|y|^2 \sinh^2(\omega)} \cosh(\omega) d\omega. \quad (8)$$

The transformed integrand satisfies the assumptions of Proposition 1. From this follows the separable Gaussian-sum approximation

$$\frac{1}{8\pi|y|} \approx \sum_{s=0}^S \omega_s \prod_{p=1}^3 e^{-\alpha_s y_p^2}, \quad (9)$$

with

$$\omega_0 = \frac{h}{8\pi^{3/2}}, \quad \alpha_0 = 0, \quad \omega_s = \frac{2h}{8\pi^{3/2}} \cosh(sh), \quad \alpha_s = \sinh^2(sh), \quad s \geq 1.$$

Multiplying the approximation (9) by $|y|^2$ yields an approximation of the biharmonic kernel $V(y) = \frac{|y|}{8\pi}$,

$$V(y) \approx V_{\text{GS}}(y) = \sum_{s=0}^S \omega_s |y|^2 e^{-\alpha_s |y|^2} = \sum_{s=0}^S \omega_s (y_1^2 + y_2^2 + y_3^2) \prod_{p=1}^3 e^{-\alpha_s y_p^2}.$$

Splitting the factor $|y|^2$ into the individual coordinates yields the separable form

$$V_{\text{GS}}(y) = \sum_{s=0}^S \sum_{q=1}^3 \omega_s \prod_{p=1}^3 \begin{cases} y_p^2 e^{-\alpha_s y_p^2}, & p = q, \\ e^{-\alpha_s y_p^2}, & p \neq q, \end{cases} \quad (10)$$

thus a sum of rank-3-separable functions. Substituting (10) into (6), the three-dimensional integral factorizes into products of one-dimensional integrals. Since the appearing factors $y_p^m e^{-\alpha_s y_p^2}$ are even in y_p , upon integration over the symmetric interval $[-1, 1]$ the sine part of $e^{-i\pi k_p y_p}$ vanishes, and only the cosine part remains. Thus, using the definitions

$$I_0(k; \alpha) = \int_0^1 2e^{-\alpha y^2} \cos(\pi k y) dy, \quad I_2(k; \alpha) = \int_0^1 2y^2 e^{-\alpha y^2} \cos(\pi k y) dy,$$

the approximation

$$\hat{V}_k \approx \hat{V}_k^{\text{GS}} = \sum_{s=0}^S \omega_s \sum_{q=1}^3 \prod_{p=1}^3 \begin{cases} I_2(k_p; \alpha_s), & p = q, \\ I_0(k_p; \alpha_s), & p \neq q. \end{cases}$$

The kernel coefficients can thus be efficiently determined in a precomputation phase.

2.4. Algorithmic Realization

The method is divided into a one-time precomputation phase for determining the kernel coefficients and an FFT-based solution phase for given densities ρ . For $N = n_1 n_2 n_3$ grid points, this yields a complexity of $\mathcal{O}(N \log N)$.

Algorithm 1 Precomputation (once per configuration (ε, B_2, N))

Require: Truncation parameter ε , Gaussian-sum rank S , sinc step size h , grid dimensions (n_1, n_2, n_3)

Ensure: Precomputed kernel coefficients $\hat{V}_k^{\text{GS}}$

- 1: Compute Gaussian-sum parameters (ω_s, α_s) , $s = 0, \dots, S$
 - 2: Compute kernel coefficients $\hat{V}_k^{\text{GS}}$ via one-dimensional quadratures
 - 3: Create FFT plans on the doubled grid
-

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Algorithm 2 Solution phase for given density ρ

Require: Sample values of ρ on the $(n_1 \times n_2 \times n_3)$ grid; precomputation results from Algorithm 1

Ensure: Approximate solution u_h on the original grid

- 1: Zero-padding of ρ to the doubled domain B_2
 - 2: Compute Fourier coefficients $\hat{\rho}_k$ by means of FFT
 - 3: Compute $\hat{u}_k = -\pi^2 |k|^2 \hat{V}_k^{\text{GS}} \hat{\rho}_k$
 - 4: Compute u by means of inverse FFT and restrict to the original grid
-

2.5. Error Analysis

The error analysis of the Poisson case consists of two components: a kernel approximation error, which arises from replacing the biharmonic kernel V by its Gaussian-sum approximation V_{GS} , and a discretization error, which results from the spectral resolution on a finite grid. The kernel error is controlled by the following localization lemma. The linear behavior $V(y) = \frac{|y|}{8\pi}$ at the origin suppresses the near-field contribution of the ball $B_\varepsilon(0)$ without near-field correction.

Lemma 2 ([10, Lemma 1]). *Let $\varepsilon > 0$, let ρ be bounded, and suppose $\left| \frac{|y|}{8\pi} - V_{\text{GS}}(y) \right| = \mathcal{O}(\varepsilon^4)$ for $|y| \in (\varepsilon, 1]$. Then for $x \in B_1$*

$$v(x) = \int_{B_2} \frac{|y|}{8\pi} \rho(x-y) dy = \int_{B_2} V_{\text{GS}}(y) \rho(x-y) dy + \mathcal{O}(\varepsilon^4).$$

Thus the kernel error of the super-potential is of fourth order in ε , uniformly in the target points $x \in B_1$. The subsequent application of the Laplace operator is carried out spectrally in the discrete method. On the space of resolved Fourier modes this operator is bounded, so that the order $\mathcal{O}(\varepsilon^4)$ is preserved according to Proposition 2 in [10].

The a priori bound [10, Thm. 3] combines the near-field term, the outer kernel error on $(\varepsilon, \delta]$, and the spectral projection error for smooth densities to

$$\|u - u_h\|_{\ell^\infty(B_1)} = \mathcal{O}(\varepsilon^4) + (\text{spectral in } N),$$

uniformly for all target points $x \in B_1$. The essential point for the subsequent chapters is that the Poisson case achieves fourth order in the truncation parameter ε through the regularity of the biharmonic kernel.

3. The Mixed-Screened Super-Potential Approach

We consider the screened Poisson equation (2) with compactly supported density $\rho \in L^\infty(\mathbb{R}^3)$, $\text{supp } \rho \subset B_1$. Since $\rho(x - y) = 0$ for $y \notin B_2$, the solution can be represented as

$$u(x) = (G * \rho)(x) = \int_{B_2} G(|y|) \rho(x - y) dy.$$

As in the Poisson case, we replace the direct evaluation of this convolution by the introduction of a super-potential with a kernel non-singular at the origin.

3.1. Kernel Construction and Fundamental Solution

Analogously to the Poisson case (cf. 2.1), we introduce a super-potential w by

$$u = -\Delta w. \tag{11}$$

In contrast to the Poisson case, an additional minus sign appears here. This choice proves to be natural for the screened Poisson equation and is motivated by the subsequent construction of the kernel W .

In order to represent w explicitly, we need a kernel W that yields the super-potential as a convolution $w = W * \rho$. We define

$$W(r) := \frac{1}{\kappa^2} (U(r) - G(r)) = \frac{1 - e^{-\kappa r}}{4\pi\kappa^2 r}.$$

The following statement justifies this definition.

Lemma 3 (W as Fundamental Solution). *The kernel W is the fundamental solution of the operator $(-\Delta)(-\Delta + \kappa^2)$, i.e. $(-\Delta)(-\Delta + \kappa^2)W = \delta_0$ in the sense of distributions.*

Proof. It is known that $-\Delta U = \delta_0$, $(-\Delta + \kappa^2)G = \delta_0$ hold in the sense of distributions, where G is the Yukawa fundamental solution. From the second identity it follows that $-\Delta G = \delta_0 - \kappa^2 G$. Therefore $-\Delta W = \frac{1}{\kappa^2}(-\Delta U + \Delta G) = \frac{1}{\kappa^2}(\delta_0 - (\delta_0 - \kappa^2 G)) = G$. Applying $(-\Delta + \kappa^2)$ yields

$$(-\Delta)(-\Delta + \kappa^2)W = (-\Delta + \kappa^2)(-\Delta W) = (-\Delta + \kappa^2)G = \delta_0. \quad \square$$

Thus $w = W * \rho$ is the desired super-potential, and from (11) follows the solution representation

$$u(x) = -\Delta w(x) = -\Delta(W * \rho)(x).$$

3. The Mixed-Screened Super-Potential Approach

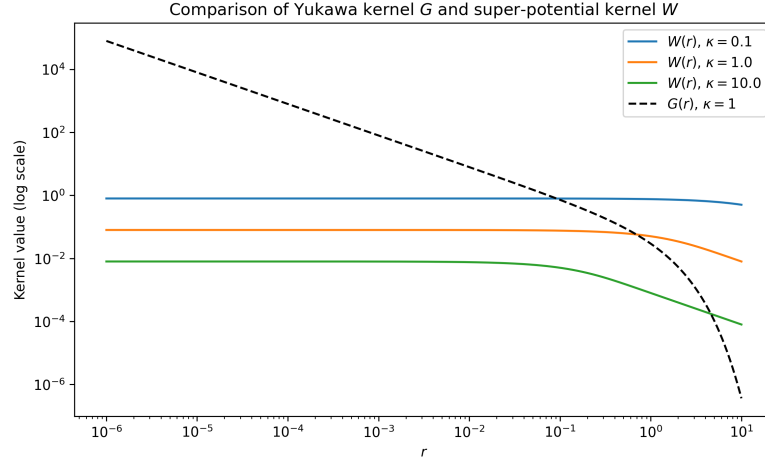


Figure 3.1.: Comparison of the super-potential kernel $W(r)$ with the Yukawa kernel $G(r)$ for various κ -values. While G grows unboundedly as $r \rightarrow 0$, W converges to the finite limit $W(0) = \frac{1}{4\pi\kappa}$.

3.2. Regularity of the Kernel and Near-Field Order

The behavior of W at the origin distinguishes the W -approach from both the Yukawa kernel G and the biharmonic kernel V of the Poisson case, and is decisive for the achievable accuracy of the Gaussian-sum approximation. Using the Taylor expansion, one obtains

$$e^{-\kappa r} = 1 - \kappa r + \frac{\kappa^2 r^2}{2} - \frac{\kappa^3 r^3}{6} + \frac{\kappa^4 r^4}{24} + \mathcal{O}(r^5),$$

from which

$$W(r) = \frac{1}{4\pi\kappa} - \frac{r}{8\pi} + \frac{\kappa r^2}{24\pi} - \frac{\kappa^2 r^3}{96\pi} + \mathcal{O}(r^4)$$

follows. In particular, $W(0) = \frac{1}{4\pi\kappa}$, so the kernel is bounded at the origin and continuously extendable. This stands in contrast to the Yukawa kernel $G(r) = \frac{e^{-\kappa r}}{4\pi r}$, which has a non-removable $1/r$ -singularity at $r = 0$ (cf. Figure 3.1). Compared to the singular kernel G , the introduction of the super-potential thus represents a substantial gain. In contrast to the biharmonic kernel $V(r) = \frac{r}{8\pi}$ of the Poisson case (cf. 2.1), however, W does not vanish at the origin, so that the near-field contribution is not suppressed by the vanishing of the kernel. The consequences of this property for the achievable error order are investigated in 3.4.2.

3.3. Gaussian-Sum Approximation of the Kernel

Analogously to the Poisson case (cf. 2.3), we approximate the kernel W by a separable Gaussian-sum of the form

$$W_{\text{GS}}(r) := \sum_{j=M_1}^{M_2} \omega_j e^{-\tau_j^2 r^2} \approx W(r), \quad r \in [\varepsilon, \delta], \quad (12)$$

in order to enable the FFT-based evaluation of the convolution $w = W * \rho$. Here $\delta > 0$ denotes an upper bound for the support of ρ and $\varepsilon > 0$ a lower bound of the approximation interval.

3.3.1. Indirect Construction

A natural approach to constructing a Gaussian-sum approximation for W consists in exploiting the decomposition $W = (U - G)/\kappa^2$. Since Gaussian-sum approximations U_{GS} and G_{GS} for the Coulomb and Yukawa kernel, respectively, are separately available, their difference

$$W_{\text{GS}}^{\text{ind}}(r) := \frac{1}{\kappa^2} (U_{\text{GS}}(r) - G_{\text{GS}}(r))$$

yields an approximation of W . For the Coulomb part, the approximation of $U(r) = \frac{1}{4\pi r}$ follows from the integral representation (8) by means of sinc quadrature with step size h :

$$U_{\text{GS}}(r) = \sum_{k=0}^S \omega_k^U e^{-(\alpha_k^U)^2 r^2}, \quad \omega_k^U = \frac{2h}{4\pi^{3/2}} \cosh(kh), \quad \alpha_k^U = \sinh(kh), \quad k > 0,$$

where $\omega_0^U = h/(4\pi^{3/2})$ and $\alpha_0^U = 0$.

For the Yukawa part, following [3, 5, 12], one obtains by the variable transformation $t = e^u$ and subsequent sinc quadrature with step size h

$$G_{\text{GS}}(r) = \sum_{m=-M_1}^{M_2} \omega_m^G e^{-(\alpha_m^G)^2 r^2}, \quad \omega_m^G = \frac{h}{2\pi^{3/2}} e^{t_m} e^{-\frac{\kappa^2}{4} e^{-2t_m}}, \quad \alpha_m^G = e^{t_m}, \quad t_m = mh.$$

By combining both representations, one obtains the Gaussian-sum approximation of W with a total of $S + M_1 + M_2 + 2$ Gaussian terms. Since the Coulomb and Yukawa kernels each satisfy the assumptions of Proposition 1 [9, 12], the quadrature error of the individual approximations U_{GS} and G_{GS} decreases exponentially in the number of terms. Since the approximations of U and G are performed independently of one another, the error estimate follows immediately from the triangle inequality

$$\sup_{r \in [\varepsilon, \delta]} |W(r) - W_{\text{GS}}^{\text{ind}}(r)| \leq \frac{1}{\kappa^2} (\varepsilon_U + \varepsilon_G),$$

where ε_U and ε_G denote the absolute approximation errors of U_{GS} and G_{GS} , respectively, on $[\varepsilon, \delta]$.

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This construction, however, exhibits structural disadvantages. For small values of κ , the kernels U and G closely approach one another, so that the computation of $W = (U - G)/\kappa^2$ relies on the difference of two nearly equal quantities. Rounding errors can be significantly amplified by cancellation, as Figure 3.2 illustrates. Furthermore, the errors ε_U and ε_G add up, and the boundedness of W at the origin is not exploited, since the approximation proceeds via the difference of two singular kernels. This motivates the development of a direct Gaussian-sum approximation of W .

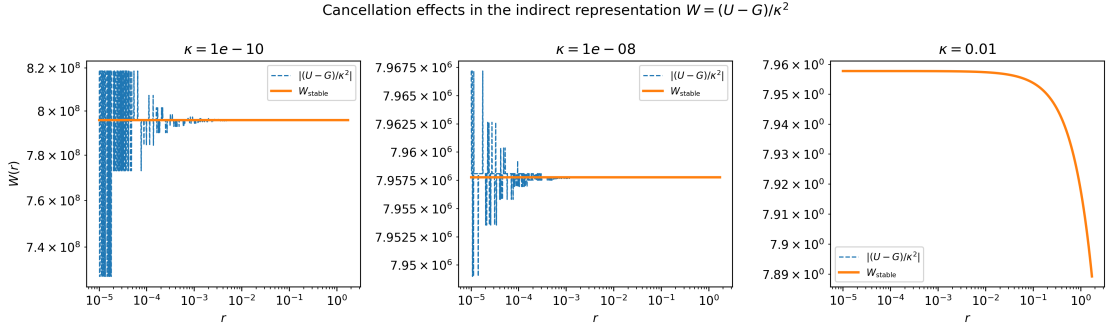


Figure 3.2.: Cancellation effects in the indirect representation $W = (U - G)/\kappa^2$ for small κ . The direct representation $W = (1 - e^{-\kappa r})/(4\pi\kappa^2 r)$ remains stable (analytically, before GS discretization).

3.3.2. Direct Construction

The starting point of the direct approximation are the standard Gaussian integral representations of the Coulomb and Yukawa kernels. We recall the Gaussian integral representation of the Coulomb kernel (cf. 2.3)

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-r^2 t^2} dt = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-r^2 e^{2u}} e^u du,$$

where the second equality follows from the substitution $t = e^u$, $dt = e^u du$. For the Yukawa kernel, the following holds (cf. [12], Eq. (2.1))

$$\frac{e^{-\kappa r}}{4\pi r} = \frac{1}{2\pi^{3/2}} \int_0^\infty e^{-r^2 t^2 - \frac{\kappa^2}{4t^2}} dt = \frac{1}{2\pi^{3/2}} \int_{\mathbb{R}} e^{-r^2 e^{2u} - \frac{\kappa^2}{4} e^{-2u}} e^u du.$$

By combining both representations and using $W(r) = \frac{1 - e^{-\kappa r}}{4\pi\kappa^2 r}$, one obtains

$$\begin{aligned} W(r) &= \frac{1}{4\pi\kappa^2} \cdot \frac{2}{\sqrt{\pi}} \left(\int_0^\infty e^{-r^2 t^2} dt - \int_0^\infty e^{-r^2 t^2 - \frac{\kappa^2}{4t^2}} dt \right) \\ &= \frac{1}{2\pi^{3/2}\kappa^2} \int_0^\infty e^{-r^2 t^2} \left(1 - e^{-\frac{\kappa^2}{4t^2}} \right) dt. \end{aligned} \quad (13)$$

3.3. Gaussian-Sum Approximation of the Kernel

Logarithmic Transformation

Analogously to the strategy in [9] for the Coulomb kernel and in [12] for the Yukawa kernel, we apply the substitution $\tau = e^u$, $d\tau = e^u du$. This transforms (13) to

$$W(r) = \frac{1}{2\pi^{3/2}\kappa^2} \int_{\mathbb{R}} f(u, r) du, \quad f(u, r) := \left(1 - e^{-\frac{\kappa^2}{4}e^{-2u}}\right) e^{-r^2 e^{2u}} e^u,$$

for $r \in [\varepsilon, \delta]$. Sinc quadrature with step size h and nodes $u_j = jh$ formally yields the Gaussian-sum structure (12) with

$$\tau_j = e^{jh}, \quad \omega_j = \frac{h}{2\pi^{3/2}\kappa^2} e^{jh} \left(1 - e^{-\frac{\kappa^2}{4}e^{-2jh}}\right).$$

The application of Proposition 1 for error analysis requires that the integrand $f(\cdot, r)$ satisfies two conditions:

1. $f(\cdot, r) \in H^1(D_\lambda)$ for some $\lambda < \pi/2$,
2. the double exponential decay condition.

However, the double exponential decay condition is satisfied for this transformation only on one side, as the following analysis shows. For $u \rightarrow +\infty$, from $r \geq \varepsilon$ and $|1 - e^{-\frac{\kappa^2}{4}e^{-2u}}| \leq 1$ it follows that

$$|f(u, r)| \leq e^u e^{-r^2 e^{2u}} \leq e^u e^{-\varepsilon^2 e^{2u}} \leq C e^{-c e^{2u}},$$

for suitable constants $C, c > 0$, hence double exponential decay. For $u \rightarrow -\infty$, on the other hand, $1 - e^{-\frac{\kappa^2}{4}e^{-2u}} \rightarrow 1$ and $e^{-r^2 e^{2u}} \rightarrow 1$, so that for sufficiently negative u

$$|f(u, r)| \leq e^u = e^{-|u|},$$

hence only singly exponential decay. The logarithmic transformation thus formally yields a Gaussian-sum structure, but not the double exponential decay structure required for Proposition 1.

Sinh Transformation

As an alternative to the logarithmic transformation, we consider the sinh transformation

$$t = \phi(u) := e^{\sigma \sinh u}, \quad \sigma > 0,$$

with Jacobian $\phi'(u) = \sigma \cosh(u) e^{\sigma \sinh u}$. Substituting into (13) yields

$$W(r) = \frac{1}{2\pi^{3/2}\kappa^2} \int_{\mathbb{R}} g(u) du, \quad g(u) := e^{-r^2 e^{2\sigma \sinh u}} \left(1 - e^{-\frac{\kappa^2}{4}e^{-2\sigma \sinh u}}\right) \sigma \cosh(u) e^{\sigma \sinh u}.$$

The truncated trapezoidal rule with step size h and nodes $u_j = jh$ yields the Gaussian-sum structure (12) with nodes and weights

$$\tau_j := e^{\sigma \sinh(jh)}, \quad \omega_j := \frac{h \sigma \cosh(jh)}{2\pi^{3/2}\kappa^2} e^{\sigma \sinh(jh)} \left(1 - e^{-\frac{\kappa^2}{4}e^{-2\sigma \sinh(jh)}}\right).$$

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This transformation generates double exponential decay in both directions. However, it is not compatible with the strip analysis of Proposition 1. For $z = u + i\lambda$ with $u \rightarrow -\infty$ we have

$$\Re(\sinh(u + i\lambda)) = \sinh(u) \cos \lambda \sim -\frac{1}{2}e^{|u|} \cos \lambda,$$

so that for $|\lambda| < \pi/2$

$$\Re(-2\sigma \sinh(u + i\lambda)) \sim \sigma e^{|u|} \cos \lambda \rightarrow +\infty.$$

The expression $e^{-2\sigma \sinh(u+i\lambda)}$ thus grows super-exponentially along the boundary lines of the strip, and the transformed integrand is not controllable there. A direct application of Proposition 1 is therefore not possible for the sinh transformation either.

Choice of Transformation

This reveals a fundamental conflict of objectives: the logarithmic transformation $\tau = e^u$ satisfies the strip condition, but does not yield double exponential decay for $u \rightarrow -\infty$. The sinh transformation generates double exponential decay in both directions, but fails the strip condition. Neither of the two transformations simultaneously satisfies all assumptions of Proposition 1.

The numerical comparison (Figure 3.3) shows that the logarithmic transformation consistently requires fewer terms in the practically relevant accuracy range ($\eta \lesssim 10^{-6}$) and reliably achieves the desired accuracy with well-controllable parameter scaling. Since it also leads to a simpler analytic structure, the error analysis in 3.4.1 is carried out exclusively for the logarithmic transformation.

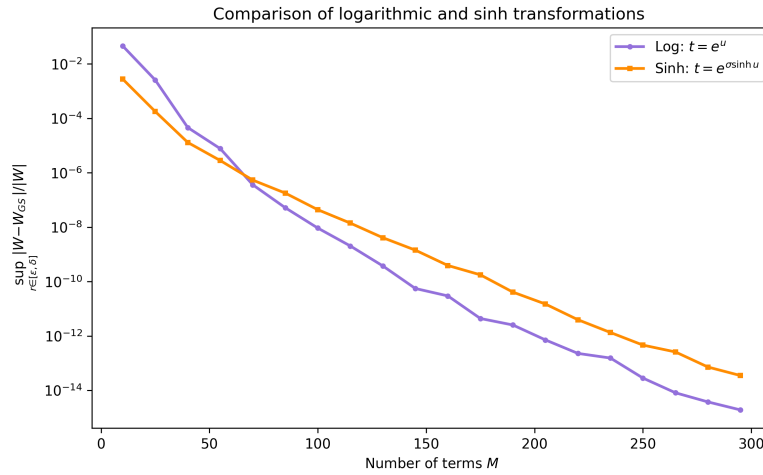


Figure 3.3.: Approximation error $\sup_{r \in [\epsilon, \delta]} |W - W_{\text{GS}}|$ as a function of the number of terms M for the logarithmic transformation and the sinh transformation, each with optimized parameters h , M_1 , M_2 (and σ for sinh).

3.4. Error Analysis

3.4.1. Error of the Gaussian-Sum Approximation

Since Proposition 1 is not directly applicable, we analyze the error of the truncated trapezoidal rule directly. For $r \in [\varepsilon, \delta]$, with the integrand $f(u, r)$ defined after the logarithmic transformation in 3.3.2, we have

$$W(r) - W_{\text{GS}}(r) = \frac{1}{2\pi^{3/2}\kappa^2} \left(\int_{\mathbb{R}} f(u, r) du - h \sum_{j=M_1}^{M_2} f(jh, r) \right).$$

For arbitrary truncation parameters $M_1, M_2 \in \mathbb{Z}$, one decomposes the difference into three contributions,

$$\begin{aligned} \int_{\mathbb{R}} f(u, r) du - h \sum_{j=M_1}^{M_2} f(jh, r) &= \underbrace{\left(\int_{\mathbb{R}} f(u, r) du - h \sum_{j \in \mathbb{Z}} f(jh, r) \right)}_{=: E_{\text{trap}}(r)} \\ &\quad + \underbrace{h \sum_{j < M_1} f(jh, r)}_{=: E_{\text{left}}(r)} + \underbrace{h \sum_{j > M_2} f(jh, r)}_{=: E_{\text{right}}(r)}. \end{aligned} \quad (14)$$

where $E_{\text{trap}}(r)$ denotes the error of the infinite trapezoidal rule and $E_{\text{left}}(r)$, $E_{\text{right}}(r)$ denote the truncation errors at the left and right boundary, respectively. Setting $\tilde{\eta} := \frac{2\pi^{3/2}\kappa^2}{3} \eta$, it suffices to bound each of the three terms by $\tilde{\eta}$, since then it follows that

$$|W(r) - W_{\text{GS}}(r)| \leq \frac{1}{2\pi^{3/2}\kappa^2} (|E_{\text{trap}}(r)| + |E_{\text{left}}(r)| + |E_{\text{right}}(r)|) \leq \eta.$$

The three contributions are estimated separately and uniformly in $r \in [\varepsilon, \delta]$ in what follows.

Error Estimate for the Trapezoidal Rule

To estimate the trapezoidal error, we first examine the analytic properties of the transformed integrand. This subsequently enables the application of a general result for analytic functions in complex strips.

Proposition 4 (Analytic Properties of the Integrand). *Let $0 < \varepsilon < \delta < \infty$, $\kappa > 0$ and $0 < \lambda < \pi/4$. For the integrand*

$$f(u, r) := (1 - e^{-\kappa^2 e^{-2u}/4}) e^{-r^2 e^{2u}} e^u, \quad u \in \mathbb{R}, \quad r \in [\varepsilon, \delta],$$

the following statements hold.

- (i) $f(\cdot, r)$ has a holomorphic continuation to $D_\lambda := \{z \in \mathbb{C} : |\Im z| < \lambda\}$.

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(ii) $f(u + i\sigma, r) \rightarrow 0$ as $|u| \rightarrow \infty$, uniformly in $\sigma \in (-\lambda, \lambda)$ and $r \in [\varepsilon, \delta]$.

(iii) With $c_\lambda := \varepsilon^2 \cos(2\lambda) > 0$ we have

$$\sup_{r \in [\varepsilon, \delta]} \int_{\mathbb{R}} |f(u + i\sigma, r)| du \leq \frac{\sqrt{\pi}}{\sqrt{c_\lambda}} \quad \text{for all } \sigma \in (-\lambda, \lambda).$$

Proof. (i) Since e^{2z} , e^{-2z} and e^z are entire functions and sums, products, and compositions of holomorphic functions remain holomorphic, $f(\cdot, r)$ is holomorphic in D_λ .

(ii) and (iii) Let $z = u + i\sigma$ with $|\sigma| < \lambda < \pi/4$. Then $\cos(2\sigma) \geq \cos(2\lambda) > 0$. For the first factor, one obtains due to $\Re(e^{-2z}) = e^{-2u} \cos(2\sigma) \geq 0$

$$\left| e^{-\kappa^2 e^{-2z}/4} \right| = \exp\left(-\frac{\kappa^2}{4} e^{-2u} \cos(2\sigma)\right) \leq 1.$$

Therefore it follows from the triangle inequality that $\left| 1 - e^{-\kappa^2 e^{-2z}/4} \right| \leq 2$. For the second factor, since $r \geq \varepsilon$:

$$\left| e^{-r^2 e^{2z}} \right| = \exp(-r^2 e^{2u} \cos(2\sigma)) \leq \exp(-\varepsilon^2 e^{2u} \cos(2\lambda)) = e^{-c_\lambda e^{2u}},$$

where $c_\lambda := \varepsilon^2 \cos(2\lambda) > 0$. For the third factor we have $|e^z| = e^u$, so that altogether the pointwise bound is obtained:

$$|f(u + i\sigma, r)| \leq 2e^u e^{-c_\lambda e^{2u}}. \quad (15)$$

For $u \rightarrow -\infty$ we have $e^u \rightarrow 0$. For $u \rightarrow +\infty$ the factor $e^{-c_\lambda e^{2u}}$ dominates super-exponentially. It therefore follows from (15) that

$$f(u + i\sigma, r) \rightarrow 0 \quad (|u| \rightarrow \infty)$$

uniformly in $\sigma \in (-\lambda, \lambda)$ and $r \in [\varepsilon, \delta]$. This proves (ii). Integrating (15) and the substitution $t = e^u$ yield

$$\int_{\mathbb{R}} |f(u + i\sigma, r)| du \leq \int_{\mathbb{R}} 2e^u e^{-c_\lambda e^{2u}} du = 2 \int_0^\infty e^{-c_\lambda t^2} dt = \frac{\sqrt{\pi}}{\sqrt{c_\lambda}}.$$

Since the right-hand side is independent of r and σ , (iii) follows. $\square$

The following error estimate for the infinite trapezoidal rule is due to Trefethen and Weideman [16].

Theorem 5 ([16, Theorem 5.1]). *Suppose w is analytic in the strip $|\operatorname{Im}(x)| < a$ for some $a > 0$. Suppose further that $w(x) \rightarrow 0$ uniformly as $|x| \rightarrow \infty$ in the strip, and for some M , it satisfies*

$$\int_{-\infty}^\infty |w(x + ib)| dx \leq M$$

for all $b \in (-a, a)$. Then, for any $h > 0$, $I_h := h \sum_{j \in \mathbb{Z}} w(jh)$ exists and satisfies

$$\left| I_h - \int_{\mathbb{R}} w(x) dx \right| \leq \frac{2M}{e^{2\pi a/h} - 1},$$

and the quantity $2M$ in the numerator is as small as possible.

Corollary 6 (Trapezoidal Error for the Integrand f). *Let $0 < \varepsilon < \delta < \infty$, $0 < \lambda < \pi/4$ and $c_\lambda := \varepsilon^2 \cos(2\lambda) > 0$. Let $f(\cdot, r)$ be as in Proposition 4. Then for every $h > 0$*

$$E_{\text{trap}}(r) := \int_{\mathbb{R}} f(u, r) du - h \sum_{j \in \mathbb{Z}} f(jh, r)$$

the uniform estimate

$$\sup_{r \in [\varepsilon, \delta]} |E_{\text{trap}}(r)| \leq \frac{2\sqrt{\pi}}{\sqrt{c_\lambda}} \frac{1}{e^{2\pi\lambda/h} - 1}$$

holds.

Proof. The conditions (i)–(iii) from Proposition 4 are precisely the assumptions of Theorem 5 with $a = \lambda$ and $M = \frac{\sqrt{\pi}}{\sqrt{c_\lambda}}$. Direct application yields the claimed bound. $\square$

The corollary provides an explicit condition on the step size h to keep the trapezoidal error below the auxiliary error $\tilde{\eta}$. Setting $C_\lambda := \frac{2\sqrt{\pi}}{\sqrt{c_\lambda}}$, the choice

$$h \leq \frac{2\pi\lambda}{\log(1 + C_\lambda/\tilde{\eta})}$$

suffices to ensure $\sup_{r \in [\varepsilon, \delta]} |E_{\text{trap}}(r)| \leq \tilde{\eta}$.

Left Truncation Error

Next, the truncation error at the left boundary of the infinite trapezoidal sum is controlled.

Proposition 7 (Left Truncation Error). *Let $0 < \varepsilon < \delta < \infty$, $h > 0$ and $f(\cdot, r)$ be as in Proposition 4. For $E_{\text{left}}(r) := h \sum_{j < M_1} f(jh, r)$ the uniform estimate*

$$\sup_{r \in [\varepsilon, \delta]} |E_{\text{left}}(r)| \leq \frac{h e^{(M_1-1)h}}{1 - e^{-h}}$$

holds for every $M_1 \in \mathbb{Z}$.

Proof. For every $j < M_1$ and every $r \in [\varepsilon, \delta]$ we have $0 \leq 1 - e^{-\kappa^2 e^{-2jh}/4} \leq 1$, $0 < e^{-r^2 e^{2jh}} \leq 1$. Therefore it follows that $|f(jh, r)| \leq e^{jh}$. Thus, with the index change $m = M_1 - 1 - j \geq 0$ and a geometric series, one obtains

$$|E_{\text{left}}(r)| \leq h \sum_{j < M_1} |f(jh, r)| \leq h \sum_{j=-\infty}^{M_1-1} e^{jh} = h e^{(M_1-1)h} \sum_{m=0}^{\infty} e^{-mh} = \frac{h e^{(M_1-1)h}}{1 - e^{-h}}.$$

Since the right-hand side is independent of r , the claimed uniform estimate follows immediately. $\square$

Therefore, the choice

$$M_1 \leq M_1^*, \quad M_1^* := \left\lceil 1 + \frac{1}{h} \log \left(\frac{\tilde{\eta}(1 - e^{-h})}{h} \right) \right\rceil$$

suffices to ensure $\sup_{r \in [\varepsilon, \delta]} |E_{\text{left}}(r)| \leq \tilde{\eta}$.

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Right Truncation Error

It remains to estimate the truncation error at the right boundary of the infinite trapezoidal sum.

Proposition 8 (Right Truncation Error). *Let $0 < \varepsilon < \delta < \infty$, $h > 0$ and $f(\cdot, r)$ be as in Proposition 4. For $E_{\text{right}}(r) := h \sum_{j > M_2} f(jh, r)$ the uniform estimate*

$$\sup_{r \in [\varepsilon, \delta]} |E_{\text{right}}(r)| \leq \frac{1}{2\varepsilon^2 e^{M_2 h}} e^{-\varepsilon^2 e^{2M_2 h}}$$

holds under the constraint $\varepsilon^2 e^{2M_2 h} \geq 1$.

Proof. For $r \in [\varepsilon, \delta]$ and all $u \in \mathbb{R}$ we have $0 \leq 1 - e^{-\kappa^2 e^{-2u}/4} \leq 1$, so that due to $r \geq \varepsilon$ $|f(u, r)| \leq e^u e^{-r^2 e^{2u}} \leq e^u e^{-\varepsilon^2 e^{2u}}$. Thus it follows that

$$|E_{\text{right}}(r)| \leq h \sum_{j=M_2+1}^{\infty} e^{jh} e^{-\varepsilon^2 e^{2jh}}.$$

With $g(u) := e^u e^{-\varepsilon^2 e^{2u}}$ we have $g'(u) = e^u e^{-\varepsilon^2 e^{2u}} (1 - 2\varepsilon^2 e^{2u})$, so g is monotonically decreasing for $\varepsilon^2 e^{2u} \geq \frac{1}{2}$. Under the constraint $\varepsilon^2 e^{2M_2 h} \geq 1 \geq \frac{1}{2}$, g is in particular monotonically decreasing for all $u \geq M_2 h$. Therefore $g(jh) \leq \frac{1}{h} \int_{(j-1)h}^{jh} g(u) du$ holds for all $j \geq M_2 + 1$, and by summation it follows that

$$h \sum_{j=M_2+1}^{\infty} g(jh) \leq \int_{M_2 h}^{\infty} g(u) du.$$

With the substitution $t = e^u$ one obtains

$$\int_{M_2 h}^{\infty} e^u e^{-\varepsilon^2 e^{2u}} du = \int_{e^{M_2 h}}^{\infty} e^{-\varepsilon^2 t^2} dt.$$

The standard estimate $\int_x^{\infty} e^{-\varepsilon^2 t^2} dt \leq \frac{1}{2\varepsilon^2 x} e^{-\varepsilon^2 x^2}$, $x > 0$, applied with $x = e^{M_2 h}$ yields

$$|E_{\text{right}}(r)| \leq \frac{1}{2\varepsilon^2 e^{M_2 h}} e^{-\varepsilon^2 e^{2M_2 h}}.$$

Since the right-hand side is independent of r , the claimed uniform estimate follows. $\square$

With $s := \varepsilon^2 e^{2M_2 h}$, the condition

$$\frac{1}{2\varepsilon^2 e^{M_2 h}} e^{-\varepsilon^2 e^{2M_2 h}} \leq \tilde{\eta} \quad \text{is equivalent to} \quad \frac{1}{2\varepsilon \sqrt{s}} e^{-s} \leq \tilde{\eta}.$$

Since under the constraint $s \geq 1$ we have $\frac{1}{\sqrt{s}} \leq 1$, the sufficient condition is $\frac{1}{2\varepsilon} e^{-s} \leq \tilde{\eta}$, i.e. $s \geq \max\{1, \ln(\frac{1}{2\varepsilon \tilde{\eta}})\}$. Thus the choice

$$M_2 := \left\lceil \frac{1}{2h} \ln \left(\frac{\max\{1, \ln(1/(2\varepsilon \tilde{\eta}))\}}{\varepsilon^2} \right) \right\rceil,$$

suffices, by which the constraint $\varepsilon^2 e^{2M_2 h} \geq 1$ is simultaneously satisfied.

Combining the Error Terms

Theorem 9 (Gaussian-Sum Approximation of the Kernel W). *Let $0 < \varepsilon < \delta < \infty$, $0 < \lambda < \pi/4$, $\kappa > 0$, and $\eta > 0$ be sufficiently small. Set $c_\lambda := \varepsilon^2 \cos(2\lambda)$, $C_\lambda := \frac{2\sqrt{\pi}}{\sqrt{c_\lambda}}$, $\tilde{\eta} := \frac{2\pi^{3/2}\kappa^2}{3} \eta$, $h := \frac{2\pi\lambda}{\ln(1+C_\lambda/\tilde{\eta})}$, and*

$$M_1 := \left\lceil 1 + \frac{1}{h} \log \left(\frac{\tilde{\eta}(1 - e^{-h})}{h} \right) \right\rceil, \quad M_2 := \left\lceil \frac{1}{2h} \ln \left(\frac{\max\{1, \ln(1/(2\varepsilon\tilde{\eta}))\}}{\varepsilon^2} \right) \right\rceil.$$

Then for the Gaussian-sum approximation

$$W_{\text{GS}}(r) := \sum_{j=M_1}^{M_2} \omega_j e^{-\tau_j^2 r^2}, \quad \tau_j := e^{jh}, \quad \omega_j := \frac{h}{2\pi^{3/2}\kappa^2} e^{jh} \left(1 - e^{-\kappa^2 e^{-2jh}/4} \right),$$

the uniform error estimate

$$\sup_{r \in [\varepsilon, \delta]} |W(r) - W_{\text{GS}}(r)| \leq \eta$$

holds. The number of terms is $M := M_2 - M_1 + 1 = \mathcal{O}(\log^2(1/\eta))$ as $\eta \downarrow 0$.

Proof. From the decomposition (14) it follows for all $r \in [\varepsilon, \delta]$ that

$$|W(r) - W_{\text{GS}}(r)| \leq \frac{1}{2\pi^{3/2}\kappa^2} \left(|E_{\text{trap}}(r)| + |E_{\text{left}}(r)| + |E_{\text{right}}(r)| \right).$$

By Corollary 6 and the choice of h we have $\sup_r |E_{\text{trap}}(r)| \leq \tilde{\eta}$. By Proposition 7 and the choice of M_1 we have $\sup_r |E_{\text{left}}(r)| \leq \tilde{\eta}$. By Proposition 8 and the choice of M_2 we have $\sup_r |E_{\text{right}}(r)| \leq \tilde{\eta}$. Thus it follows that

$$\sup_{r \in [\varepsilon, \delta]} |W(r) - W_{\text{GS}}(r)| \leq \frac{3\tilde{\eta}}{2\pi^{3/2}\kappa^2} = \eta.$$

For the number of terms we have $|M_1| = \mathcal{O}(\log(1/\tilde{\eta})/h)$ and $M_2 = \mathcal{O}(\log \log(1/\tilde{\eta})/h)$. Since $h \sim \frac{2\pi\lambda}{\log(1/\tilde{\eta})}$ as $\tilde{\eta} \rightarrow 0$, $|M_1|$ dominates and it follows that $M = \mathcal{O}(\log^2(1/\tilde{\eta}))$. Since $\log(1/\tilde{\eta}) = \log(1/\eta) + \mathcal{O}(1)$, we have $M = \mathcal{O}(\log^2(1/\eta))$. $\square$

The Gaussian-sum approximation W_{GS} is separable in the sense that each summand $e^{-\tau_j^2 r^2} = e^{-\tau_j^2 (x_1^2 + x_2^2 + x_3^2)}$ factorizes as a product of one-dimensional Gaussian functions,

$$e^{-\tau_j^2 r^2} = \prod_{k=1}^3 e^{-\tau_j^2 x_k^2}.$$

The product structure reduces the precomputation of the Fourier coefficients to products of one-dimensional integrals.

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3.4.2. Localization Lemma

Theorem 9 yields with the choice $\delta = 2$ the bound

$$\sup_{r \in [\varepsilon, 2]} |W(r) - W_{\text{GS}}(r)| \leq \eta,$$

which applies on the entire far field $B_2 \setminus B_\varepsilon(0)$, since $|y| \leq \sqrt{3} < 2$ for all $y \in B_2$. We set $w^{\text{GS}} := W_{\text{GS}} * \rho$ and estimate the error $w - w^{\text{GS}}$ on B_1 .

Lemma 10 (Convolution error of the kernel replacement). *Let $\varepsilon > 0$ and $\rho \in L^\infty(\mathbb{R}^3)$ with $\text{supp } \rho \subset B_1$. Suppose $\sup_{r \in [\varepsilon, 2]} |W(r) - W_{\text{GS}}(r)| \leq \eta$. Then for all $x \in B_1$*

$$|(W * \rho)(x) - (W_{\text{GS}} * \rho)(x)| \leq C_{\text{conv}}^W \|\rho\|_{L^\infty} (\eta + \varepsilon^3),$$

where $C_{\text{conv}}^W > 0$ is independent of x , η , and ε .

Proof. Since $\text{supp } \rho \subset B_1$, for all $x \in B_1$

$$(W * \rho)(x) - (W_{\text{GS}} * \rho)(x) = \int_{B_2} (W(|y|) - W_{\text{GS}}(|y|)) \rho(x - y) dy.$$

We decompose the integration domain into near field and far field:

$$\begin{aligned} \int_{B_2} (W(|y|) - W_{\text{GS}}(|y|)) \rho(x - y) dy &= \underbrace{\int_{B_2 \setminus B_\varepsilon(0)} (W(|y|) - W_{\text{GS}}(|y|)) \rho(x - y) dy}_{=: I_{\text{out}}} \\ &\quad + \underbrace{\int_{B_\varepsilon(0)} (W(|y|) - W_{\text{GS}}(|y|)) \rho(x - y) dy}_{=: I_{\text{in}}}. \end{aligned}$$

Far-field term I_{out} . For $y \in B_2 \setminus B_\varepsilon(0)$ we have $\varepsilon \leq |y| \leq \sqrt{3} < 2$, so that by assumption $|W(|y|) - W_{\text{GS}}(|y|)| \leq \eta$. Therefore it follows

$$|I_{\text{out}}| \leq \eta \int_{B_2 \setminus B_\varepsilon(0)} |\rho(x - y)| dy \leq \eta |B_2| \|\rho\|_{L^\infty}.$$

Near-field term I_{in} . Since W is continuous on $[0, \infty)$ with finite limit $W(0) = \frac{1}{4\pi\kappa}$, there exists a constant $C_W > 0$ with $\sup_{r \in [0, \varepsilon]} |W(r)| \leq C_W$. For W_{GS} , since $\omega_j \geq 0$ and $e^{-\tau_j^2 r^2} \leq 1$

$$|W_{\text{GS}}(r)| \leq \sum_{j=M_1}^{M_2} \omega_j e^{-\tau_j^2 r^2} \leq \sum_{j=M_1}^{M_2} \omega_j = W_{\text{GS}}(0) =: C_{\text{GS}}^W.$$

Since $W_{\text{GS}}(0) = \sum_j \omega_j$ represents the trapezoidal sum approximation of $W(0) = \frac{1}{4\pi\kappa}$ and converges to $W(0)$ as $\eta \rightarrow 0$, C_{GS}^W is uniformly bounded in η and ε . With $|B_\varepsilon(0)| = \frac{4\pi}{3} \varepsilon^3$ it follows

$$|I_{\text{in}}| \leq (C_W + C_{\text{GS}}^W) \|\rho\|_{L^\infty} |B_\varepsilon(0)| =: C_{\text{near}}^W \|\rho\|_{L^\infty} \varepsilon^3.$$

Combining both estimates yields

$$|(W * \rho)(x) - (W_{\text{GS}} * \rho)(x)| \leq |B_2| \|\rho\|_{L^\infty} \eta + C_{\text{near}}^W \|\rho\|_{L^\infty} \varepsilon^3 \leq C_{\text{conv}}^W \|\rho\|_{L^\infty} (\eta + \varepsilon^3),$$

with $C_{\text{conv}}^W := \max(|B_2|, C_{\text{near}}^W) > 0$, independent of x , η , and ε . $\square$

Under the coupling condition $\eta \leq C_{\text{coup}}^W \varepsilon^3$, the error order simplifies as follows.

Corollary 11. *If one chooses $\eta \leq C_{\text{coup}}^W \varepsilon^3$ with a constant $C_{\text{coup}}^W > 0$, then under the assumptions of Lemma 10*

$$\sup_{x \in B_1} |(W * \rho)(x) - (W_{\text{GS}} * \rho)(x)| \leq C_{\text{pot}}^W \|\rho\|_{L^\infty} \varepsilon^3,$$

where $C_{\text{pot}}^W := C_{\text{conv}}^W(1 + C_{\text{coup}}^W) > 0$ is independent of ε and x .

Proof. From $\eta \leq C_{\text{coup}}^W \varepsilon^3$ it follows that $\eta + \varepsilon^3 \leq (C_{\text{coup}}^W + 1) \varepsilon^3$. Substituting into the bound from Lemma 10 yields the claim with $C_{\text{pot}}^W := C_{\text{conv}}^W(1 + C_{\text{coup}}^W)$. $\square$

3.4.3. A Priori Error Estimate

Corollary 11 provides a bound for the error of the super-potential $w = W * \rho$ in the ℓ^∞ -norm on B_1 . The numerical solution u_h is however only obtained by the spectral application of the Laplace operator to a Gaussian-sum convolution with the discretized density. The total error $\|u - u_h\|_{\ell^\infty(B_1)}$ therefore consists of a kernel approximation error and a spectral discretization error. We first establish the spectral framework in which the discretization statements are formulated.

For $s \geq 0$, the Sobolev space $H^s(\mathbb{T}^3)$ is defined by the Fourier norm

$$\|\rho\|_{H^s(\mathbb{T}^3)}^2 = \sum_{k \in \mathbb{Z}^3} (1 + |k|^2)^s |\hat{\rho}_k|^2.$$

Let S_N be the space of trigonometric polynomials with frequencies $-N \leq k_j \leq N - 1$ in each coordinate, and let P_N be the L^2 -orthogonal projection onto S_N . The following classical approximation estimate is needed in the proof of the main theorem.

Lemma 12 ([4, Eq. (5.8.4)]). *Let $s \geq m \geq 0$ and $\rho \in H^s(\mathbb{T}^3)$. Then*

$$\|\rho - P_N \rho\|_{H^m(\mathbb{T}^3)} \leq C N^{m-s} \|\rho\|_{H^s(\mathbb{T}^3)},$$

where $C > 0$ is independent of N and ρ .

In the following theorem, the complete a priori bound is derived. It combines the contributions of kernel approximation and spectral discretization into a single inequality.

Theorem 13 (Total Error Estimate, W -Method). *Let $\mu > \frac{3}{2}$ be fixed, $\rho \in H^s(\mathbb{T}^3)$ with $s > \mu$ and $\text{supp } \rho \subset B_1$. The Gaussian-sum approximation W_{GS} is constructed according to Theorem 9 with accuracy $\eta \leq C_{\text{coup}}^W \varepsilon^3$. Let w_h be the grid function computed by*

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Gaussian-sum FFT convolution with W_{GS} , and let $u_h := -\Delta_h w_h$ be the result of the spectral Laplace application. Then

$$\|u - u_h\|_{\ell^\infty(B_1)} \leq C_\Delta(N) C_{\text{pot}}^W \|\rho\|_{L^\infty(\mathbb{T}^3)} \varepsilon^3 + C_{\text{proj}}^W N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)},$$

where $C_{\text{pot}}^W, C_{\text{proj}}^W > 0$ are constants independent of ε and N , and $C_\Delta(N) = \mathcal{O}(N^2)$ denotes the operator norm of the spectral Laplace operator on S_N .

Proof. The total error is decomposed into two contributions by introducing the auxiliary quantity $u^{\text{GS}} := -\Delta(W_{\text{GS}} * \rho)$:

$$u - u_h = \underbrace{(u - u^{\text{GS}})}_{\text{kernel error}} + \underbrace{(u^{\text{GS}} - u_h)}_{\text{grid error}}.$$

Here u^{GS} denotes the continuous solution with approximated kernel and exact source density. Both contributions are estimated separately.

Kernel error. We identify $w := W * \rho$ and $w^{\text{GS}} := W_{\text{GS}} * \rho$ with their trigonometric interpolants in the space S_N and continue to use the same notation. Since the spectral Laplace operator $-\Delta_h$ on S_N corresponds to the Fourier multiplier $|k|^2$, it coincides with the continuous Laplace operator on S_N . Since $|k|^2 \leq 3N^2$ for all k with $-N \leq k_j \leq N-1$, $-\Delta_h$ defines a bounded linear operator with constant $C_\Delta(N) = \mathcal{O}(N^2)$ (cf. Proposition 2 in [10]), that is $\|-\Delta_h f\|_{\ell^\infty} \leq C_\Delta(N) \|f\|_{\ell^\infty}$ for all $f \in S_N$. It follows that

$$\|u - u^{\text{GS}}\|_{\ell^\infty(B_1)} \leq C_\Delta(N) \|w - w^{\text{GS}}\|_{\ell^\infty(B_1)}.$$

Since $\eta \leq C_0 \varepsilon^3$ is assumed, Corollary 11 and Lemma 10 yield for all grid points $x \in B_1$

$$\|u - u^{\text{GS}}\|_{\ell^\infty(B_1)} \leq C_\Delta(N) \|w - w^{\text{GS}}\|_{\ell^\infty(B_1)} \leq C_\Delta(N) C_{\text{pot}}^W \|\rho\|_{L^\infty(\mathbb{T}^3)} \varepsilon^3.$$

Grid error. We model the numerical solution as

$$u_h = T_{\text{GS}}(P_N \rho) = -\Delta(W_{\text{GS}} * P_N \rho),$$

where $T_{\text{GS}} f := -\Delta(W_{\text{GS}} * f)$ denotes the solution operator induced by the Gaussian-sum approximation. Since convolution and the Laplace operator are linear, it holds that

$$u^{\text{GS}} - u_h = -\Delta(W_{\text{GS}} * (\rho - P_N \rho)) = T_{\text{GS}}(\rho - P_N \rho).$$

Since derivatives commute with convolution, T_{GS} is a convolution operator with kernel $K_{\text{GS}} := -\Delta W_{\text{GS}}$:

$$T_{\text{GS}} f = (-\Delta W_{\text{GS}}) * f = K_{\text{GS}} * f.$$

Since W_{GS} is a finite sum of smooth Gaussian functions, K_{GS} is also smooth and in particular integrable, hence $K_{\text{GS}} \in L^1(\mathbb{T}^3)$. From Young's convolution inequality and the Sobolev embedding $H^\mu(\mathbb{T}^3) \hookrightarrow L^\infty(\mathbb{T}^3)$ for $\mu > \frac{3}{2}$ (cf. [1]), that is $\|f\|_{L^\infty} \leq C_{\text{Sob}}^W \|f\|_{H^\mu}$, it follows that

$$\|T_{\text{GS}} f\|_{L^\infty(\mathbb{T}^3)} \leq \|K_{\text{GS}}\|_{L^1(\mathbb{T}^3)} \|f\|_{L^\infty(\mathbb{T}^3)} \leq \|K_{\text{GS}}\|_{L^1(\mathbb{T}^3)} C_{\text{Sob}} \|f\|_{H^\mu(\mathbb{T}^3)} =: C \|f\|_{H^\mu(\mathbb{T}^3)}.$$

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Applied to $f = \rho - P_N \rho$ this yields

$$\|u^{\text{GS}} - u_h\|_{\ell^\infty(B_1)} \leq \|u^{\text{GS}} - u_h\|_{L^\infty(\mathbb{T}^3)} = \|T_{\text{GS}}(\rho - P_N \rho)\|_{L^\infty(\mathbb{T}^3)} \leq C \|\rho - P_N \rho\|_{H^\mu(\mathbb{T}^3)}.$$

Lemma 12 with $m = \mu$ finally yields

$$\|u^{\text{GS}} - u_h\|_{\ell^\infty(B_1)} \leq C N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)} =: C_{\text{proj}} N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)}, \quad s > \mu > \frac{3}{2}.$$

Combination. For the kernel error it was shown that $\|u - u^{\text{GS}}\|_{\ell^\infty(B_1)} \leq C_\Delta(N) C_{\text{pot}}^W \|\rho\|_{L^\infty(\mathbb{T}^3)} \varepsilon^3$, and for the grid error $\|u^{\text{GS}} - u_h\|_{\ell^\infty(B_1)} \leq C_{\text{proj}}^W N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)}$, $s > \mu > \frac{3}{2}$. Together, an application of the triangle inequality yields the total error estimate

$$\|u - u_h\|_{\ell^\infty(B_1)} \leq C_\Delta(N) C_{\text{pot}}^W \|\rho\|_{L^\infty(\mathbb{T}^3)} \varepsilon^3 + C_{\text{proj}}^W N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)}.$$

□

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We continue to consider the screened Poisson equation (2) with compactly supported density $\rho \in L^\infty(\mathbb{R}^3)$, $\text{supp } \rho \subset B_1$.

4.1. Kernel Construction and Fundamental Solution

In the previous chapter, the mixed factorization $(-\Delta)(-\Delta + \kappa^2)W = \delta_0$ was used, which leads to the solution representation $u = -\Delta(W * \rho)$. We now replace this by a construction in which the screened operator is applied twice:

$$(-\Delta + \kappa^2)^2 H = \delta_0, \quad u = (-\Delta + \kappa^2)(H * \rho).$$

This corresponds to the natural generalization of the Poisson construction from 2.1, in which the super-potential is characterized by $-\Delta^2 V = \delta_0$ and the solution is subsequently obtained by $u = \Delta(V * \rho)$.

We define the kernel H as the fundamental solution of

$$(-\Delta + \kappa^2)^2 H = \delta_0.$$

The following lemma gives an explicit representation of H and justifies this definition.

Lemma 14 (H as Fundamental Solution). *The kernel*

$$H(r) = \frac{e^{-\kappa r}}{8\pi\kappa}, \quad r = |x|,$$

is the fundamental solution of the operator $(-\Delta + \kappa^2)^2$, i.e. $(-\Delta + \kappa^2)^2 H = \delta_0$ in the sense of distributions.

Proof. Since $(-\Delta + \kappa^2)G = \delta_0$ holds for the Yukawa fundamental solution $G(r) = e^{-\kappa r}/(4\pi r)$, it suffices to show $(-\Delta + \kappa^2)H = G$. From this it follows immediately that

$$(-\Delta + \kappa^2)^2 H = (-\Delta + \kappa^2)((-\Delta + \kappa^2)H) = (-\Delta + \kappa^2)G = \delta_0.$$

A direct computation yields for $r > 0$

$$\Delta H(r) = -\frac{e^{-\kappa r}}{4\pi r} + \frac{\kappa e^{-\kappa r}}{8\pi},$$

4.2. Regularity of the Kernel and Near-Field Order

and thus

$$(-\Delta + \kappa^2)H = \frac{e^{-\kappa r}}{4\pi r} - \frac{\kappa e^{-\kappa r}}{8\pi} + \kappa^2 \cdot \frac{e^{-\kappa r}}{8\pi\kappa} = \frac{e^{-\kappa r}}{4\pi r} = G(r).$$

Since H is bounded at the origin, this pointwise identity extends to the sense of distributions. $\square$

Setting $s := H * \rho$, it follows that $(-\Delta + \kappa^2)^2 s = ((-\Delta + \kappa^2)^2 H) * \rho = \delta_0 * \rho = \rho$, and thus

$$u := (-\Delta + \kappa^2) s = (-\Delta + \kappa^2)(H * \rho)$$

satisfies the screened Poisson equation (2).

4.2. Regularity of the Kernel and Near-Field Order

Like the kernels V and W before, H also has no singularity at the origin.

Using the Taylor expansion $e^{-\kappa r} = 1 - \kappa r + \frac{\kappa^2 r^2}{2} - \frac{\kappa^3 r^3}{6} + \mathcal{O}(r^4)$ it follows that

$$H(r) = \frac{1}{8\pi\kappa} - \frac{r}{8\pi} + \frac{\kappa r^2}{16\pi} - \frac{\kappa^2 r^3}{48\pi} + \mathcal{O}(r^4).$$

In particular, $H(0) = \frac{1}{8\pi\kappa} \neq 0$, so that the kernel H is bounded at the origin. The consequences of this property for the convolution error analysis are examined in 4.4.2.

4.3. Gaussian-Sum Approximation of the Kernel

The decisive structural advantage of the kernel H over the W -approach lies in its integral representation: the transformed integrand fully satisfies the assumptions of Proposition 1, so that the Gaussian-sum approximation manages without the error decomposition into three terms required in the W -case.

The starting point is the Gaussian integral representation of the Yukawa kernel [5, 12]

$$\frac{e^{-\kappa r}}{4\pi r} = \frac{1}{2\pi^{3/2}} \int_0^\infty e^{-r^2\mu^2 - \kappa^2/(4\mu^2)} d\mu.$$

By the substitution $t = \kappa/(2r\mu)$ and subsequent multiplication by $4\pi r$ one obtains for $r > 0$

$$e^{-\kappa r} = \frac{\kappa}{\sqrt{\pi}} \int_0^\infty t^{-2} e^{-r^2 t^2 - \kappa^2/(4t^2)} dt,$$

and thus

$$H(r) = \frac{e^{-\kappa r}}{8\pi\kappa} = \frac{1}{8\pi^{3/2}} \int_0^\infty t^{-2} e^{-r^2 t^2 - \kappa^2/(4t^2)} dt. \quad (16)$$

The logarithmic transformation $t = e^u$, $dt = e^u du$ transforms (16) into

$$H(r) = \frac{1}{8\pi^{3/2}} \int_{\mathbb{R}} f_H(u, r) du, \quad f_H(u, r) := e^{-u} e^{-r^2 e^{2u} - \frac{\kappa^2}{4}} e^{-2u}. \quad (17)$$

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The sinc quadrature with step size h and symmetric truncation $|j| \leq S$ yields from this the Gaussian-sum approximation

$$H_{\text{GS}}(r) = \sum_{|j| \leq S} \omega_j e^{-\tau_j^2 r^2}, \quad \tau_j = e^{jh}, \quad \omega_j = \frac{h}{8\pi^{3/2}} e^{-jh} e^{-\frac{\kappa^2}{4} e^{-2jh}}. \quad (18)$$

4.4. Error Analysis

4.4.1. Error of the Gaussian-Sum Approximation

To apply Proposition 1 we examine the properties of the transformed integrand f_H from (17). On the one hand, for $u \rightarrow +\infty$, since $r \geq \varepsilon > 0$,

$$|f_H(u, r)| \leq e^{-u} e^{-\varepsilon^2 e^{2u}} \leq C e^{-b e^{2u}}$$

for every $b < \varepsilon^2$ and sufficiently large u . On the other hand, for $u \rightarrow -\infty$ we use the estimate $e^{-r^2 e^{2u}} \leq 1$. Thus it follows that

$$|f_H(u, r)| \leq e^{-u} e^{-\frac{\kappa^2}{4} e^{-2u}} = e^{|u|} e^{-\frac{\kappa^2}{4} e^{2|u|}} \leq C e^{-b e^{2|u|}}$$

for every $b < \kappa^2/4$ and sufficiently large $|u|$, since the term $\kappa^2 e^{2|u|}/4$ dominates the prefactor $e^{|u|}$. In summary, for every $b < \min(\varepsilon^2, \kappa^2/4)$ and sufficiently large $|u|$

$$|f_H(u, r)| \leq C \exp(-b e^{a|u|}), \quad a = 2,$$

uniformly in $r \in [\varepsilon, \delta]$. This essentially distinguishes the H -case from the W -case: the integrand there contains, after logarithmic transformation, the factor $1 - e^{-\kappa^2 e^{-2u}/4}$, which tends to 1 as $u \rightarrow -\infty$, so that no double exponential decay is present at the left boundary.

To verify the strip condition, let $z = u + iy$ with $|y| < \lambda < \pi/4$. Then $\cos(2y) \geq \cos(2\lambda) > 0$, and with $\Re(e^{\pm 2z}) = e^{\pm 2u} \cos(2y)$ it follows for $r \in [\varepsilon, \delta]$ that

$$|f_H(z, r)| = e^{-u} e^{-r^2 e^{2u} \cos(2y) - \frac{\kappa^2}{4} e^{-2u} \cos(2y)} \leq e^{-u} e^{-\varepsilon^2 e^{2u} \cos(2\lambda) - \frac{\kappa^2}{4} e^{-2u} \cos(2\lambda)}.$$

The right-hand side is integrable on $\mathbb{R}$, since the double exponential decay in both directions dominates the prefactor e^{-u} . Since $\cos(2y)$ is even in y , this bound holds identically for $y = +\lambda$ and $y = -\lambda$, so that

$$N(f_H, D_\lambda) = \int_{\mathbb{R}} (|f_H(u + i\lambda, r)| + |f_H(u - i\lambda, r)|) du < \infty$$

uniformly in $r \in [\varepsilon, \delta]$. Since $f_H(\cdot, r)$ is analytic as a composition of entire functions, $f_H(\cdot, r) \in H^1(D_\lambda)$ holds for $0 < \lambda < \pi/4$. Thus all assumptions of Proposition 1 are satisfied.

Theorem 15 (Gaussian-Sum Approximation of the Kernel H). *Let $0 < \varepsilon < \delta < \infty$, $\kappa > 0$ and $0 < \lambda < \pi/4$. With $a = 2$, $b \in (0, \min(\varepsilon^2, \kappa^2/4))$ and the step size*

$$h = \frac{\ln(2\pi aS/b)}{aS}$$

the following uniform error estimate holds for the Gaussian-sum approximation (18)

$$\sup_{r \in [\varepsilon, \delta]} |H(r) - H_{\text{GS}}(r)| \leq C_{\text{GS}}^H \exp\left(-\frac{2\pi\lambda aS}{\ln(2\pi aS/b)}\right),$$

where $C_{\text{GS}}^H > 0$ depends on ε , δ , κ and λ , but is independent of S . For a target accuracy $\eta > 0$ the choice

$$S = \mathcal{O}(\log(1/\eta) \log \log(1/\eta))$$

suffices.

Proof. By the preceding discussions, f_H satisfies the assumptions of Proposition 1: holomorphy in D_λ for $0 < \lambda < \pi/4$, $N(f_H, D_\lambda) < \infty$ uniformly in r , and double exponential decay with $a = 2$ and $b < \min(\varepsilon^2, \kappa^2/4)$. Since f_H decays in both directions with the same rate $a = 2$, a symmetrically truncated trapezoidal rule can be used. The direct application of Proposition 1 yields the claimed error estimate. For the number of terms one sets $S = c \log(1/\eta) \log \log(1/\eta)$ with sufficiently large $c > 0$. Then $\ln(2\pi aS/b) = \mathcal{O}(\log \log(1/\eta))$ and thus

$$\frac{2\pi\lambda aS}{\ln(2\pi aS/b)} = \mathcal{O}(\log(1/\eta)),$$

so that the error bound reaches the magnitude η . □

The number-of-terms asymptotics $S = \mathcal{O}(\log(1/\eta) \log \log(1/\eta))$ represents a substantial advantage over the W -approach, which, due to the absence of double exponential decay at the left boundary, requires a manual error decomposition and needs $\mathcal{O}(\log^2(1/\eta))$ terms (cf. Theorem 9). At the same time, the separability decisive for the FFT evaluation is preserved, since each summand

$$e^{-\tau_j^2 r^2} = \prod_{p=1}^3 e^{-\tau_j^2 x_p^2}$$

factorizes as a product of one-dimensional Gaussian functions. The precomputation of the Fourier coefficients therefore proceeds analogously to the W -approach via one-dimensional integrals.

4.4.2. Convolution Error

Since H is bounded at the origin with $H(0) = \frac{1}{8\pi\kappa}$ and the weights ω_j of the Gaussian-sum approximation H_{GS} are non-negative, the convolution error analysis from the W -case can be transferred directly (cf. Lemma 10).

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Lemma 16 (Convolution Error of the Kernel Replacement). *Let $\varepsilon > 0$ and $\rho \in L^\infty(\mathbb{R}^3)$ with $\text{supp } \rho \subset B_1$. Suppose $\sup_{r \in [\varepsilon, 2]} |H(r) - H_{\text{GS}}(r)| \leq \eta$. Then for all $x \in B_1$*

$$|(H * \rho)(x) - (H_{\text{GS}} * \rho)(x)| \leq C_{\text{conv}}^H \|\rho\|_{L^\infty} (\eta + \varepsilon^3),$$

where $C_{\text{conv}}^H > 0$ is independent of x , η , and ε .

Proof. The proof follows that of Lemma 10, where the near-field term is controlled by the boundedness of H with $H(0) = \frac{1}{8\pi\kappa}$ and the uniform boundedness of $H_{\text{GS}}(0) = \sum_j \omega_j$. $\square$

Under the coupling condition $\eta \leq C_{\text{coup}}^H \varepsilon^3$, the error order simplifies as in the W -case.

Corollary 17. *If one chooses $\eta \leq C_{\text{coup}}^H \varepsilon^3$ with a constant $C_{\text{coup}}^H > 0$, then under the assumptions of Lemma 16*

$$\sup_{x \in B_1} |(H * \rho)(x) - (H_{\text{GS}} * \rho)(x)| \leq C_{\text{pot}}^H \|\rho\|_{L^\infty} \varepsilon^3,$$

where $C_{\text{pot}}^H := C_{\text{conv}}^H(1 + C_{\text{coup}}^H) > 0$ is independent of ε and x .

4.4.3. A Priori Error Estimate

We use the spectral framework from 3.4.3 and obtain a total error estimate that is structurally analogous to the W -method. The only difference lies in the application of the operator $(-\Delta_h + \kappa^2)$ instead of $-\Delta_h$. On S_N this corresponds to the Fourier multiplier $|k|^2 + \kappa^2$ with the same asymptotic operator norm $C_\Delta(N) = \mathcal{O}(N^2)$.

Theorem 18 (Total Error Estimate, H -Method). *Let $\mu > \frac{3}{2}$ be fixed, $\rho \in H^s(\mathbb{T}^3)$ with $s > \mu$ and $\text{supp } \rho \subset B_1$. Let the Gaussian-sum approximation H_{GS} be constructed according to Theorem 15 with accuracy $\eta \leq C_{\text{coup}}^H \varepsilon^3$. Let s_h be the grid function computed by Gaussian-sum FFT convolution with H_{GS} and $u_h := (-\Delta_h + \kappa^2) s_h$. Then*

$$\|u - u_h\|_{\ell^\infty(B_1)} \leq C_\Delta(N) C_{\text{pot}}^H \|\rho\|_{L^\infty(\mathbb{T}^3)} \varepsilon^3 + C_{\text{proj}}^H N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)},$$

where $C_{\text{pot}}^H, C_{\text{proj}}^H > 0$ are constants independent of ε and N , and $C_\Delta(N) = \mathcal{O}(N^2)$ denotes the operator norm of $(-\Delta_h + \kappa^2)$ on S_N .

Proof. The proof proceeds in a structurally analogous manner to Theorem 13. With $s^{\text{GS}} := H_{\text{GS}} * \rho$, $u^{\text{GS}} := (-\Delta + \kappa^2) s^{\text{GS}}$ and the decomposition

$$u - u_h = \underbrace{(u - u^{\text{GS}})}_{\text{kernel error}} + \underbrace{(u^{\text{GS}} - u_h)}_{\text{grid error}}$$

we analyse both contributions.

Kernel error. As in the W -case, the kernel error is interpreted on the discrete spectral space S_N . We apply not the continuous operator $-\Delta + \kappa^2$ to the mere L^∞ -error $s - s^{\text{GS}}$, but the discrete operator $-\Delta_h + \kappa^2$ to the corresponding spectral grid function. On S_N

4.4. Error Analysis

this coincides with the Fourier multiplier $|k|^2 + \kappa^2$. Since $|k|^2 + \kappa^2 \leq 3N^2 + \kappa^2$ holds for all k with $-N \leq k_j \leq N-1$, it has there the operator norm $C_\Delta(N) = \mathcal{O}(N^2)$. Therefore it follows with Corollary 17 that

$$\|u - u^{\text{GS}}\|_{\ell^\infty(B_1)} \leq C_\Delta(N) \|s - s^{\text{GS}}\|_{\ell^\infty(B_1)} \leq C_\Delta(N) C_{\text{pot}}^H \|\rho\|_{L^\infty(\mathbb{T}^3)} \varepsilon^3.$$

Grid error. We define the solution operator $T_{\text{GS}}^H f := (-\Delta + \kappa^2)(H_{\text{GS}} * f)$. With the identification $u_h = T_{\text{GS}}^H(P_N \rho)$ one obtains by linearity $u^{\text{GS}} - u_h = T_{\text{GS}}^H(\rho - P_N \rho)$. Since derivatives commute with the convolution, T_{GS}^H is a convolution operator with kernel $K_{\text{GS}}^H := (-\Delta + \kappa^2)H_{\text{GS}}$. This consists of finitely many terms of the form $\omega_j(6\tau_j^2 - 4\tau_j^4|x|^2 + \kappa^2)e^{-\tau_j^2|x|^2}$, that is, of polynomial-times-Gaussian terms, and therefore belongs to $L^1(\mathbb{T}^3)$. Young's convolution inequality and the Sobolev embedding $H^\mu(\mathbb{T}^3) \hookrightarrow L^\infty(\mathbb{T}^3)$ for $\mu > \frac{3}{2}$ (cf. [1]) yield

$$\|T_{\text{GS}}^H f\|_{L^\infty(\mathbb{T}^3)} \leq \|K_{\text{GS}}^H\|_{L^1(\mathbb{T}^3)} C_{\text{Sob}}^H \|f\|_{H^\mu(\mathbb{T}^3)} =: C^H \|f\|_{H^\mu(\mathbb{T}^3)}.$$

Applied to $f = \rho - P_N \rho$ and with Lemma 12 it follows that

$$\|u^{\text{GS}} - u_h\|_{\ell^\infty(B_1)} \leq C_{\text{proj}}^H N^{\mu-s} \|\rho\|_{H^s(\mathbb{T}^3)}, \quad s > \mu > \frac{3}{2}.$$

Combination. The triangle inequality yields the claim. □

5. Numerical Results

5.1. Experimental Setup

All numerical experiments concern the screened Poisson equation

$$(-\Delta + \kappa^2)u = \rho \quad \text{in } \mathbb{R}^3$$

(cf. 1.1) with density $\rho \in L^\infty(\mathbb{R}^3)$, $\text{supp } \rho \subset B_1$, where $B_1 \subset \mathbb{R}^3$ denotes an axis-aligned rectangular domain. The numerical solution is computed on a uniform $N \times N \times N$ grid on B_1 . For the FFT solver, B_1 is extended by zero-padding to $B_2 = 2 \cdot B_1$. The source code of both solvers, the parameter selection routines, and the benchmark runner is provided in Appendix A.

5.1.1. Reference Solutions and Error Measure

For all source densities ρ considered in 5.3, the exact solution u^* is known analytically. The error measure used is the relative ℓ^∞ -error on B_1 ,

$$E_\infty := \frac{\|u^* - u_h\|_{\ell^\infty(B_1)}}{\|u^*\|_{\ell^\infty(B_1)}} = \frac{\max_{x \in \mathcal{T}_h} |u^*(x) - u_h(x)|}{\max_{x \in \mathcal{T}_h} |u^*(x)|},$$

where u_h denotes the computed grid solution and $\mathcal{T}_h$ denotes the set of all grid points on the discrete computational grid.

5.1.2. Choice of Gaussian-Sum Parameters

The construction of the Gaussian-sum approximation K_{GS} of the kernel $K \in \{W, H\}$ is operated in two modes, which are aimed at different purposes.

In the verification experiments (cf. 5.2), the parameters (h, M_1, M_2) for W_{GS} and (h, S) for H_{GS} , respectively, are determined according to the a priori formulas from Theorem 9 and Theorem 15, respectively. This choice of parameters allows direct coupling with the theoretical error bounds.

In the benchmarks (cf. 5.3), the parameters are determined by a numerical grid search procedure: For each κ , (h, M_1, M_2) and (h, S) , respectively, are chosen such that

$$\sup_{r \in [\varepsilon_{\text{gs}}, \delta_{\text{gs}}]} |K(r) - K_{\text{GS}}(r)| \leq \text{tol}$$

is satisfied with minimal number of terms. Here $\varepsilon_{\text{gs}} = 10^{-5}$ denotes the near-field cutoff, $\text{tol} = 10^{-16}$ the target accuracy, and $\delta_{\text{gs}} = \max_{y \in B_1} |y|$ the Euclidean half-diagonal of B_1 .

5.2. Verification of the Theoretical Results

For both methods, the same grid search procedure is applied on the same interval $[\varepsilon_{\text{gs}}, \delta_{\text{gs}}]$. Runtime and accuracy comparisons between the W - and H -approach are therefore directly comparable and independent of the method-specific theoretical constants.

5.1.3. Runtime Measurement

Two timing quantities are reported. The precomputation time t_{pre} comprises the one-time computation of the Fourier coefficients $\widehat{K}$ of the kernel and of the spectral multiplier. It is incurred once per grid/parameter configuration and is not recomputed upon repeated solving. The precomputation phase is structurally analogous to 2.4 and [10, Alg. 1], respectively, where the biharmonic kernel V_{GS} is replaced by $K_{\text{GS}} \in \{W_{\text{GS}}, H_{\text{GS}}\}$ and the spectral Laplace multiplier is replaced by the operator responsible for the respective approach. The mean solver time t_{avg} is the arithmetic mean over ten repetitions of the actual FFT convolution including the spectral operator application and the back-projection onto B_1 .

5.1.4. Implementation

All computations were carried out in Python (NumPy/SciPy) in double precision (`float64`). Runtimes were measured with `time.perf_counter`. The experiments were carried out on a MacBook Air (2022) with Apple M2 chip (8 CPU cores), 8 GB of RAM, and the operating system macOS Tahoe 26.5.

5.2. Verification of the Theoretical Results

5.2.1. Mixed-Screened Super-Potential Approach W

The following experiments verify the theoretical results from Section 3 in the order of their derivation.

The numerical results confirm the statements of Theorem 9 for the tested choice of parameters (Figure 5.1). The parameters (h, M_1, M_2) chosen according to the theorem reliably satisfy the prescribed target accuracy η . Furthermore, the theoretically predicted complexity $M = \mathcal{O}(\log^2(1/\eta))$ is observed. The linear fit in the transformed variables yields a coefficient of determination of $R^2 = 0.993$.

The spatial error profile $|W(r) - W_{\text{GS}}(r)|$ for various target accuracies is shown in Figure 5.2. For all considered tolerances, the error remains uniformly below the prescribed bound η over the entire investigated range. This numerically confirms the uniform error estimate from Theorem 9.

The effects of the cancellation discussed in 3.3.1 are shown in Figure 5.3. For small values of κ , the indirect approximation $W_{\text{GS}}^{\text{ind}}$ exhibits a significantly larger relative error than the direct approximation $W_{\text{GS}}^{\text{dir}}$. Here, the error of $W_{\text{GS}}^{\text{ind}}$ increases in particular for decreasing values of r , while $W_{\text{GS}}^{\text{dir}}$ achieves errors close to the prescribed target accuracy over the entire considered range. With increasing κ , the difference between both constructions decreases.

5. Numerical Results

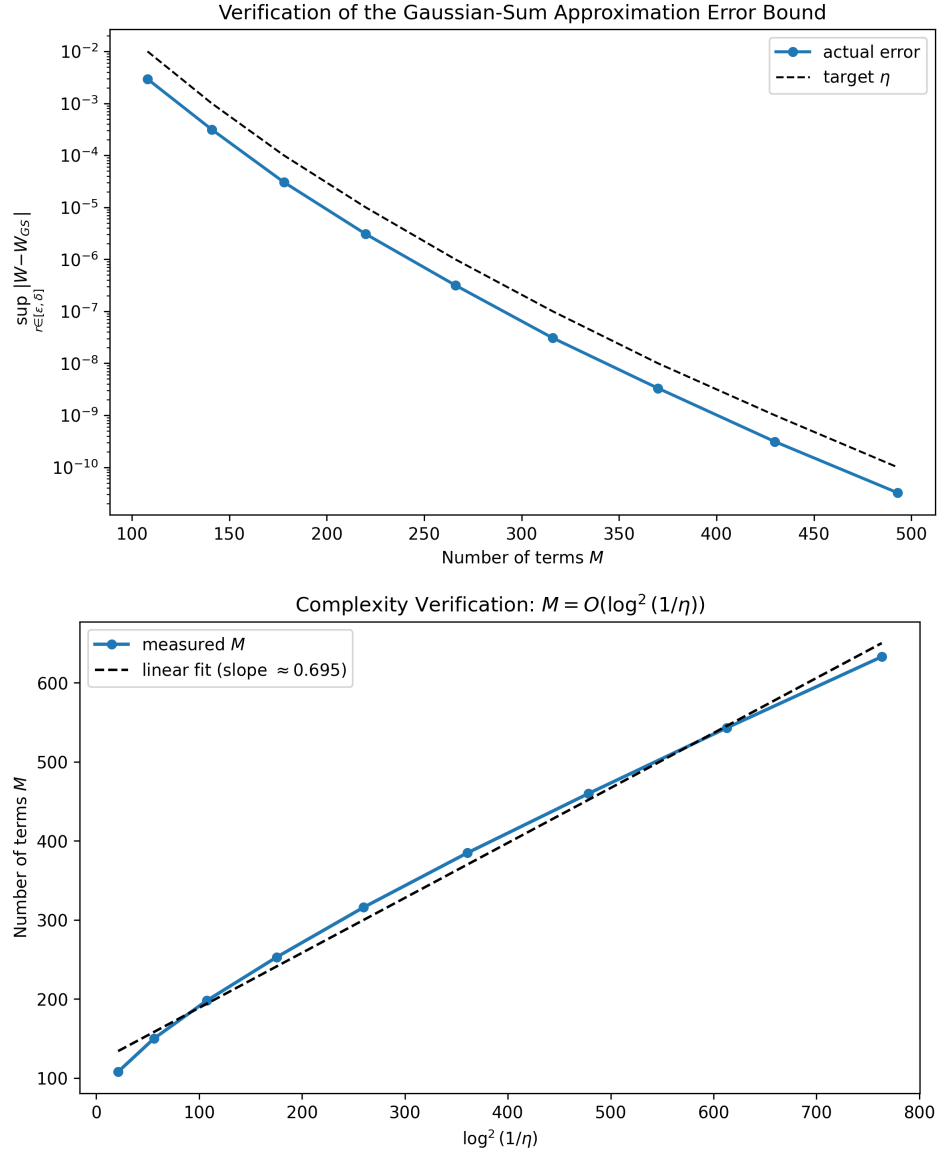


Figure 5.1.: Verification of Theorem 9. Top: Error $\sup_{r \in [\varepsilon, \delta]} |W - W_{GS}|$ as a function of the number of terms M for various target accuracies η . Bottom: Number of terms M versus $\log^2(1/\eta)$ with linear fit.

5.2. Verification of the Theoretical Results

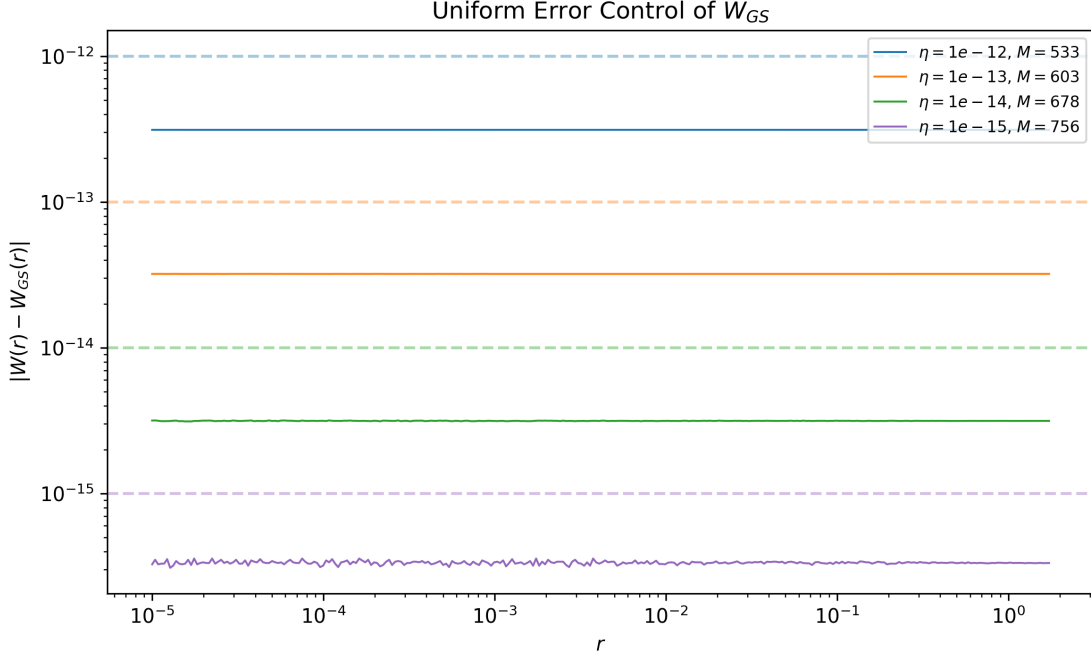


Figure 5.2.: Absolute error $|W(r) - W_{GS}(r)|$ for various target accuracies η .

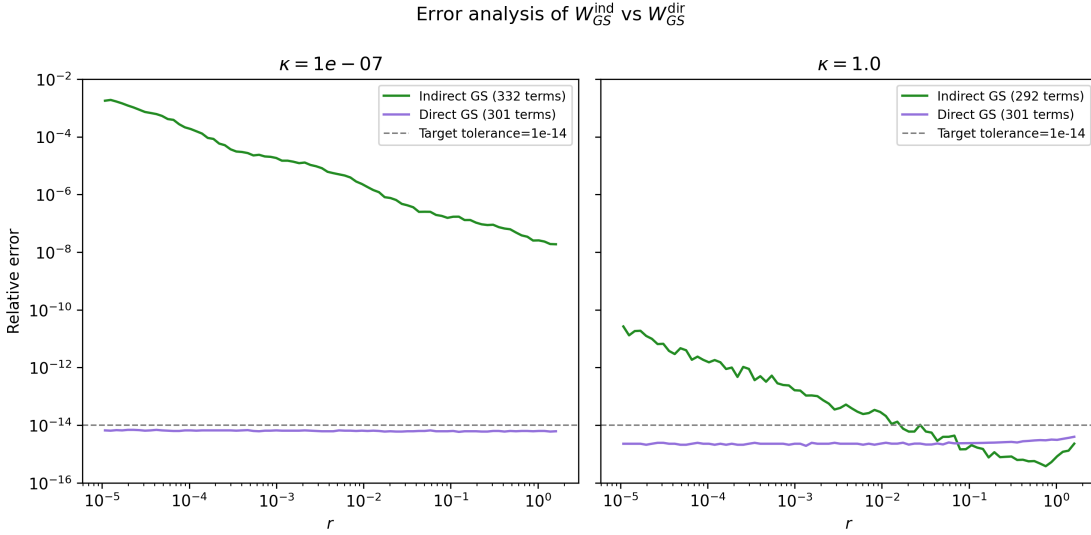


Figure 5.3.: Relative error of W_{GS}^{ind} (green) and W_{GS}^{dir} (purple) for $\kappa \in \{10^{-7}, 1\}$ at $\varepsilon = 10^{-5}$ and $\delta = \sqrt{3}$.

5. Numerical Results

The error order $\mathcal{O}(\varepsilon^3)$ predicted in Corollary 11 is confirmed in Figure 5.4. The measured global slope in the double logarithmic scale is 2.985, while the local slopes lie in the interval $[2.90, 3.09]$. This numerically confirms cubic convergence over the entire considered range $\varepsilon \in [10^{-4}, 10^{-1}]$.

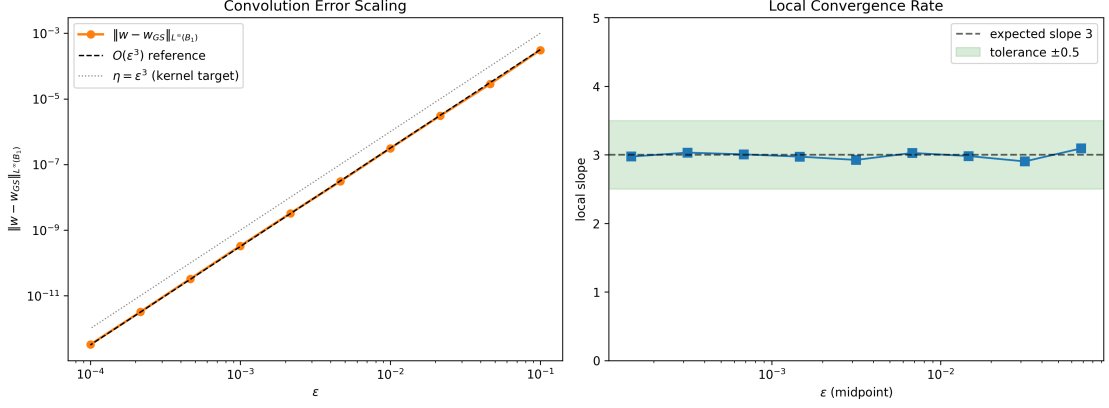


Figure 5.4.: Verification of Corollary 11. Left: Error $\|w - w_{GS}\|_{\ell^\infty(B_1)}$ versus ε with $\mathcal{O}(\varepsilon^3)$ reference. Right: Local convergence rates.

The two-term structure of the total error predicted in Theorem 13 is consistent with the numerical results (cf. Figure 5.5). For small grid sizes N , the error decreases rapidly. For large N , the error transitions into an ε -dependent plateau, where smaller values of ε lead to lower plateau values. This behavior is consistent with the error decomposition from Theorem 13: for small N , the discretization-induced part of the error dominates, while for large N , the kernel error depending on ε becomes visible.

5.2.2. Double-Screened Super-Potential Approach H

The following experiments verify the theoretical results from Section 4 in the order of their derivation.

The numerical results confirm the statements of Theorem 15 for the tested choice of parameters (Figure 5.6). The parameters (h, S) chosen according to the theorem reliably satisfy the prescribed target accuracy η . The observed error lies significantly below the prescribed bound, which reflects the conservative character of the a priori sinc quadrature estimate. The complexity measurement is consistent with the theoretical prediction $S = \mathcal{O}(\log(1/\eta) \log \log(1/\eta))$. The linear fit in the transformed variables yields a coefficient of determination of $R^2 = 0.998977$.

The error order $\mathcal{O}(\varepsilon^3)$ predicted in Corollary 17 is confirmed in Figure 5.7. In the double logarithmic scale, the measured convolution error follows the $\mathcal{O}(\varepsilon^3)$ reference over the considered range. The global slope determined from the measurement data is approximately 3.16, consistent with the theoretically predicted cubic error order.

The two-term structure of the total error predicted in Theorem 18 is consistent with the numerical results (cf. Figure 5.8). For small grid sizes N , the error decreases significantly

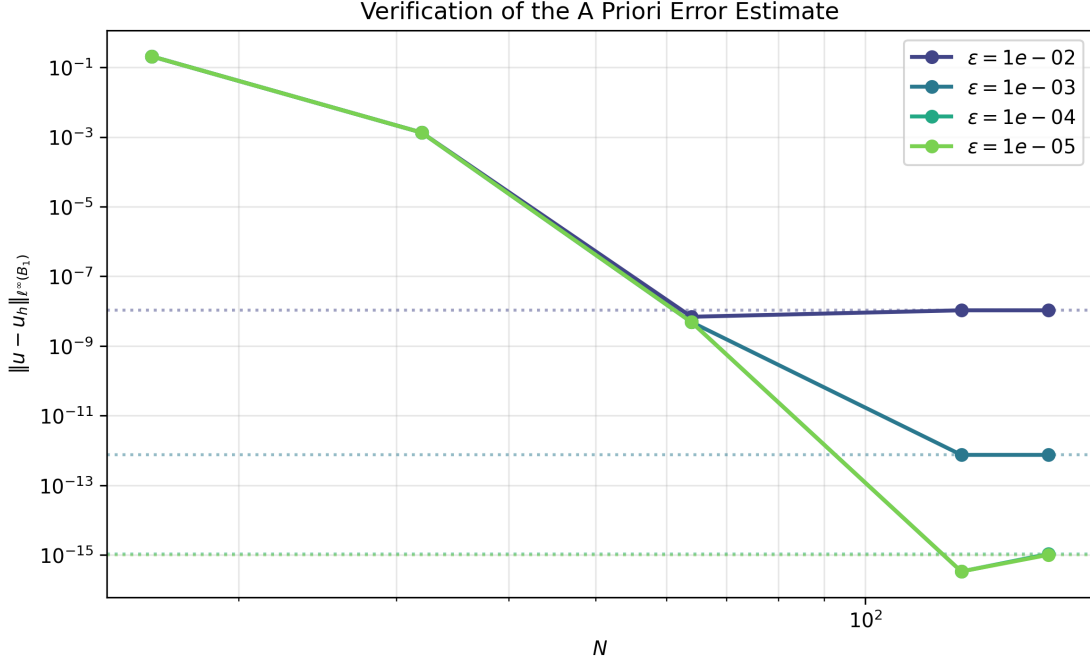


Figure 5.5.: Verification of Theorem 13. Error $\|u - u_h\|_{\ell^\infty(B_1)}$ versus grid size N for various values of ε . The dashed lines mark the observed plateau values.

upon grid refinement. For large N , the error transitions into a plateau depending on ε , where smaller values of ε produce lower plateau values. This behavior corresponds to the error decomposition from Theorem 18: initially, the discretization error dominates, while for sufficiently large grid resolutions, the error contribution determined by the Gaussian-sum approximation becomes visible.

5.3. Benchmarks

In this section, various test problems are considered. For each benchmark, the results of the Mixed-Screened super-potential approach (W -approach) and the Double-Screened super-potential approach (H -approach) are presented.

5.3.1. Gaussian source

Cubic Domain

As the first benchmark, we consider the Gaussian density

$$\rho(x) = \frac{1}{(2\pi)^{3/2}\sigma^3} \exp\left(-\frac{|x - c|^2}{2\sigma^2}\right), \quad (19)$$

5. Numerical Results

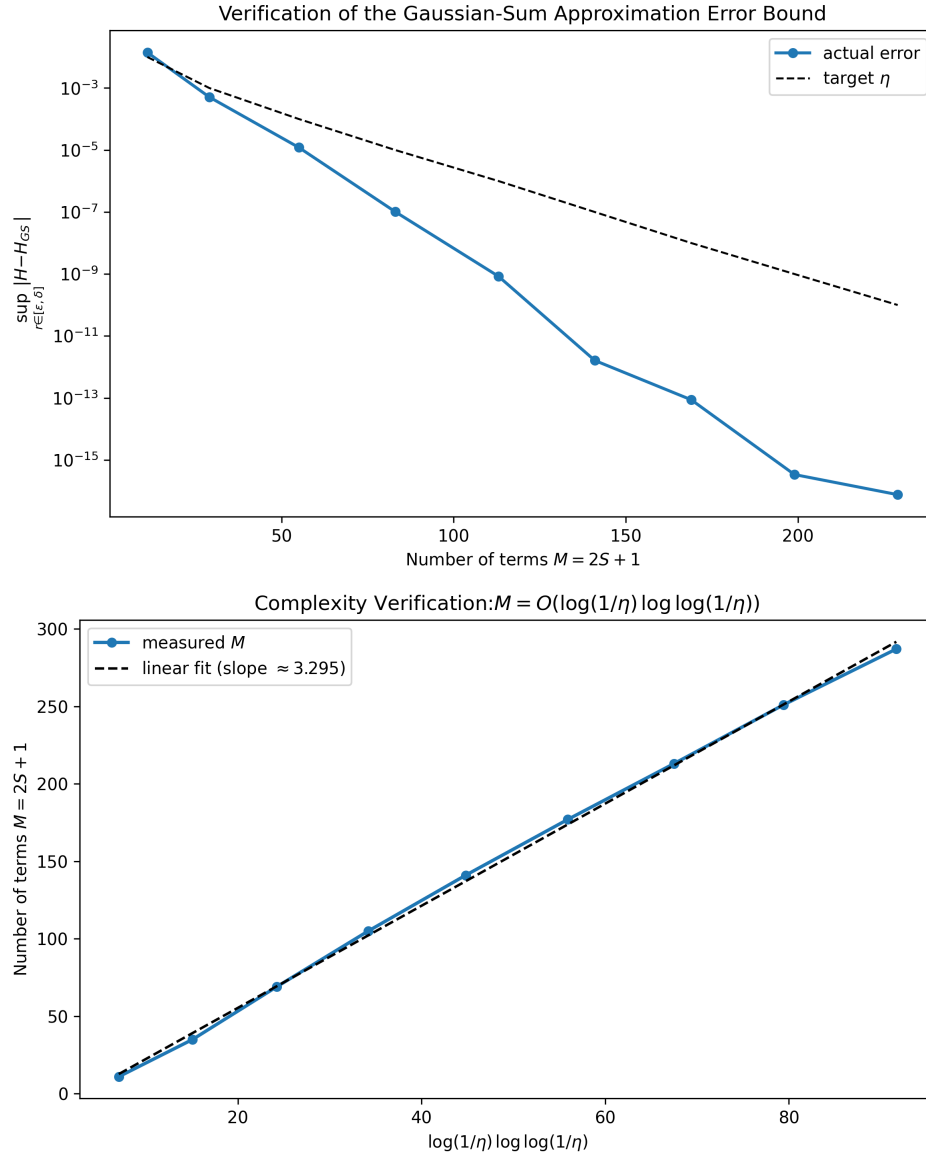


Figure 5.6.: Verification of Theorem 15. Top: Error $\sup_{r \in [\varepsilon, \delta]} |H - H_{GS}|$ versus the number of terms M . Bottom: Number of terms M versus $\log(1/\eta) \log \log(1/\eta)$.

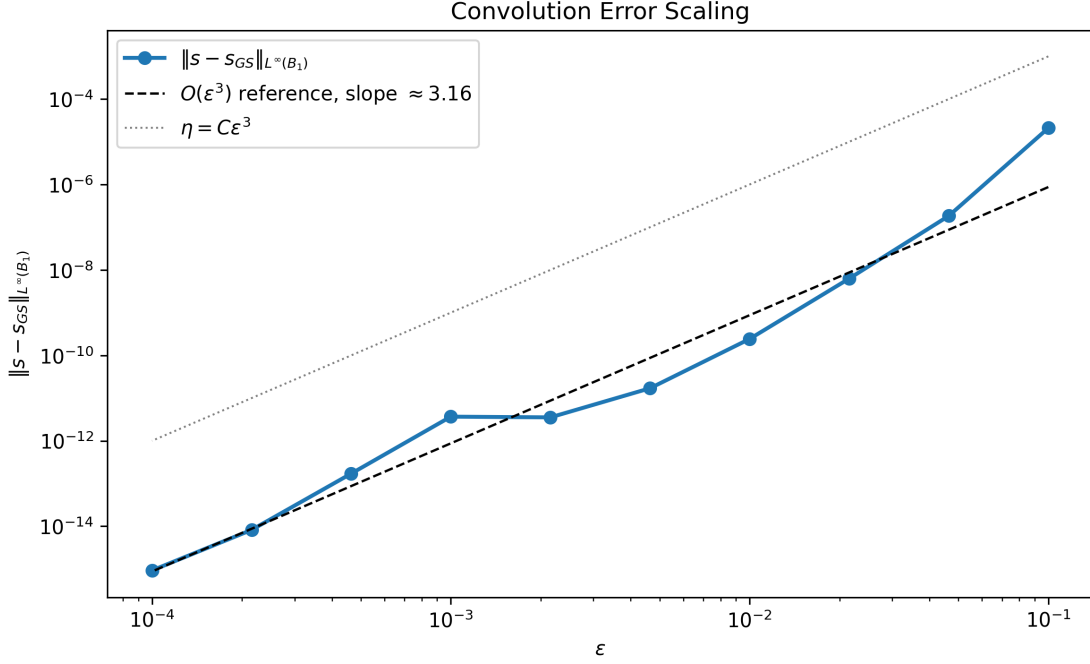


Figure 5.7.: Verification of Corollary 17. Error $\|s - s_{GS}\|_{\ell^\infty(B_1)}$ versus ϵ with $\mathcal{O}(\epsilon^3)$ reference.

where c denotes the center of the computational domain. The corresponding exact solution reads

$$u^*(x) = \frac{e^{\kappa^2 \sigma^2 / 2}}{8\pi|x-c|} \left[e^{-\kappa|x-c|} \operatorname{erfc}\left(\frac{\kappa\sigma^2 - |x-c|}{\sqrt{2}\sigma}\right) - e^{\kappa|x-c|} \operatorname{erfc}\left(\frac{\kappa\sigma^2 + |x-c|}{\sqrt{2}\sigma}\right) \right]. \quad (20)$$

We first consider the cubic domain $B = [-2, 2]^3$. The experiments are carried out for $\kappa = 1$ and various values of σ . The results are compiled in Tables 5.1a and 5.1b.

Rectangular Domain

Next, we consider the same Gaussian source from equation (19) on the rectangular domain $B = (-3, 2) \times (-2, 3.5) \times (-1, 5)$ for the case $\kappa = 1$ and $\sigma = 0.20$. The numerical results are compiled in Tables 5.2a and 5.2b.

Variation of the Screening Parameter

Subsequently, the influence of the screening parameter κ is examined. For this purpose, the parameters $\sigma = 0.20$ and $N = 128$ are fixed, while κ is varied. The corresponding results are listed in Tables 5.3a and 5.3b.

5. Numerical Results

(a) W -approach					
σ	N	M	E_∞	t_{pre} [s]	t_{avg} [s]
0.20	16	401	2.631×10^{-3}	2.998×10^{-3}	2.582×10^{-3}
	32	401	9.269×10^{-9}	5.504×10^{-3}	1.415×10^{-2}
	64	401	7.798×10^{-16}	2.494×10^{-2}	1.361×10^{-1}
	128	401	3.231×10^{-15}	2.432×10^{-1}	3.207
0.15	16	401	3.303×10^{-2}	4.584×10^{-3}	7.857×10^{-3}
	32	401	8.380×10^{-6}	6.848×10^{-3}	4.225×10^{-2}
	64	401	1.009×10^{-15}	3.637×10^{-2}	2.075×10^{-1}
	128	401	1.575×10^{-15}	6.873×10^{-1}	1.884
0.10	16	401	3.689×10^{-1}	1.926×10^{-3}	2.564×10^{-3}
	32	401	2.392×10^{-3}	4.800×10^{-3}	1.438×10^{-2}
	64	401	8.606×10^{-9}	2.219×10^{-2}	1.161×10^{-1}
	128	401	1.840×10^{-15}	2.023×10^{-1}	1.206
(b) H -approach					
σ	N	M	E_∞	t_{pre} [s]	t_{avg} [s]
0.20	16	241	2.631×10^{-3}	2.059×10^{-3}	7.534×10^{-4}
	32	241	9.269×10^{-9}	2.542×10^{-3}	5.921×10^{-3}
	64	241	6.684×10^{-16}	1.575×10^{-2}	5.808×10^{-2}
	128	241	3.119×10^{-15}	1.401×10^{-1}	5.680×10^{-1}
0.15	16	241	3.303×10^{-2}	1.061×10^{-3}	7.463×10^{-4}
	32	241	8.380×10^{-6}	2.440×10^{-3}	5.558×10^{-3}
	64	241	4.726×10^{-16}	1.403×10^{-2}	5.603×10^{-2}
	128	241	1.733×10^{-15}	1.631×10^{-1}	5.074×10^{-1}
0.10	16	241	3.689×10^{-1}	8.827×10^{-4}	7.063×10^{-4}
	32	241	2.392×10^{-3}	2.336×10^{-3}	5.407×10^{-3}
	64	241	8.606×10^{-9}	1.350×10^{-2}	5.497×10^{-2}
	128	241	5.934×10^{-16}	1.290×10^{-1}	5.148×10^{-1}

Table 5.1.: Results for the Gaussian source (19) on the cubic domain $B = [-2, 2]^3$ for $\kappa = 1$.

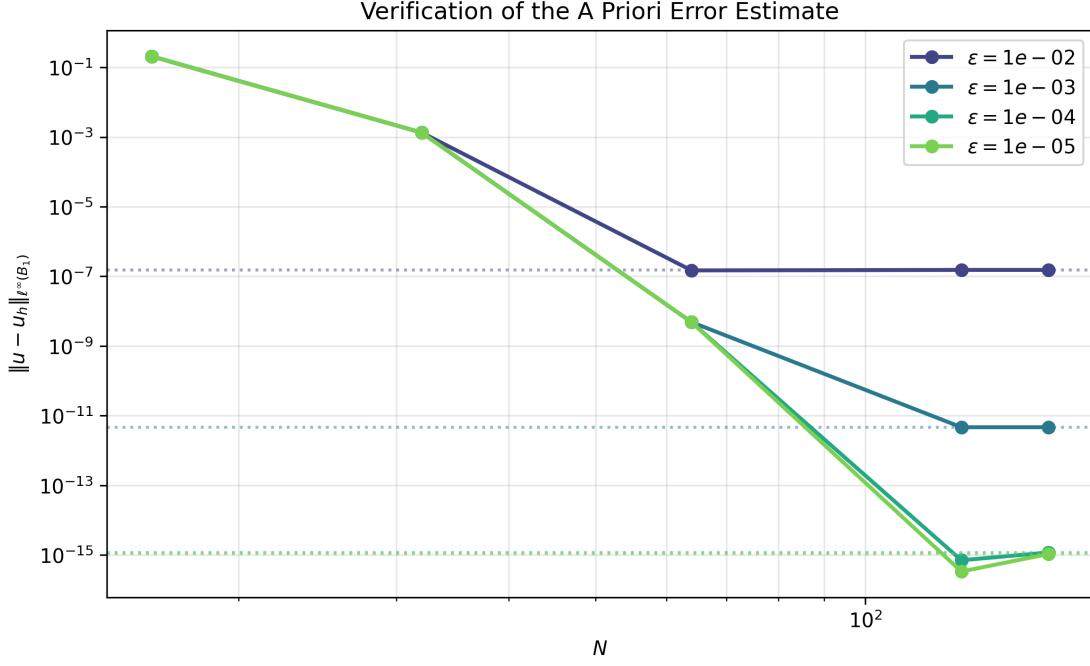


Figure 5.8.: Verification of Theorem 18. Error $\|u - u_h\|_{\ell^\infty(B_1)}$ versus grid size N for various values of ϵ . The dotted lines mark the observed plateau values.

(a) W -approach

σ	N	M	E_∞	t_{pre} [s]	t_{avg} [s]
0.20	16	381	4.700×10^{-2}	3.777×10^{-3}	2.541×10^{-3}
	32	381	2.818×10^{-5}	4.711×10^{-3}	1.398×10^{-2}
	64	381	4.434×10^{-14}	2.460×10^{-2}	1.137×10^{-1}
	128	381	2.005×10^{-15}	2.122×10^{-1}	3.238

(b) H -approach

σ	N	M	E_∞	t_{pre} [s]	t_{avg} [s]
0.20	16	221	4.700×10^{-2}	1.053×10^{-3}	7.024×10^{-4}
	32	221	2.818×10^{-5}	3.473×10^{-3}	5.750×10^{-3}
	64	221	4.423×10^{-14}	1.615×10^{-2}	5.727×10^{-2}
	128	221	2.005×10^{-15}	1.339×10^{-1}	5.201×10^{-1}

Table 5.2.: Results for the Gaussian source (19) on the rectangular domain $B = (-3, 2) \times (-2, 3.5) \times (-1, 5)$ for $\kappa = 1$.

5. Numerical Results

(a) W -approach					
κ	N	M	E_∞	t_{pre} [s]	t_{avg} [s]
0.5	128	401	1.582×10^{-15}	1.620×10^{-1}	8.672×10^{-1}
1.0	128	401	3.231×10^{-15}	2.155×10^{-1}	7.911×10^{-1}
2.0	128	401	2.096×10^{-15}	2.045×10^{-1}	7.887×10^{-1}
5.0	128	381	2.412×10^{-15}	1.966×10^{-1}	7.649×10^{-1}
10.0	128	461	5.698×10^{-15}	2.313×10^{-1}	8.040×10^{-1}

(b) H -approach					
κ	N	M	E_∞	t_{pre} [s]	t_{avg} [s]
0.5	128	201	1.582×10^{-15}	1.538×10^{-1}	5.982×10^{-1}
1.0	128	241	3.119×10^{-15}	2.797×10^{-1}	6.975×10^{-1}
2.0	128	231	2.096×10^{-15}	2.454×10^{-1}	5.717×10^{-1}
5.0	128	281	2.666×10^{-15}	2.569×10^{-1}	6.584×10^{-1}
10.0	128	441	5.837×10^{-15}	2.778×10^{-1}	5.820×10^{-1}

Table 5.3.: Results for the Gaussian source (19) for varying values of κ on the cubic domain $B = [-2, 2]^3$ and $\sigma = 0.20$.

5.3.2. Superposition of Two Gaussian Sources

Next, we consider the superposition of two Gaussian sources $\rho(x) = \frac{1}{2}(\rho_1(x) + \rho_2(x))$, where

$$\rho_i(x) = \frac{1}{(2\pi)^{3/2}\sigma_i^3} \exp\left(-\frac{|x - c_i|^2}{2\sigma_i^2}\right), \quad i = 1, 2.$$

The corresponding exact solution follows, by linearity of the screened Poisson equation, as the superposition of the corresponding individual solutions from equation (20). The results are compiled in Tables 5.4a and 5.4b.

5.3.3. Anisotropic Gaussian Source (Manufactured Solution)

For the following experiments, the exact solution

$$u^*(x) = \exp\left(-\frac{(x - c_x)^2}{\sigma_x^2} - \frac{(y - c_y)^2}{\sigma_y^2} - \frac{(z - c_z)^2}{\sigma_z^2}\right) \quad (21)$$

is prescribed. The corresponding right-hand side is determined by $\rho = (-\Delta + \kappa^2)u^*$:

$$\rho(x) = \left(\frac{4(x - c_x)^2}{\sigma_x^4} + \frac{4(y - c_y)^2}{\sigma_y^4} + \frac{4(z - c_z)^2}{\sigma_z^4} - \frac{2}{\sigma_x^2} - \frac{2}{\sigma_y^2} - \frac{2}{\sigma_z^2} + \kappa^2\right) u^*(x).$$

Table 5.5 shows the results for the cubic domain for $\kappa = 1$ and $\sigma = (0.3, 0.2, 0.28)$.

(a) W -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	401	4.508×10^{-2}	3.154×10^{-3}	1.607×10^{-3}
32	401	9.404×10^{-4}	5.050×10^{-3}	8.599×10^{-3}
64	401	4.061×10^{-9}	1.708×10^{-2}	7.343×10^{-2}
128	401	1.476×10^{-15}	1.683×10^{-1}	7.840×10^{-1}

(b) H -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	241	4.508×10^{-2}	3.899×10^{-3}	7.095×10^{-4}
32	241	9.404×10^{-4}	2.709×10^{-3}	5.511×10^{-3}
64	241	4.061×10^{-9}	1.515×10^{-2}	5.915×10^{-2}
128	241	1.186×10^{-15}	1.487×10^{-1}	5.478×10^{-1}

Table 5.4.: Results for two superposed Gaussian sources on the cubic domain $B = [-2, 2]^3$ for $\kappa = 1$ and $\sigma = (0.2, 0.1)$.

(a) W -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	401	1.684×10^{-1}	1.529×10^{-3}	1.651×10^{-3}
32	401	1.313×10^{-4}	3.628×10^{-3}	9.074×10^{-3}
64	401	9.015×10^{-14}	1.779×10^{-2}	7.664×10^{-2}
128	401	2.127×10^{-15}	1.578×10^{-1}	9.203×10^{-1}

(b) H -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	241	1.684×10^{-1}	1.137×10^{-3}	7.346×10^{-4}
32	241	1.313×10^{-4}	2.543×10^{-3}	5.727×10^{-3}
64	241	9.015×10^{-14}	1.486×10^{-2}	5.680×10^{-2}
128	241	4.441×10^{-16}	1.389×10^{-1}	5.604×10^{-1}

Table 5.5.: Results for the Manufactured Anisotropic Gaussian (21) on $B = [-2, 2]^3$ for $\kappa = 1$ and $\sigma = (0.3, 0.2, 0.28)$.

5. Numerical Results

5.3.4. Bump Function

Next, we consider a compactly supported reference solution. For $r = |x - c|$ let

$$u^*(x) = \begin{cases} \exp\left(-\frac{d}{1 - r^2/R^2}\right), & r < R, \\ 0, & r \geq R. \end{cases} \quad (22)$$

The corresponding right-hand side is defined by $\rho(x) = (-\Delta + \kappa^2)u^*(x)$. The experiments are carried out on the domain $B = [-4, 2] \times [-3, 4] \times [-3, 5]$. The results are compiled in Tables 5.6a and 5.6b.

(a) W -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	421	4.281×10^{-3}	1.212×10^{-3}	1.639×10^{-3}
32	421	3.630×10^{-5}	3.411×10^{-3}	8.778×10^{-3}
64	421	1.984×10^{-8}	1.714×10^{-2}	7.153×10^{-2}
128	421	1.069×10^{-12}	1.517×10^{-1}	7.114×10^{-1}

(b) H -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	231	4.281×10^{-3}	6.362×10^{-3}	7.410×10^{-4}
32	231	3.630×10^{-5}	3.655×10^{-3}	5.905×10^{-3}
64	231	1.984×10^{-8}	1.508×10^{-2}	6.033×10^{-2}
128	231	1.069×10^{-12}	1.395×10^{-1}	5.765×10^{-1}

Table 5.6.: Results for the bump function (22) on $B = [-4, 2] \times [-3, 4] \times [-3, 5]$ with $\kappa = 1$, $R = 2$ and $d = 10$.

5.3.5. Oscillatory Manufactured Solution

As the last benchmark, we consider an oscillatory analytical reference solution of the form

$$u^*(x) = e^{-|x-c|^2/\sigma^2} \cos(\omega|x-c|^2). \quad (23)$$

The corresponding right-hand side is defined by $\rho(x) = (-\Delta + \kappa^2)u^*(x)$. The experiments are carried out on the domain $B = [-2, 2]^3$. The results are compiled in Tables 5.7a and 5.7b.

5.4. Comparison of the Approaches

In this section, the results of both approaches are directly compared using the benchmark data collected in 5.3. The quantities compared are the average solver time t_{avg} , the

5.4. Comparison of the Approaches

(a) W -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	401	1.036×10^0	1.185×10^{-3}	1.626×10^{-3}
32	401	3.688×10^{-3}	3.268×10^{-3}	8.660×10^{-3}
64	401	2.929×10^{-8}	1.718×10^{-2}	7.469×10^{-2}
128	401	8.281×10^{-15}	1.678×10^{-1}	7.273×10^{-1}

(b) H -approach				
N	M	E_∞	t_{pre} [s]	t_{avg} [s]
16	241	1.036×10^0	1.086×10^{-3}	7.203×10^{-4}
32	241	3.688×10^{-3}	2.499×10^{-3}	5.607×10^{-3}
64	241	2.929×10^{-8}	1.545×10^{-2}	5.660×10^{-2}
128	241	2.220×10^{-16}	1.403×10^{-1}	5.745×10^{-1}

Table 5.7.: Results for the oscillatory density (23) on $B = [-2, 2]^3$ with $\kappa = 1$, $\sigma = 0.3$ and $\omega = 20$.

relative ℓ^∞ -error E_∞ , and the number of Gaussian terms M for all configurations in which both methods were evaluated under identical parameters. Figure 5.9 contrasts the kernels G , W and H for $\kappa = 1$.

In the direct runtime comparison (Figure 5.10), the majority of points lie below the diagonal, i.e. the H -approach exhibits a shorter average solver time than the W -approach for the predominant part of the evaluated configurations.

The accuracy comparison in Figure 5.11 shows that for almost all configurations the points lie on or very close to the diagonal. Points that deviate slightly from the diagonal in the near-machine-precision regime correspond to configurations in which both methods achieve errors close to machine precision.

The predominant part of the points in Figure 5.12 lies in the upper right quadrant, i.e. the H -approach requires fewer Gaussian terms and simultaneously achieves a shorter solver time. Configurations to the left of the vertical line, for which the H -approach requires slightly more terms, exhibit no noteworthy runtime disadvantage.

5. Numerical Results

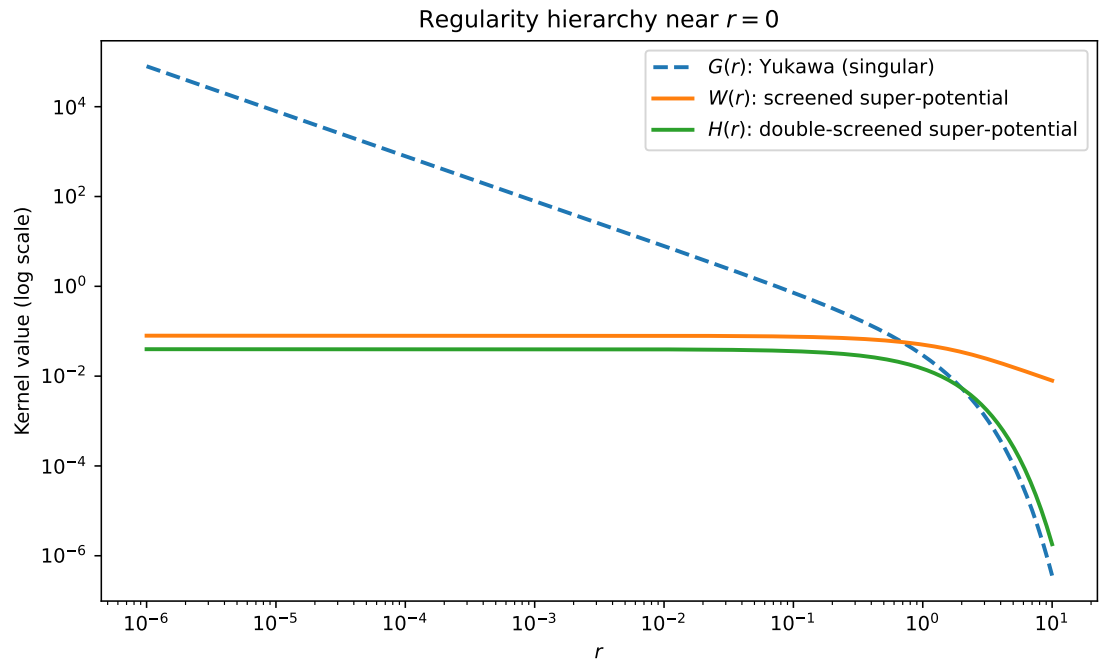


Figure 5.9.: Regularity hierarchy of the kernels G , W and H for $\kappa = 1$.

5.4. Comparison of the Approaches

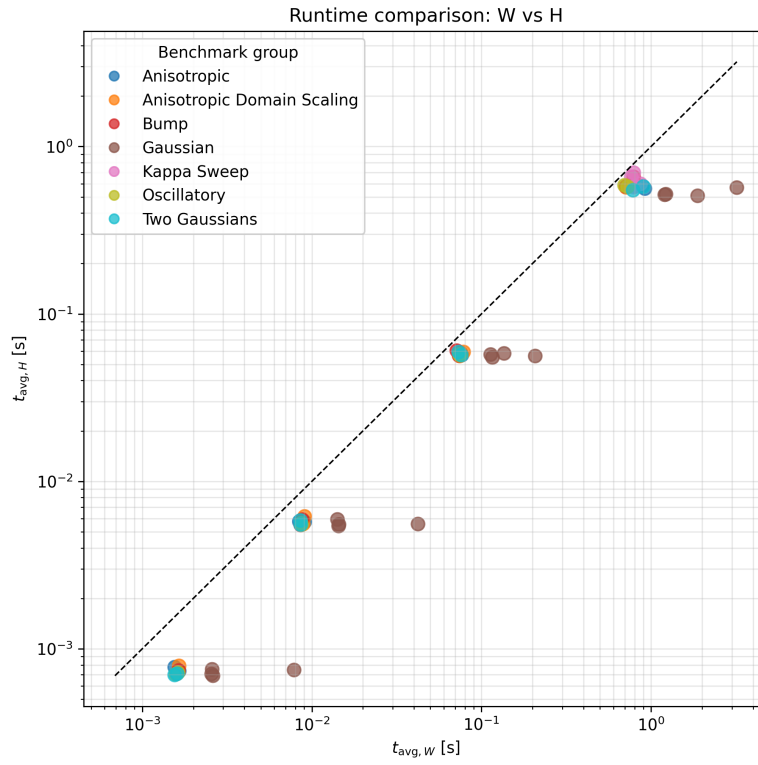


Figure 5.10.: Direct runtime comparison of the average solver times $t_{\text{avg},W}$ and $t_{\text{avg},H}$ across all benchmark configurations on a double logarithmic scale.

5. Numerical Results

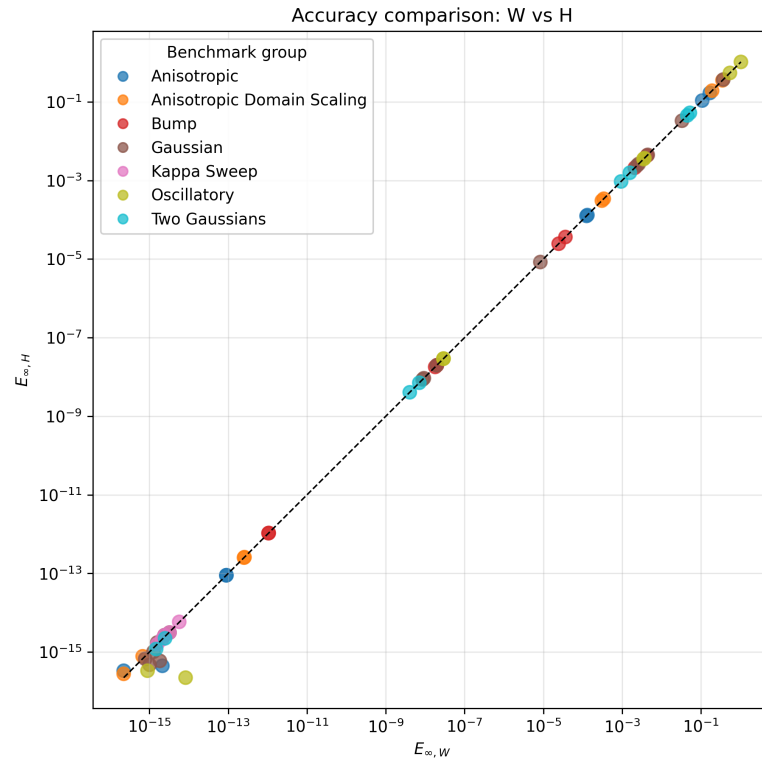


Figure 5.11.: Direct accuracy comparison of the relative ℓ^∞ -errors $E_{\infty,W}$ and $E_{\infty,H}$ across all benchmark configurations on a double logarithmic scale. The dashed line marks $E_{\infty,W} = E_{\infty,H}$.

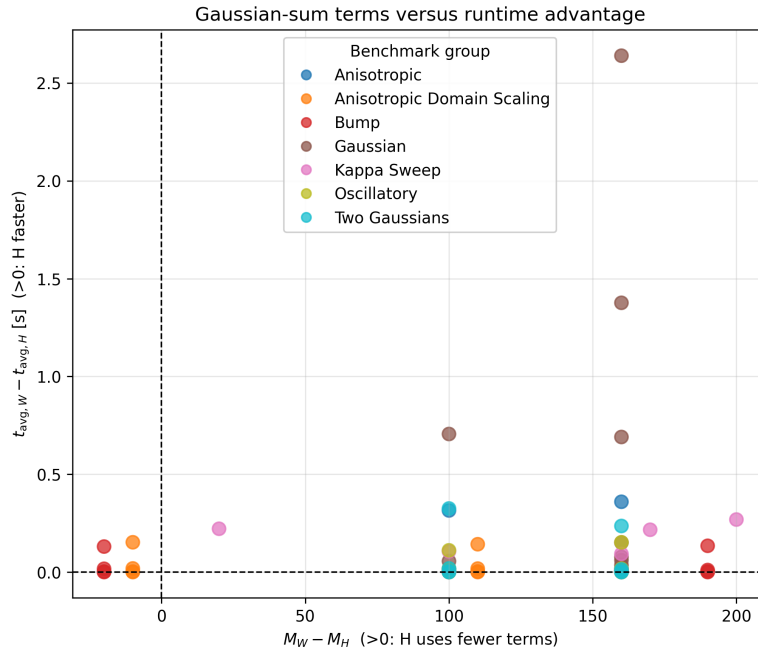


Figure 5.12.: Difference of the numbers of Gaussian terms $M_W - M_H$ versus the difference of the average solver times $t_{\text{avg},W} - t_{\text{avg},H}$ across all benchmark configurations.

6. Conclusion

6.1. Summary

This work develops and analyzes two FFT-based methods for the efficient numerical solution of the free-space equation $(-\Delta + \kappa^2)u = \rho$ in $\mathbb{R}^3$ with compactly supported source density $\rho \in L^\infty(\mathbb{R}^3)$. Both methods are based on the super-potential method, in which the direct convolution with the singular Yukawa kernel $G(r) = e^{-\kappa r}/(4\pi r)$ is avoided by convolution with a more regular surrogate kernel. The spectral evaluation is performed by means of separable Gaussian-sum approximations of the kernels and an FFT-based convolution computation.

The main results are:

- **Kernel construction and regularity.** The W -approach (Mixed-Screened) uses the super-potential $u = -\Delta(W * \rho)$, where W is the fundamental solution of the operator $(-\Delta)(-\Delta + \kappa^2)$. The H -approach (Double-Screened) uses $u = (-\Delta + \kappa^2)(H * \rho)$, where H is the fundamental solution of $(-\Delta + \kappa^2)^2$. Both kernels are bounded at the origin, in contrast to the non-removable singularity of the Yukawa kernel G .
- **Gaussian-sum approximation.** For the W -approach, a Gaussian-sum approximation is derived via a logarithmic transformation. Since Proposition 1 is not directly applicable to the transformed integrand, the error analysis is carried out by a manual decomposition into three terms, yielding a complexity of $M = \mathcal{O}(\log^2(1/\eta))$ terms for a target accuracy η . For the H -approach, the transformed integrand fully satisfies the assumptions of Proposition 1, so that the error analysis can be applied directly and the improved complexity $S = \mathcal{O}(\log(1/\eta) \log \log(1/\eta))$ follows.
- **Error analysis and a priori bounds.** For both approaches, a complete a priori bound for the total error $\|u - u_h\|_{\ell^\infty(B_1)}$ is derived, which exhibits a two-term structure: a near-field term of order $\mathcal{O}(\varepsilon^3)$ and a spectral discretization term that decays with the grid size N for smooth densities. The order $\mathcal{O}(\varepsilon^3)$ is one order below that of the Poisson case ($\mathcal{O}(\varepsilon^4)$), since both kernels do not vanish at the origin and the near-field contribution is not suppressed by the kernel behavior.
- **Numerical verification.** The numerical experiments confirm the central theoretical predictions. The Gaussian-sum approximation meets the prescribed target accuracies uniformly, and the measured complexities agree with the theoretical predictions. The cubic near-field convergence of both approaches is confirmed in the double logarithmic scale. The two-term structure of the total error is compatible with the numerical data in both cases.

- **Benchmarks.** Both methods achieve relative ℓ^∞ -errors near machine accuracy for grid sizes $N = 128$ across various test problems, including Gaussian sources, anisotropic and compactly supported manufactured solutions, as well as oscillating reference solutions. Both approaches deliver nearly identical accuracy at the same configurations. The H -approach consistently requires fewer Gauss terms and achieves shorter mean solve times for the majority of the evaluated configurations.

The results show that both approaches enable the numerical solution of the screened Poisson equation in free-space geometry with accuracy near machine precision. The H -approach offers structural advantages over the W -approach in the error analysis and a more favorable number-of-terms asymptotics, which is reflected in the benchmarks for the majority of the considered configurations in shorter runtimes.

6.2. Outlook

The present work raises several follow-up questions that go beyond the treated framework.

Sharpness of the $\mathcal{O}(\varepsilon^3)$ bound. Both kernels W and H are bounded at the origin and do not vanish there. In contrast to the Poisson case, where $V(y) = \mathcal{O}(|y|)$ for $|y| \rightarrow 0$ holds and the near-field term yields order $\mathcal{O}(\varepsilon^4)$, the boundedness of the kernels at the origin gives rise to an a priori bound of order $\mathcal{O}(\varepsilon^3)$ for W and H . Whether this bound is sharp remains open. Likewise, it is unclear whether a construction exists in which the super-potential kernel for the screened Poisson equation vanishes at the origin and thereby restores $\mathcal{O}(\varepsilon^4)$.

Error analysis of the W -approach. The error analysis of the W -approach required a manual decomposition into three terms, since none of the transformations examined satisfies all assumptions of Proposition 1: the logarithmic transformation violates the double exponential decay condition at the left boundary, while the sinh-transformation fails at the strip condition. It remains an open question whether a transformation exists that satisfies both conditions simultaneously and thereby enables a more direct analysis, as was possible for the H -approach.

Generalization of the operator factorization. The H -approach is based on the factorization $(-\Delta + \kappa^2)^2 H = \delta_0$, which can be understood as a generalization of the Poisson construction $-\Delta^2 V = \delta_0$. The principle used, of reducing the solution of $Lu = \rho$ via a factorization $\tilde{L} \cdot L \cdot K = \delta_0$ to the convolution with a more regular kernel K , is not restricted to the operators considered here. A natural extension concerns operators of the form $(-\Delta + \kappa^2)^n$ for $n \geq 3$, for which analogous fundamental solutions are explicitly known. More generally, the approach appears transferable to elliptic operators whose fundamental solution is bounded at the origin.

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A. Source Code Listings

Appendix A.1 lists the core functions of the Mixed-Screened approach (W -approach), Appendix A.2 those of the Double-Screened approach (H -approach), and Appendix A.3 documents the benchmark methodology together with the Gaussian source experiment.

A.1. The Mixed-Screened Super-Potential Method

Listing A.1: Numerically stable evaluation of $W(r; \kappa)$ and the naive indirect form $(U - G)/\kappa^2$ illustrating cancellation for small κ .

```
1 def W(r, kappa):
2     with np.errstate(invalid='ignore', divide='ignore'):
3         val = (1.0 - np.exp(-kappa * r)) / (4.0 * np.pi * kappa**2
4         * r)
5     return np.where(r < 1e-14, 1.0 / (4.0 * np.pi * kappa), val)
6
7 def W_stable(r, kappa):
8     return (-np.expm1(-kappa * r)) / (4.0 * np.pi * kappa**2 * r)
9
10 def W_naive_indirect(r, kappa):
11     U = 1.0 / (4.0 * np.pi * r)
12     G_kern = np.exp(-kappa * r) / (4.0 * np.pi * r)
13     return (U - G_kern) / kappa**2
```

Listing A.2: Direct Gaussian-sum approximation $W_{\text{GS}}(r) = \sum_{j=M_1}^{M_2} \omega_j e^{-\tau_j^2 r^2}$ with nodes τ_j and weights ω_j from the logarithmic transformation.

```
1 @dataclass(frozen=True)
2 class WDirectGSPParams:
3     kappa: float; h: float; M1: int; M2: int
4     tau: np.ndarray; omega: np.ndarray
5
6 def build_W_direct_gs_params(kappa, h, M1, M2) -> WDirectGSPParams:
7     j = np.arange(M1, M2 + 1, dtype=np.float64)
8     tau = np.exp(j * float(h))
9     omega = (float(h) / (2.0 * np.pi**1.5 * float(kappa)**2)
10     * tau
11     * (-np.expm1(-(float(kappa)**2 / 4.0) * np.exp(-2.0 *
12     j * float(h)))))
13     return WDirectGSPParams(kappa=float(kappa), h=float(h), M1=M1,
14     M2=M2,
```

A.1. The Mixed-Screened Super-Potential Method

```

13         tau=tau, omega=omega)
14
15 def W_direct_gs_r(gs: WDirectGSParams, r) -> np.ndarray:
16     r2 = np.atleast_1d(np.asarray(r, dtype=np.float64))**2
17     return (gs.omega[:, None] * np.exp(-(gs.tau[:, None]**2) * r2[
        None, :]))).sum(axis=0)

```

Listing A.3: Fourier integral $I_0(k; \alpha)$ evaluated across four numerical regimes, and separable assembly of $\hat{W}_k$ via Kronecker products.

```

1  LARGE_ALPHA_THRESHOLD = 50.0
2  SMALL_ALPHA_THRESHOLD = 1e-8
3
4  def build_I_tables(alphas_scaled: np.ndarray, kmax: int, nq: int =
    256,
5                      need_I2: bool = True):
6      alphas = np.asarray(alphas_scaled, dtype=np.float64)
7      k = np.arange(0, kmax + 1, dtype=np.float64)
8      K = k.shape[0]
9      S = alphas.shape[0]
10     I0 = np.empty((K, S), dtype=np.float64)
11     I2 = np.empty((K, S), dtype=np.float64) if need_I2 else None
12     zero_mask = (alphas == 0.0)
13     small_mask = (alphas > 0) & (alphas < SMALL_ALPHA_THRESHOLD)
14     large_mask = (alphas >= LARGE_ALPHA_THRESHOLD)
15     mid_mask = (alphas >= SMALL_ALPHA_THRESHOLD) & (alphas <
        LARGE_ALPHA_THRESHOLD)
16     cos_pik = np.cos(np.pi * k) # (K,)
17     pk = np.pi * k
18     # alpha = 0
19     if zero_mask.any():
20         idx0 = np.where(zero_mask)[0]
21         k_is_zero = (k == 0.0)
22         I0_0 = np.where(k_is_zero, 2.0, 0.0)
23         with np.errstate(divide="ignore", invalid="ignore"):
24             I2_0 = np.where(k_is_zero, 2.0/3.0,
25                             2.0*(np.sin(pk)/pk + 2*np.cos(pk)/pk
26                                 **2 - 2*np.sin(pk)/pk**3))
27         I0[:, idx0] = I0_0[:, None]
28         if need_I2:
29             I2[:, idx0] = I2_0[:, None]
30     # alpha small: Taylor
31     if small_mask.any():
32         idx_s = np.where(small_mask)[0]
33         a_s = alphas[small_mask] # (Ss,)
34         k_is_zero = (k == 0.0)
35         I0_0 = np.where(k_is_zero, 2.0, 0.0)
36         with np.errstate(divide="ignore", invalid="ignore"):
37             I2_0 = np.where(k_is_zero, 2.0/3.0,

```

A. Source Code Listings

```

37         2.0*(np.sin(pk)/pk + 2*np.cos(pk)/pk
38             **2 - 2*np.sin(pk)/pk**3))
39     # I0(k, alpha) ca I0(k, 0) - alpha * I2(k, 0)
40     I0[:, idx_s] = I0_0[:, None] - a_s[None, :] * I2_0[:, None]
41     ]
42     if need_I2:
43         I2[:, idx_s] = np.broadcast_to(I2_0[:, None], (K, a_s.
44             shape[0])).copy()
45     # alpha big: Gaussian-asymptotic (faster than wofz, neglect
46     the term on the edge ~e^{-alpha})
47     if large_mask.any():
48         idx_L = np.where(large_mask)[0]
49         a_L = alphas[large_mask] # (SL,)
50         sq = np.sqrt(np.pi / a_L) # (SL
51         ,)
52         exp_k = np.exp(-(np.pi**2) * k[:, None]**2 / (4.0 * a_L[
53             None, :])) # (K, SL)
54         I0[:, idx_L] = sq[None, :] * exp_k
55     if need_I2:
56         # I2 = I0/(2alpha) * (1 - pi^2k^2/(2alpha)) - e^{-
57         alpha} cos(pik)/alpha
58         I2[:, idx_L] = (I0[:, idx_L] / (2.0 * a_L[None, :])) \
59             * (1.0 - (np.pi**2) * k[:, None]**2 /
60                 (2.0 * a_L[None, :]))
61     # alpha middle: analytic via Faddeeva
62     if mid_mask.any():
63         idx_m = np.where(mid_mask)[0]
64         a_m = alphas[mid_mask] # (Sm,)
65         sa = np.sqrt(a_m)
66         b = (np.pi * k[:, None]) / (2.0 * sa[None, :]) # (K, Sm
67         )
68         z = sa[None, :] + 1j * b
69         W = _wofz(1j * z)
70         phase = cos_pik[:, None] # (K, 1)
71         , +/-1
72         re_term = np.exp(-a_m)[None, :] * phase * np.real(W)
73         re_erf_times_expmb2 = np.exp(-b*b) - re_term
74         I0_m = np.sqrt(np.pi / a_m)[None, :] * re_erf_times_expmb2
75         I0[:, idx_m] = I0_m
76     if need_I2:
77         I2[:, idx_m] = (I0_m / (2.0 * a_m[None, :])) \
78             * (1.0 - (np.pi**2) * k[:, None]**2 /
79                 (2.0 * a_m[None, :])) \
80             - (np.exp(-a_m) / a_m)[None, :] *
81             cos_pik[:, None]
82
83     return I0, I2

```

Listing A.4: FFT-based solver for $u_h = -\Delta_h(W_{GS} * \rho)$ via spectral Laplacian multiplier.

```

1 def build_W_multiplier(W_hat, setup):
2     return -setup.lap_mult * W_hat
3
4 def solve_superpotential(setup, gs, rho_B1):
5     nt = setup.nt
6     n = setup.n
7     sl = b1_center_slices(n)
8     rho_B2 = np.zeros(nt, dtype=np.float64)
9     rho_B2[sl.sx, sl.sy, sl.sz] = rho_B1
10    W_hat = precompute_W_hat(setup, gs)
11    G = build_W_multiplier(W_hat, setup)
12    rho_hat = np.fft.fftn(rho_B2)
13    u_B2 = np.fft.ifftn(rho_hat * G).real
14    return u_B2[sl.sx, sl.sy, sl.sz].copy()

```

A.2. The Double-Screened Super-Potential Method

Listing A.5: Gaussian-sum approximation $H_{\text{GS}}(r) = \sum_{j=-S}^S \omega_j e^{-\tau_j^2 r^2}$ and parameter selection implementing the $\mathcal{O}(\log(1/\eta) \log \log(1/\eta))$ complexity bound.

```

1 @dataclass(frozen=True)
2 class HDoubleScreenedGSPParams:
3     kappa: float
4     h: float
5     S: int
6     tau: np.ndarray
7     omega: np.ndarray
8
9 def build_H_double_screened_gs_params(kappa, h, S) ->
10    HDoubleScreenedGSPParams:
11    kappa = float(kappa)
12    h = float(h)
13    S = int(S)
14    j = np.arange(-S, S + 1, dtype=np.float64)
15    tau = np.exp(j * h)
16    omega = (
17        h / (8.0 * np.pi**1.5)
18        * np.exp(-j * h)
19        * np.exp(-(kappa**2 / 4.0) * np.exp(-2.0 * j * h))
20    )
21    return HDoubleScreenedGSPParams(
22        kappa=kappa,
23        h=h,
24        S=S,
25        tau=tau,
26        omega=omega,

```

A. Source Code Listings

```

26     )
27
28 def H_double_screened_gs_r(gs: HDoubleScreenedGSParams, r) -> np.
    ndarray:
29     r2 = np.atleast_1d(np.asarray(r, dtype=np.float64))**2
30     return (
31         gs.omega[:, None]
32         * np.exp(-(gs.tau[:, None]**2) * r2[None, :])
33     ).sum(axis=0)

```

Listing A.6: FFT-based solver for $u_h = (-\Delta_h + \kappa^2)(H_{\text{GS}} * \rho)$ via screened spectral multiplier $((2\pi)^2|k|^2 + \kappa^2)\hat{H}_k$.

```

1 def build_H_screened_multiplier(H_hat: np.ndarray, setup: FFTSetup
    , kappa: float) -> np.ndarray:
2     screened_mult = -setup.lap_mult + float(kappa)**2
3     return screened_mult * H_hat
4
5 def solve_double_screened_superpotential(
6     setup: FFTSetup,
7     gs: HDoubleScreenedGSParams,
8     rho_B1: np.ndarray,
9 ) -> np.ndarray:
10     nt = setup.nt
11     n = setup.n
12     sl = b1_center_slices(n)
13     rho_B2 = np.zeros(nt, dtype=np.float64)
14     rho_B2[sl.sx, sl.sy, sl.sz] = rho_B1
15     H_hat = precompute_H_hat(setup, gs)
16     G = build_H_screened_multiplier(H_hat, setup, gs.kappa)
17     rho_hat = np.fft.fftn(rho_B2)
18     u_B2 = np.fft.ifftn(rho_hat * G).real
19     return u_B2[sl.sx, sl.sy, sl.sz].copy()

```

A.3. Benchmark Methodology and Gaussian Source Experiment

Listing A.7: Benchmark runner measuring precomputation time and averaged solver time separately, with GS parameters cached per kappa.

```

1 def benchmark_table_H(*, name, B, Ns, param_list, rho_fn,
2     u_exact_fn, eps_gs=1e-5, tol=1e-14,
3     delta_gs=np.sqrt(3.0), repeats=5, nq=256):
4     # Cache GS parameters per kappa to avoid redundant computation
5     gs_cache = {}
6     for params in param_list:
7         kappa = float(params["kappa"])

```

A.3. Benchmark Methodology and Gaussian Source Experiment

```

8         if kappa not in gs_cache:
9             h_gs, S = eps_to_h_S_H_direct(kappa=kappa, eps=eps_gs,
10                                             delta=delta_gs, tol=tol
11                                             )
12             gs_cache[kappa] = build_H_double_screened_gs_params(
13                 kappa, h_gs, S)
14         gs = gs_cache[kappa]
15         # Precompute kernel and measure t_pre per grid size
16         for N in Ns:
17             setup = build_fft_setup(N, N, N, DomainBox(*B))
18             t0 = time.perf_counter()
19             H_hat = precompute_H_hat(setup, gs, nq=nq)
20             G = build_H_screened_multiplier(H_hat, setup, gs.
21                                             kappa)
22             t_pre = time.perf_counter() - t0
23
24             rho_B1 = rho_fn(setup, params)
25             u_ex_B1 = u_exact_fn(setup, params)
26             sl = b1_center_slices(setup.n)
27             rho_B2 = np.zeros(setup.nt, dtype=np.float64)
28             rho_B2[sl.sx, sl.sy, sl.sz] = rho_B1
29             # Average solver time over repeated runs
30             t0 = time.perf_counter()
31             for _ in range(repeats):
32                 rho_hat = np.fft.fftn(rho_B2)
33                 u_B2 = np.fft.ifftn(rho_hat * G).real
34                 u_num_B1 = u_B2[sl.sx, sl.sy, sl.sz].copy()
35             t_avg = (time.perf_counter() - t0) / repeats
36             E_inf = relerr_inf(u_ex_B1, u_num_B1)

```

Listing A.8: Gaussian source density ρ and closed-form exact solution u^* , evaluated using `erfcx` to avoid overflow with a L'Hôpital limit at $r = 0$.

```

1 def rho_gaussian(setup: FFTSetup, p: dict) -> np.ndarray:
2     sigma = float(p["sigma"])
3     cx, cy, cz = map(float, p.get("center", setup.B1.center))
4     X, Y, Z, _ = B1_coords_from_setup(setup, return_mesh=True)
5     r2 = (X - cx)**2 + (Y - cy)**2 + (Z - cz)**2
6     pref = 1.0 / ((2.0 * np.pi)**1.5 * sigma**3)
7     return pref * np.exp(-r2 / (2.0*sigma**2))
8
9 def u_exact_gaussian_screened(setup: FFTSetup, p: dict) -> np.
10 ndarray:
11     sigma = float(p["sigma"])
12     kappa = float(p["kappa"])
13     cx, cy, cz = map(float, p.get("center", setup.B1.center))
14     A = np.exp(kappa**2 * sigma**2 / 2.0)
15     X, Y, Z, _ = B1_coords_from_setup(setup, return_mesh=True)
16     r = np.sqrt((X - cx)**2 + (Y - cy)**2 + (Z - cz)**2)

```

A. Source Code Listings

```

16     sq2 = np.sqrt(2.0)
17     # Limit at r=0 via L'Hopital
18     u0 = (1.0 / (4.0 * np.pi)) * (
19         -kappa * A * erfc(kappa * sigma / sq2)
20         + np.sqrt(2.0 / np.pi) / sigma
21     )
22     with np.errstate(over="ignore", invalid="ignore", divide="
        ignore"):
23         a1 = (kappa * sigma**2 - r) / (sq2 * sigma)
24         a2 = (kappa * sigma**2 + r) / (sq2 * sigma)
25         B = kappa**2 * sigma**2 / 2.0
26         term1 = np.exp(B - kappa * r - a1**2) * erfcx(a1)
27         term2 = np.exp(B + kappa * r - a2**2) * erfcx(a2)
28         u = (term1 - term2) / (8.0 * np.pi * r)
29     return np.where(r < 1e-10, u0, u)

```

Listing A.9: Benchmark Example: Gaussian source on a cubic domain, four grid sizes, four parameter pairs, averaged over 10 solver runs.

```

1  B = (-2., 2., -2., 2., -2., 2.)
2  records_H += benchmark_table_H(
3      name="Gaussian source on B=[-2,2]^3",
4      B=B,
5      Ns=[16, 32, 64, 128],
6      param_list=[
7          {"kappa": 1.0, "sigma": 0.20},
8          {"kappa": 1.0, "sigma": 0.15},
9          {"kappa": 1.0, "sigma": 0.10},
10         {"kappa": 5.0, "sigma": 0.20},
11     ],
12     label_fn=lambda p: f"kappa={p['kappa']}, sigma={p['sigma']}",
13     header_left="(kappa, sigma)",
14     rho_fn=rho_gaussian,
15     u_exact_fn=u_exact_gaussian_screened,
16     eps_gs=1e-5,
17     tol=1e-16,
18     delta_gs=box_radius(B),
19     repeats=10,
20 )

```