On the efficient computation of multidimensional singular sums

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by

Andreas Alexander Buchheit

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Dean of the faculty:	Prof. Dr. Thomas Schuster

Examination committee

Chair:	Prof. Dr. Alfred K. Louis
First reviewer:	Prof. Dr. Sergej Rjasanow
Second reviewer:	Prof. Dr. Matthias Ehrhardt
Third reviewer:	Prof. Dr. Frank Wilhelm-Mauch
Scientific assistant:	Dr. Dimitri Rothermel

Abstract

This thesis is concerned with the development of the singular Euler–Maclaurin expansion, a novel method that allows for the efficient evaluation of large sums over values of functions with singularities. The method offers an approximation to the sum whose runtime is independent of the number of summands and whose error falls of exponentially with the expansion order. Hereby, a powerful numerical tool is provided whose applications range from fast multidimensional summation methods in numerical analysis over the analysis of long-range interactions in condensed matter systems to the evaluation of partition functions in quantum physics. The numerical performance of the new method is demonstrated by precisely computing the forces in a topological defect in a one-dimensional chain of long-range interacting particles. Furthermore, prototypical sums in an infinite two-dimensional lattice are efficiently evaluated. In the derivation of the multidimensional expansion, a deep connection between our new method to analytical number theory is revealed. This connection provides tools for the efficient computation of the operator coefficients that appear in the expansion. On the other hand, the expansion yields new globally convergent representations of the Riemann zeta function and its generalisation to higher dimensions.

Kurzzusammenfassung

Die vorliegende Arbeit beschäfigt sich mit der Entwicklung der singulären Euler–Maclaurin Entwicklung, einer neuen Methode zur effizienten Auswertung großer Summen über Werte von Funktionen mit Singularitäten. Die Methode ermöglicht eine Approximation der Summe mit einem von der Anzahl an Summanden unabhängigen numerischen Aufwand, deren Approximationsfehler zudem exponentiell mit der Entwicklungsordnung abfällt. Hierdurch wird ein mächtiges numerisches Werkzeug bereitgestellt, dessen Anwendungen von der effizienten Auswertung großer mehrdimensionaler Summen in der Numerik über die Analyse von langreichweitigen Wechselwirkungen in Festkörpern bis hin zur Auswertung von Zustandssummen in der Quantenmechanik reichen. Die numerische Leistungsstärke der neuen Methode wird anhand der präzisen Auswertung von langreichweitigen Kräften innerhalb eines topologischen Defekts in einer eindimensionalen Kette aufgezeigt. Weiterhin werden prototypische Summen in einem unendlichen zweidimensionalen Gitter effizient berechnet. In der Herleitung der mehrdimensionalen Entwicklung tritt eine tiefgehende Verbindung zur analytischen Zahlentheorie zutage. Diese Verbindung kann einerseits genutzt werden, um die Operatorkoeffizienten der Entwicklung effizient zu berechnen. Andererseit stellt die Entwicklung neue global konvergente Darstellungen der Riemann Zeta Funktion und ihrer Verallgemeinerung auf höhere Raumdimensionen bereit.

List of publications and joint publication statement

The contents of this thesis are based on the research published in the following two articles [6, 7]:

[6] Andreas A. Buchheit and Torsten Keßler.
Singular Euler-Maclaurin expansion.
In review, *arXiv preprint arXiv:2003.12422*, 2020,

[7] Andreas A. Buchheit and Torsten Keßler.
Singular Euler-Maclaurin expansion
on multidimensional lattices.
In review, *arXiv preprint arXiv:2102.10941*, 2021.

During the work on this thesis, I have furthermore published a third article [8] together with my supervisor Prof. Sergej Rjasanow in the field of nonlinear condensed matter and quantum physics,

[8] Andreas A. Buchheit and Sergej Rjasanow.
Ground state of the Frenkel–Kontorova model with a globally deformable substrate potential.
Physica D: Nonlinear Phenomena, 406:132298, 2020.

Nowadays, excellent research is often based on great teamwork. This is certainly true for above articles, out of which [6] and [7] are joint works with my colleague Torsten Keßler. In accordance to the Plagiarism Policy of the Faculty of Mathematics and Computer Science of Saarland University, Revision 2020-01-15, I now discuss the individual contributions to the publications [6] and [7]:

I developed the idea for the new expansion and set it into context with open problems in condensed matter physics. In the next step, I laid out a strategy on how to approach the problem, wrote early first versions of the manuscripts, provided first proofs of the theorems, and verified working assumptions on the expansion by extensive numerical experiments in case of the one-dimensional problem [6] and for the generalisation to higher dimensions in [7]. My colleague Torsten Keßler and I thereafter contributed equally to the publications [6, 7]. We finalised the proofs, analysed the numerical results, and jointly created the final version of the two articles.

In a footnote on the first page of each chapter of the thesis, I explicitly state the respective publication on which the chapter is based.

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The past two years have, in many regards, been quite a challenging yet rewarding journey. I have to thank many friends and colleagues that accompanied me on the way, made it both enjoyable and enriching, and lent support when it was needed. First of all, I would like to thank my respected colleagues Torsten Keßler, Daniel Seibel, Jan Schmitz, Christian Michel, Steffen Weißer, and Darya Apushkinskaya, for a great time in and outside of the office and for bringing my mathematical knowledge to a new level. In particular, I am highly grateful to my colleagues and friends Torsten Keßler and Daniel Seibel for many hours of helpful discussions. I also want to thank Jan Schmitz for his amazing job as a system administrator. Never before have I experienced such an inspiring working atmosphere as in this group, where everyone is willing to freely share their extensive knowledge in many different fields of expertise. The most important feature of this work environment is that everyone is conducting free, curiosity driven research, which is not all that common in these times. This atmosphere is, of course, a consequence of the work of my highly respected supervisor Prof. Sergej Rjasanow. I am highly grateful for your continued and unconditional support. You made it possible for me to to freely pursue the high-risk but high-reward project that resulted in this thesis and offered help whenever needed. Thank you for everything.

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Thanks to Dominik Kirst for introducing me to the taekwondo club and for organising the regular piano concerts; music has certainly been an inspiration. Also thanks to Marina Gogelgans, who taught me how to make Beethoven sound like it should. The third sonata will soon be ready to go.

Last but not least, a big thank you goes to my family! First, let me thank my sister Carolin, who has been a role model to look up to and a good friend all my life! A big thanks goes to to Michael, who makes the best drinks and the best fireworks. I am grateful to Ron; let's soon find use for the Schwenker again. Thanks to my dear grandma Roswitha, who makes the best food in all of Saarland. Finally, a big thank you goes to my mother Birgit, for your love and for teaching me the most important things in life. Thank you all for your lifelong support.

Contents

Motivation and overview

This thesis is concerned with the efficient computation of numerically challenging sums that appear in physical applications. Addition is among the most basic and historically most ancient of all mathematical operations. By repeated addition of the number 1 to itself, we can count, and from counting, the natural numbers $\mathbb{N} = \{1, 2, 3, \dots\}$ are created. If you can count, you can make predictions on the future. It is the starting point of all scientific progress.

While the addition of two numbers is a basic operation, the computation of a large sum can turn into a challenging problem, as it is difficult to improve upon the numerical efficiency of the underlying operation. The main approach for computing sums with a large number of addends is to approximate them by an integral, which is possible if the summands are based on function values. This integral is subsequently computed by means of quadrature rules, which finally results again in a sum, but with a smaller number of addends [13].

However, it is a priori not clear how to quantify the approximation error of the integral approximation to the sum. A first step towards an answer to this question was provided by Euler and Maclaurin in the 18th century, who discovered that the difference between sum and integral of a sufficiently smooth function can be expanded in terms of derivatives of the summand function [1]. The resulting expansion is called the Euler–Maclaurin expansion, which is discussed in more detail in Chapter 1. This expansion offers, in principle, an efficient way to express sums in terms of integrals and local derivatives. However, it exhibits two severe problems that stop it from being applicable to physically relevant problems. First, the expansion does not converge for summand functions that include singularities [1]. Unfortunately, all relevant physical interactions, e.g. the electromagnetic and the gravitational interaction, are of this kind. Second, the Euler–Maclaurin expansion offers an expansion of a one-dimensional sum, whereas most physical problems are high-dimensional. While early first steps towards a solution of the first problem were made by Navot [42] and to the second by Müller [41] and Freeden [23], a satisfactory solution to both problems remained to be found. A more detailed review of generalised Euler–Maclaurin expansions is given in Sections 1.1 and 2.1. In this thesis, the multidimensional singular Euler–Maclaurin expansion is developed, which resolves both problems mentioned above and makes the expansion applicable to realistic physical problems.

In nature, we regularly encounter the situation that a system can be understood as the sum of a macroscopic number of microscopic individual and irreducible parts, whose interplay determine the system properties [10]. The most basic example is given by the condensed matter that surrounds us. A few grams of a solid consist of a number of atoms in the range of the Avogadro constant $N_A \approx 6 \times 10^{23}$. The pairwise interactions between the atoms or molecules inside a solid, for instance a crystal, in principal give rise to its macroscopic properties. Although we are well aware of these microscopic interactions [24], e.g. of the Coulomb interaction that acts between charged ions, it is a challenging task to derive from them the properties of the material at the macro- (or even meso) scale due to the sheer number of particles that are involved. Continuum limits are challenging if long-range interactions are present, see e.g. [35] for a discussion of the nonlinear Schrödinger equation in a charged DNA string. Large sums also appear in case of microscopic interactions in spin lattices. Topological excitations in spin lattices, so called Skyrmions, are promising candidates for efficiently storing and moving information in spintronics devices [12] and could become a part in a new spin-based IT infrastructure. Metamaterials [50], which promise the creation of flat lenses and new tools for manipulating light in general, are composed of mesoscopic structures, where the number of particles is too small for standard continuum limits yet too large to be efficiently computable. Finally, sums with large number of addends typically arise in partition functions in statistical physics and quantum mechanics from which the thermodynamic properties of the system under consideration can be determined [9].

All these examples from condensed matter and statistical physics share a fundamental granularity in their description. Discreteness is also found on a more basic level, as the universe itself consists of interacting elementary particles. Some theories go even further and consider discreteness not only of particles, but also of space and/or time. For instance a discretisation of space-time is a well known numerical method in quantum field theory, which regularises divergent path integrals [46]. Loop quantum gravity on the other hand introduces a granularity at the Planck scale in order to reconcile quantum mechanics and general relativity [15, 45].

The method developed in this thesis can be used for rigorous derivations of precise continuum limits of discrete systems even in case that singular interactions are present. Higher orders of the expansion describe finite size effects in increasing detail. In this thesis, the new method is applied to two physical examples. In Chapter 1.3, we efficiently compute the full nonlinear forces that act in a topological defect in a one-dimensional chain of charged particles, see [37] for a review on topological defects. In Chapter 4.4, we then move on to a prototypical two dimensional sum that appears in the evaluation of forces in spin lattices. While in both cases, the evaluation of the exact sum is a challenging numerical problem, the singular Euler–Maclaurin expansion offers a precise approximation to the sum with a runtime that does not depend on the particle number and with an error that decreases exponentially in the expansion order.

The derivation of the singular Euler–Maclaurin expansion in this work is structured as follows. In Chapter 1, the one-dimensional singular Euler–Maclaurin (SEM) expansion is developed, extending the validity of the traditional Euler–Maclaurin (EM) summation formula to functions with singularities. By including the singular function factor in a generalisation of the periodised Bernoulli functions, the convergence properties of the expansion are restored. Thus, the SEM expansion is applicable and useful for physical systems that exhibit singular interactions, e.g. due to long-ranged particle interactions. We derive bounds for the approximation error and lay out under which conditions the expansion order can be taken to infinity, namely if the function under consideration is of exponential type. This condition is subsequently interpreted as a definition for physically meaningful interpolation functions that vary at a scale larger than the grid spacing. In the numerics section, we demonstrate the performance of the expansion by computing the full nonlinear long-range forces in a macroscopic crystal. The SEM expansion yields, under the condition of a physically meaningful interpolation function, an efficiently computable approximation to the sum for all interaction exponents, especially for the notoriously difficult case where the interaction exponent is equal to the dimension of the system.

Chapter 2 is concerned with the extension of the traditional EM expansion (for functions without singularities) to multidimensional lattices. This provides a powerful analytical tool that is subsequently applied in the derivation of the multidimensional SEM expansion in the following chapter. Using results on the regularity of elliptic partial differential operators, we deduce the properties of the generalisation of the periodised Bernoulli functions to higher dimensions. Differences between lattice sums and related integrals, we call them sum-integrals, are then approximated by a surface integral over derivatives of the summand function. The multidimensional Bernoulli functions form the coefficients of the associated differential operator. We provide sharp bounds for the approximation error of the expansion.

Further improving on the EM expansion in higher dimensions, we set out to derive the SEM expansion on multidimensional lattices in Chapter 3. Following the same strategy as in one dimension, we aim at including the singularity inside a generalisation of the multidimensional Bernoulli functions, the Bernoulli-$\mathcal{A}$ functions. In higher dimensions, we construct these functions by carefully combining fundamental solutions to the poly-Laplace operator with the interaction. Infinite sums over fundamental solutions are needed, which can be made well-defined by a particular regularisation method that makes use of sum-integrals that include a superpolynomially decaying regularisation. The multidimensional SEM expansion then takes a similar form as the EM expansion in higher dimensions, where the surface integral is now taken over derivatives of the smooth factor of the summand function only. We improve the method further by introducing the SEM expansion for interior lattice points that works even if the singularity lies within the integration region and where an additional parameter ε arises.

In Chapter 4, we remove the free parameter ε by means of the Hadamard integral. The resulting hypersingular Euler–Maclaurin expansion (HSEM) is able to approximate the difference between sum and integral by a single local differential operator in case that the integration region equals $\mathbb{R}^d$. We discover a deep connection of our theory to analytical number theory, showing that regularised differences between sums and integrals can be used to generate analytic continuations of Dirichlet series. This allows us to use tools from number theory in order to efficiently compute the coefficients of the differential operator. As a by-product of the expansion, new globally convergent representations of the Riemann zeta function and its generalisations to higher dimensions are found. Finally, we show the numerical performance of the HSEM expansion by computing lattice sums in an infinite two-dimensional lattice, which appear in a number of different fields of research. The error scaling of the multidimensional EM expansion in Chapter 2 is recovered, showing that the singularity has been properly absorbed in the Bernoulli-$\mathcal{A}$ functions. Here, the approximation error decreases polynomially with the width of the interpolating function and exponentially with the expansion order, with a runtime that is independent of the particle number.

We draw our conclusions in Chapter 5 and give an outlook on applications of the new expansions in pure and applied mathematics, condensed matter, and quantum physics.

CHAPTER 1

Singular Euler–Maclaurin expansion

We present the one-dimensional singular Euler–Maclaurin expansion, a method that allows to represent large scale sums in terms of integral and differential operators. The new expansion extends the applicability of the classical Euler–Maclaurin summation formula to sums whose addends are formed by the product of a sufficiently differentiable function, we call it the interpolating function, and an asymptotically smooth interaction function that includes all relevant physical interaction potentials and forces. First, a generalisation of the periodised Bernoulli polynomials, the Bernoulli–$\mathcal{A}$ functions, is introduced in which all information about the interaction is encoded. The difference between sum and integral is then described by a differential operator, whose coefficients are the Bernoulli–$\mathcal{A}$ functions, and a remainder integral. The operator acts only on the interpolating function thereby avoiding derivatives of the interaction, whose fast increase with the derivative order leads to the breakdown of the standard Euler–Maclaurin summation formula. The slower the derivatives of the interpolating function increase with the derivative order, the better are the resulting rates of convergence. If this increase is sufficiently slow, the expansion order can be taken to infinity. The coefficients of the differential operator follow from a generating function and are therefore easily accessible. We provide analytical formulas for the differential operator for standard interactions. Finally, we show that the singular Euler–Maclaurin expansion can be used as a powerful numerical tool in condensed matter physics. It allows us to evaluate large scale force sums with a runtime that does not depend on the particle number. As a proof of numerical performance, we compute the nonlinear forces in a macroscopic one-dimensional crystal composed of 2×10^{10} particles. We provide a reference implementation in *Mathematica* online[1].

This chapter is based on the publication [6].

[1] `https://github.com/andreasbuchheit/singular_euler_maclaurin`

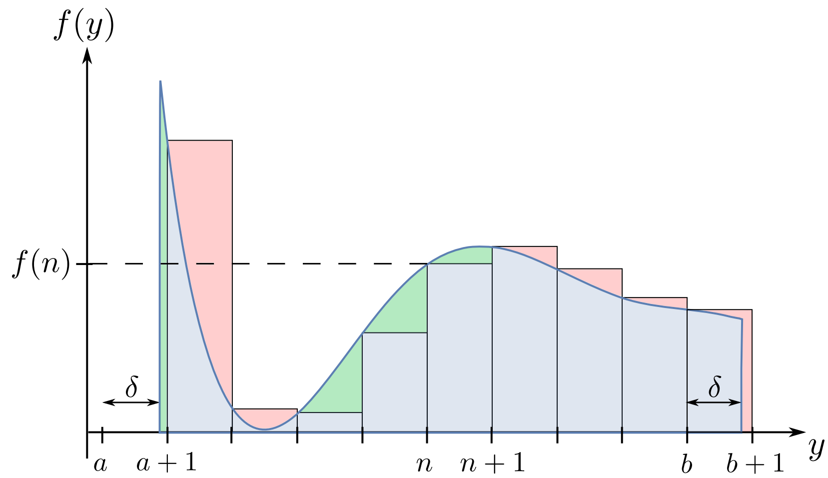

FIGURE 1. Approximation of a sum by an integral as described by the Euler–Maclaurin expansion (1.1). In the red areas, the addends are larger than the corresponding integral, whereas the integral exceeds the addend in the green areas.

1. Introduction

When we try to simulate the dynamics of the discrete particles inside a body of macroscopic size, we encounter a serious computational problem, if the forces acting between particles are long-ranged. In order to determine the force acting on one specific particle, a sum has to be evaluated where the number of addends scales with the number of particles. A fast, yet precise computation of this sum is challenging, even if the microscopic observable, e.g. the displacement of particles from a reference position in a crystal, can be described by a smooth interpolating function. It is often easier to evaluate an integral than a sum, either because efficient quadrature rules can be applied or because analytical simplifications are possible. However, the precise relation between sums and integrals is difficult to establish. Fig. 1 schematically displays the approximation of a sum by an integral. The surface area of the rectangles are the summands and the blue area is the value the integral. In the green regions, the integral overestimates the sum, whereas in the red parts, the integral is smaller than the sum.

A first step in the quantification of the error when approximating sums by integrals and vice versa was given by Leonard Euler in 1736 and by Colin Maclaurin in 1742, see the review [1]. The Euler–Maclaurin (EM) expansion allows us to write the difference between sum and integral as derivatives of the summand function, evaluated at the limits of integration, together with a remainder integral.

Before presenting the EM expansion, we review the following standard notations. For an open and possibly unbounded set $I \subseteq \mathbb{R}$ and $\ell \in \mathbb{N}_0$ or $\ell = \infty$, $C^\ell(I)$ shall denote the vector space of all ℓ-times continuously differentiable functions. The vector space $C^\ell(\bar{I})$, where $\bar{I}$ is the closure of I, is composed of those functions in $C^\ell(I)$ whose derivatives have continuous extensions from I to $\bar{I}$. Furthermore we set $C^{-1}(I)$ as the space of regulated functions,

$$C^{-1}(I) = \left\{ f : I \to \mathbb{C} : \forall y_0 \in I : \lim_{y \nearrow y_0} f(y),\ \lim_{y \searrow y_0} f(y) \text{ exist} \right\},$$

where

$$\lim_{y \nearrow y_0}, \quad \lim_{y \searrow y_0}$$

are the one-sided limits from left and right. Regulated functions are continuous up to a countable set of points.

Let $a, b \in \mathbb{Z}$, with $a < b$, $\delta \in (0,1]$, and $\ell \in \mathbb{N}_0$. The EM expansion for a function $f \in C^{\ell+1}[a+\delta, b+\delta]$ then reads [1, 40]

$$\sum_{n=a+1}^{b} f(n) = \int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y - \sum_{k=0}^{\ell} \frac{(-1)^k}{k!} \frac{B_{k+1}(1+y-\lceil y \rceil)}{k+1} f^{(k)}(y) \Big|_{y=a+\delta}^{y=b+\delta} + \frac{(-1)^\ell}{\ell!} \int_{a+\delta}^{b+\delta} \frac{B_{\ell+1}(1+y-\lceil y \rceil)}{\ell+1} f^{(\ell+1)}(y)\,\mathrm{d}y. \tag{1.1}$$

Here $\lceil y \rceil$ is the smallest integer larger than or equal to y. The Bernoulli polynomials $B_\ell : \mathbb{R} \to \mathbb{R}$ are defined via the recurrence relation

$$B_0(y) = 1, \quad B_\ell'(y) = \ell B_{\ell-1}(y), \quad \int_0^1 B_\ell(y)\,\mathrm{d}y = 0, \quad \ell \in \mathbb{N}. \tag{1.2}$$

A derivation of the EM expansion together with a brief introduction to its history are provided in [1].

The EM expansion allows to write sums in terms of integral and differential operators, which, after discarding the remainder integral on the right hand side of (1.1), provide an efficiently computable approximation to the sum. The usefulness of the formula relies on the convergence of the expansion, meaning that the limit $\ell \to \infty$ is well defined. Let us consider a smooth function f. By using the scaling of the Bernoulli polynomials [36],

$$\max_{y \in [0,1]} \frac{|B_\ell(y)|}{\ell!} \sim (2\pi)^{-\ell}, \quad \ell \in \mathbb{N}_0,$$

we find that the derivatives of the function f may increase at most exponentially in the derivative order with

$$\left|f^{(\ell)}(y)\right| \sim \sigma^{\ell}, \quad \ell \in \mathbb{N}_0,$$

and $\sigma < 2\pi$. This condition in particular excludes functions f that involve a singular factor $y^{-\nu}$, with $\nu > 0$, whose derivatives grow with the factorial of ℓ. The fast increase of the derivatives with the derivative order is typical for many physical interaction energies and forces, and thus the EM expansion cannot be applied in these cases.

Over the years, several extensions of the classical EM expansion have been developed. A significant contribution has been provided by Navot [42], where the expansion is generalised to branch singularities at the limits of integration. An approach using Hadamard finite-part integrals has been provided by Monegato and Lyness [40]. Also higher dimensional generalisation of the expansion have been derived [34]. Recently, an alternative approach has been presented by Pinelis, which relies on the use of integral instead of differential operators [44].

The EM expansion fails to converge for asymptotically smooth functions, see Definition 1.1, which are, unfortunately, of high practical interest as singular physical interaction forces belong to this set of functions. In the following, we present the singular Euler–Maclaurin (SEM) expansion, which converges, even if the summand function includes a factor that is an asymptotically smooth function.

This chapter is organised as follows. In Section 2, we present the SEM expansion and offer the reader all tools required for its application. In Section 3, we conduct a numerical study using the SEM expansion and efficiently perform force calculations in a macroscopic crystal with long-range interactions. In Section 4, we prove the main theorems and propositions of this chapter. Technical details needed in the derivation are relegated to Section 5. In Section 6, conclusions are drawn.

2. Main result and notation

In the following, we present the SEM expansion. Consider an interval $[a+\delta, b+\delta]$, with $a, b \in \mathbb{Z}$, $a < b$, and an offset $\delta \in (0,1]$. Let the addends of a sum be given by a function f,

$$f : [a+\delta, b+\delta] \to \mathbb{C}.$$

In order to overcome the convergence problems of the standard EM expansion, we now apply the following strategy. We take the function f and split it into two factors

$$f(y) = s(y-x)g(y), \quad y \in [a+\delta, b+\delta], \tag{1.3}$$

where $x \in \mathbb{Z}$, $s \in C^\infty(\mathbb{R} \setminus \{0\})$ and $g : [a+\delta, b+\delta] \to \mathbb{C}$ is a sufficiently differentiable function. Now, all functions whose derivatives increase quickly with the derivative order and are thus not suitable for the standard EM expansion, e.g. singularities at x, are included in the function s. This function will require special treatment. In practice, the function s often describes a pairwise interaction potential or an interaction force that follows from a potential. For this reason, we call s the interaction. The remaining well-behaved function factors are collected in g, which typically includes the interpolation of a discrete observable, e.g. a particle displacement. We call g the interpolating function. The slower the increase in the derivatives of g with the derivative order, the better will be the convergence rates that the SEM expansion is able to offer.

We now provide a roadmap for our presentation of the SEM expansion. First, the admissible set of functions for the interaction s is introduced. Then an exponential regularisation is added to the interaction, making it an integrable function on $[1,\infty)$. Subsequently, we use the integrability of the regularised interaction and quantify the difference between sum and integral of the interaction in a function that we call $\mathcal{C}$. From the function $\mathcal{C}$ we deduce a generalisation of the periodised Bernoulli polynomials, the Bernoulli–$\mathcal{A}$ functions, which include all information about the interaction. The Bernoulli–$\mathcal{A}$ functions then form the coefficients of the SEM differential operator, which acts on g only, avoiding derivatives of s and thus also the divergence of the remainder that is caused by their unfavourable scaling. Finite order approximations of the SEM operator then lead to the finite order SEM. If the function g is smooth and the scaling of its derivatives is sufficiently favourable, then the order of the expansion can be extended to infinity, yielding the infinite order SEM.

Before we formulate the SEM expansion, we specify the admissible function set for the interaction, namely the set of asymptotically smooth functions [3, Sec. 3.2].

Definition 1.1 (Asymptotically smooth functions). We call a function $s \in C^\infty(\mathbb{R} \setminus \{0\})$ asymptotically smooth if there exist $c > 0$ and $\gamma \ge 1$ such that

$$\left|s^{(\ell)}(y)\right| \le c\,\ell!\,\gamma^\ell\,|y|^{-\ell}\,|s(y)|, \tag{1.4}$$

for all $y \in \mathbb{R} \setminus \{0\}$ and $\ell \in \mathbb{N}_0$. We denote the vector space of all asymptotically smooth functions by S.

The asymptotically smooth functions include entire functions, like polynomials, but also many singular functions. Examples for asymptotically smooth functions are

$$s(y) = |y|^{-\nu}, \quad y \in \mathbb{R} \setminus \{0\}, \tag{1.5}$$

for $\nu \in \mathbb{R}$. In the physical case $\nu > 0$, where the interaction decreases with distance $|y|$, they exhibit a singularity at zero.

Remark 1.2. For s in (1.5), the constant γ in (1.4) equals 1 in the case $\nu \leq 1$. For $\nu > 1$, then $\gamma = 1 + \varepsilon$ for an arbitrary $\varepsilon > 0$, see the proof at the beginning of the Section 5.

Asymptotically smooth functions have two important properties that we are going to use. First, their derivatives may only increase with the factorial of the derivative order with an additional exponential growth for $\gamma \neq 1$, but not faster. Second, the growth rate of the interaction s at infinity is polynomial in y. We use this scaling as a way to further classify asymptotically smooth functions.

Definition 1.3. We define S_α, $\alpha \in \mathbb{R}$, as the vector space of all $s \in S$ for which there exists $c_0 > 0$ such that

$$|s(y)| \leq c_0 |y|^\alpha, \quad |y| > 1. \tag{1.6}$$

Remark 1.4. From Grönwall's lemma follows immediately that

$$S = \bigcup_{\alpha \in \mathbb{R}} S_\alpha, \tag{1.7}$$

see Section 5 for a proof.

In order to avoid the breakdown of the EM expansion, derivatives of s have to be avoided. It is possible to integrate s instead. In order to make s integrable on $[1, \infty)$, which is not always possible (take for instance $\nu = 1$ in (1.5)), we introduce an exponentially decreasing weighting.

Notation 1.5. Let $s \in S$. The exponentially weighted interaction reads

$$s_\beta(y) = s(y) e^{-\beta |y|}, \quad y \in \mathbb{R} \setminus \{0\}, \tag{1.8}$$

with $\beta \geq 0$.

The parameter β restricts the range of the interaction, we call it the shielding. In the limit $\beta \searrow 0$ the shielding is removed and the interaction regains its full range. It is important to note that the shielded interaction s_β remains asymptotically smooth for all $\beta \geq 0$.

We first quantify the difference between sum and integral of the shielded interaction through the function $\mathcal{C}$.

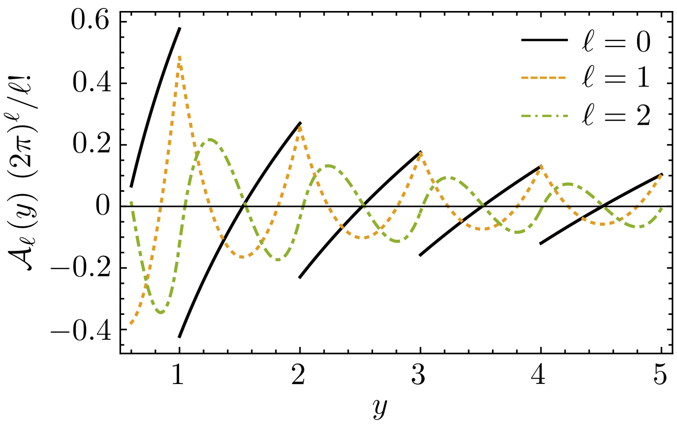

FIGURE 2. Generalised Bernoulli functions $\mathcal{A}_\ell$ for $s(y) = |y|^{-1}$.

DEFINITION 1.6. Let $s \in S$. We define $\mathcal{C} : \mathbb{R}_+ \times \mathbb{R}_+ \to \mathbb{C}$ as

$$\mathcal{C}(y,\beta) = \sum_{n=\lceil y \rceil}^{\infty} s_\beta(n) - \int_y^\infty s_\beta(z)\,\mathrm{d}z, \tag{1.9}$$

with $\mathbb{R}_+$ the positive real numbers.

We use calligraphic notation for objects that include the interaction s. From the function $\mathcal{C}$ follow the Bernoulli–$\mathcal{A}$ functions, which serve as a replacement for the periodised Bernoulli polynomials in (1.1). The shielding β here plays a special role as it allows to generate the Bernoulli–$\mathcal{A}$ functions via an exponential generating function.

DEFINITION 1.7 (Bernoulli–$\mathcal{A}$ functions). Let $s \in S$. The Bernoulli–$\mathcal{A}$ functions,

$$\mathcal{A}_\ell : \mathbb{R}_+ \to \mathbb{C}, \quad \ell \in \mathbb{N}_0,$$

are defined as the coefficients in the power series

$$e^{\beta\xi}\mathcal{C}(\xi,\beta) = \sum_{\ell=0}^{\infty} \mathcal{A}_\ell(\xi)\frac{\beta^\ell}{\ell!}, \quad \xi > 0.$$

We say that the sequence $(\mathcal{A}_\ell(\xi))_{\ell\in\mathbb{N}_0}$ is exponentially generated by

$$\mathcal{G}_\xi(\beta) = e^{\beta\xi}\mathcal{C}(\xi,\beta)$$

and refer to $\mathcal{G}_\xi$ as the generating function.

The first three Bernoulli–$\mathcal{A}$ functions are displayed for $s(y) = |y|^{-1}$ in Fig. 2.

REMARK 1.8. In the case $s = 1$, we reobtain the periodised Bernoulli polynomials,

$$\mathcal{A}_\ell(y) = \frac{B_{\ell+1}(1 + y - \lceil y \rceil)}{\ell + 1}, \quad \ell \in \mathbb{N}_0,\ y > 0.$$

PROOF. Let $y > 0$ and $\beta > 0$. Then

$$\begin{aligned} e^{\beta y}\mathcal{C}(y,\beta) &= e^{\beta y}\sum_{n=\lceil y\rceil}^{\infty} e^{-\beta n} - e^{\beta y}\int_y^\infty e^{-\beta z}\,\mathrm{d}z = \frac{e^{\beta(1+y-\lceil y\rceil)}}{e^\beta - 1} - \frac{1}{\beta} \\ &= \frac{1}{\beta}\left(\frac{\beta e^{\beta(1+y-\lceil y\rceil)}}{e^\beta - 1} - 1\right). \end{aligned}$$

We find that the first term inside the brackets equals the exponential generating function for the Bernoulli polynomials evaluated at $1+y-\lceil y\rceil$ [21, Sec. 1.13, Eq. (2)]. As $B_0 = 1$, we obtain

$$e^{\beta y}\mathcal{C}(y,\beta) = \sum_{\ell=1}^{\infty} B_\ell(1 + y - \lceil y\rceil)\frac{\beta^{\ell-1}}{\ell!} = \sum_{\ell=0}^{\infty}\frac{B_{\ell+1}(1 + y - \lceil y\rceil)}{\ell+1}\frac{\beta^\ell}{\ell!}.$$

□

We use the Bernoulli–$\mathcal{A}$ functions and define the SEM operator, a differential operator of infinite order, and finite order approximations thereof.

DEFINITION 1.9 (SEM operator). For $s \in S$ and $\xi \in \mathbb{R}_+$, we define the differential operator of infinite order

$$\mathcal{D}_\xi = \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\mathcal{A}_\ell(\xi)\,(-D)^\ell, \tag{1.10}$$

where D is the derivative operator. We call $\mathcal{D}_\xi$ the SEM operator. It formally reads

$$\mathcal{D}_\xi = \mathcal{G}_\xi(-D),$$

and for $\ell \in \mathbb{N}_0$ the finite order approximations $\mathcal{D}_\xi^{(\ell)}$ are given by

$$\mathcal{D}_\xi^{(\ell)} = \sum_{k=0}^{\ell}\frac{1}{k!}\mathcal{A}_k(\xi)\,(-D)^k.$$

With the Bernoulli–$\mathcal{A}$ functions and the SEM operator, we can now formulate the finite order SEM expansion.

THEOREM 1.10 (Finite order SEM). *For $x, a, b \in \mathbb{Z}$, with $x \le a < b$, and $\delta \in (0, 1]$, let f factor into*

$$f(y) = s(y - x)g(y),$$

where $s \in S$ *and* $g \in C^{\ell+1}[a+\delta, b+\delta]$, $\ell \in \mathbb{N}_0$. *Then,*

$$\sum_{n=a+1}^{b} f(n) = \int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y - \Big(\mathcal{D}^{(\ell)}_{y-x} g\Big)(y)\Big|_{y=a+\delta}^{y=b+\delta} + \frac{(-1)^{\ell}}{\ell!} \int_{a+\delta}^{b+\delta} \mathcal{A}_{\ell}(y-x) g^{(\ell+1)}(y)\,\mathrm{d}y.$$

Note that the SEM operator only acts on g, not on s. Therefore, the convergence problems of the classic EM expansion are avoided. If we would like to take the limit of the expansion order to infinity, the function g has to belong to a specific set of functions, which restricts the scaling of its derivatives. Namely, the function g has to be of exponential type.

Definition 1.11 (Functions of exponential type). Let g be entire. If there exists $\sigma > 0$ such that for every $\epsilon > 0$, there is $M_\epsilon > 0$ with

$$\left|g^{(\ell)}(y)\right| \le M_\epsilon (\sigma+\epsilon)^{\ell} e^{(\sigma+\epsilon)|y|}, \quad y \in \mathbb{R},\ \ell \in \mathbb{N}_0,$$

we say that g is of exponential type σ. By E_σ we denote the vector space of all functions of exponential type σ.

For a review of functions of exponential type, see [11]. The parameter σ describes the largest angular wavenumber for oscillations of the function g. It depends on the parameter γ in Definition 1.1, but always has to be smaller than 2π. This restriction is physically meaningful, as the function g serves as an interpolation between discrete points, e.g. particle displacements in a physical setting. Consider Fig. 3 where we interpolate the blue points by two different interpolating functions of exponential type. Interpolations that include oscillations with wavelengths smaller than the separation of the discrete points can be considered unphysical. Thus in black, we see a physically meaningful interpolation of the blue points ($\sigma < 2\pi$) and an unphysical interpolation in red ($\sigma > 2\pi$).

We now formulate the infinite order SEM expansion.

Theorem 1.12 (Infinite order SEM). *For* $x, a, b \in \mathbb{Z}$, *with* $x \le a < b$, *and* $\delta \in (0,1]$, *let* f *factor into*

$$f(y) = s(y-x)g(y),$$

where $s \in S$ *and* $g \in E_\sigma$ *with* $\sigma < 2\pi/(1+\gamma)$. *Then,*

$$\sum_{n=a+1}^{b} f(n) = \int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y - \Big(\mathcal{D}_{y-x} g\Big)(y)\Big|_{y=a+\delta}^{y=b+\delta}. \tag{1.11}$$

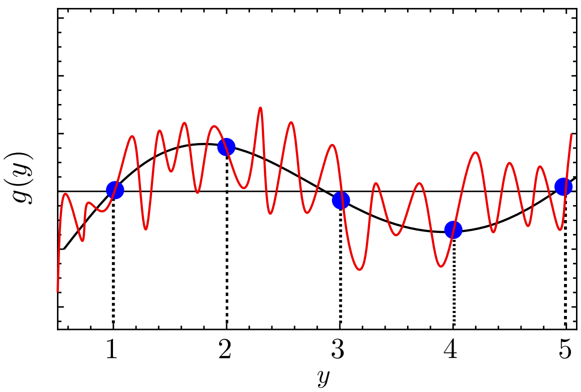

FIGURE 3. Different choices for a smooth interpolation of the blue points by a function $g \in E_\sigma$. The black line shows a physically meaningful interpolation with $\sigma < 2\pi$, the red line an unphysical interpolation where $\sigma > 2\pi$.

REMARK 1.13. Both Theorems 1.10 and 1.12 require that x is positioned to the left of the interval $[a+1,b]$. We can however also apply the SEM in the case that x is positioned to the right of the interval by reflecting the interval about x. Take for instance $a < b < x$. The reflected interval is $[\tilde{a}+1,\tilde{b}]$, with

$$\tilde{a} = 2x - (b+1), \quad \tilde{b} = 2x - (a+1),$$

where $x \le \tilde{a} < \tilde{b}$. The sum can then be rewritten as

$$\sum_{n=a+1}^{b} s(n-x)g(n) = \sum_{n=\tilde{a}+1}^{\tilde{b}} \tilde{s}(n-x)\tilde{g}(n), \tag{1.12}$$

with $\tilde{s} \in S$ and $\tilde{g}$ given by

$$\tilde{s}(y) = s(-y), \quad \tilde{g}(y) = g(2x-y).$$

The SEM expansion can then be applied to (1.12).

REMARK 1.14. Consider $s \in S$ of the form

$$s(y) = |y|^{-\nu}, \quad y \in \mathbb{R} \setminus \{0\},$$

where $\nu \in \mathbb{R}$. Then we can improve the restriction on σ to $\sigma < 2\pi$, which can be deduced from the following example.

EXAMPLE 1.15. Take $s(y) = |y|^{-\nu}$, $y \in \mathbb{R} \setminus \{0\}$, with $\nu \in \mathbb{R}$. Then the radius of convergence of the exponential generating function $\mathcal{G}_y$ equals 2π and the Bernoulli–$\mathcal{A}$ functions follow as

$$\mathcal{A}_\ell(y) = \sum_{k=0}^{\ell} (-1)^k \binom{\ell}{k} y^{\ell-k} \left(\zeta(\nu-k,\lceil y \rceil) - \frac{y^{-(\nu-k-1)}}{\nu-k-1} \right), \quad \ell \in \mathbb{N}_0, \tag{1.13}$$

where $\zeta(\cdot,\cdot)$ is the Hurwitz zeta function,

$$\zeta(z,q) = \sum_{n=0}^{\infty} \frac{1}{(n+q)^z}, \quad z > 1, \quad q > 0, \tag{1.14}$$

which can be analytically continued to the complex plane for all $z \neq 1$ [21, Sec. 1.10]. In the case $\nu \in \mathbb{N}_0$ we obtain

$$\lim_{\nu \to k+1} \left(\zeta(\nu - k, \lceil y \rceil) - \frac{y^{-(\nu-k-1)}}{\nu - k - 1} \right) = \gamma_e - H_{\lceil y \rceil - 1} - \log y, \quad k \in \mathbb{N}_0,$$

with γ_e the Euler–Mascheroni constant and where H_k is the kth harmonic number,

$$H_k = \sum_{j=1}^{k} \frac{1}{j}.$$

3. Numerical application

We apply the SEM expansion to the calculation of the nonlinear long-range forces that act inside a one-dimensional crystal of macroscopic size. As the SEM is applicable to all asymptotically smooth interactions, we can use it to simulate all physically relevant cases. In this study, we focus in particular on the 3D Coulomb repulsion restricted to a one-dimensional line manifold. In this case, the interaction potential decays algebraically with an exponent ν that equals the dimension of the system manifold. The treatment of this case is particularly challenging, both analytically and numerically, as the discreteness of the material has an observable effects at all scales [14].

Let the crystal be composed of $2N+1$ particles, with $N \in \mathbb{N}_0$. We write the particle positions as $x_j \in \mathbb{R},\ j = -N, \dots, N$. The particles are displaced from an equidistant crystal configuration with lattice constant $h > 0$ such that

$$x_j = jh + u(jh), \quad j = -N, \dots, N, \tag{1.15}$$

with a smooth function u that interpolates the particles displacements.

Let $V \in S$ be the pairwise interaction energy between two particles, which decays algebraically with the inter-particle distance x,

$$V(x) = c_\nu |x|^{-\nu}, \quad \nu > 0. \tag{1.16}$$

The force that acts on the particle at reference position x then equals

$$F(x) = -\sum_{\substack{n=-N \\ n \neq x/h}}^{N} V'\Big(x - hn + u(x) - u(hn)\Big), \quad x \in h\{-N, \dots, N\}. \tag{1.17}$$

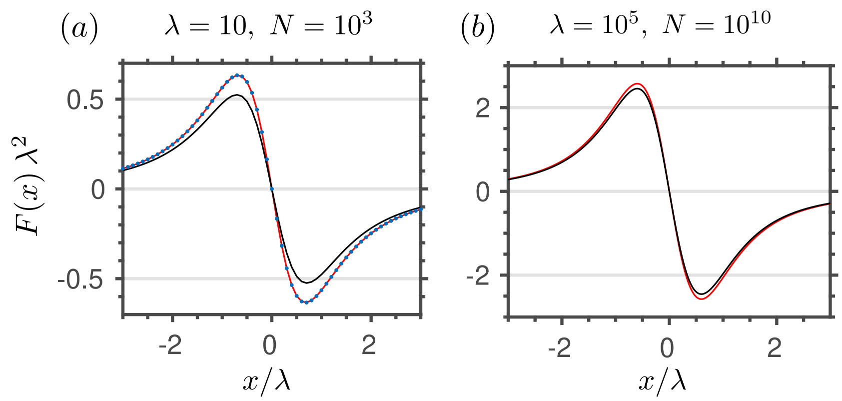

FIGURE 4. Force F as a function of distance x from the centre of the crystal for different values of the kink width λ and the particle number N. The black line gives the integral approximation, the first order singular Euler–Maclaurin expansion is shown in red, and the blue dots display the exact forces. In (a), the maximum absolute error for the first order singular Euler–Maclaurin expansion is smaller than 3×10^{-7} for all forces and the relative error does not exceed 8×10^{-5}.

We now remove all physical dimensions by writing positions in units of h and forces in units of $V''(h)h$. The forces then read

$$F(x) = \sum_{n=-N}^{x-1} f(n) + \sum_{n=x+1}^{N} f(n), \quad x \in \{-N, \dots, N\}, \tag{1.18}$$

with a function f that factors into

$$f(y) = s(y-x)g(y) \tag{1.19}$$

where we define $s \in S$ and g smooth as

$$s(y) = \operatorname{sgn}(y)\, |y|^{-(\nu+1)}, \quad g(y) = -\frac{1}{\nu+1}\left(1 + \frac{u(y)-u(x)}{y-x}\right)^{-(\nu+1)}. \tag{1.20}$$

We choose the exponent $\nu = 1$, which corresponds to 3D Coulomb interaction restricted to a 1D line. For the interpolating function u, we take

$$u(y) = \frac{1}{\pi}\int_{-\infty}^{y/\lambda} \frac{1}{1+z^2}\,\mathrm{d}z, \tag{1.21}$$

which is a simplified profile of a domain wall, also called kink, in a crystal with

$$\lim_{y\to\infty} u(y) = 1, \qquad \lim_{y\to-\infty} u(y) = 0. \tag{1.22}$$

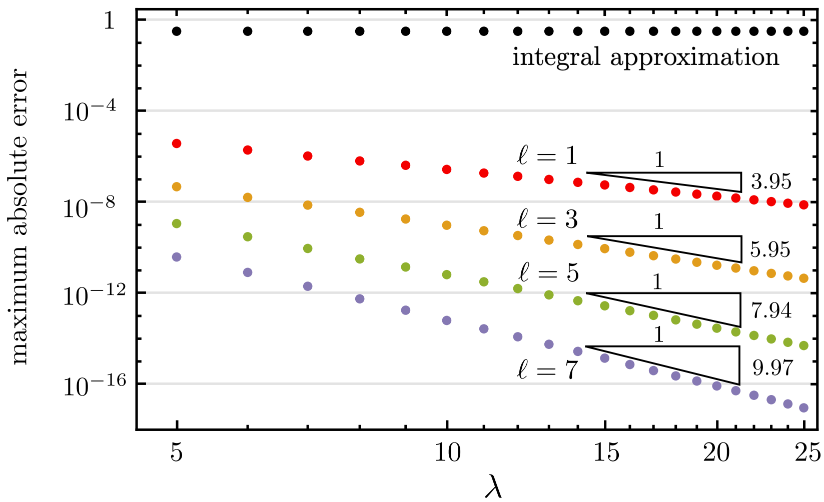

FIGURE 5. Maximum absolute error for $N = 200$ as a function of λ for different orders ℓ of the singular Euler–Maclaurin expansion.

For an overview of kinks in condensed matter physics, see [37]. They typically arise through an additional nonlinearity that is applied to the crystal, for instance through the interaction with a substrate crystal. The parameter $\lambda > 0$ scales the width of the kink.

A reference implementation of the SEM expansion in *Mathematica*, which allows to reproduce the following results, is provided online[2]. The nonlinear forces in the crystal are computed numerically by using the SEM expansion up to order ℓ with $\delta = 1$. The integral is evaluated using global adaptive quadrature. We first compute the coefficients of the SEM differential operator. Then the operator is applied to the function g, where the differentiation is carried out symbolically. We discard the remainder integral and compute the forces. Here, the computational time for a single force evaluation using the SEM expansion does not depend on the number of particles.

We then compute the forces inside the centre of a crystal with a kink of width λ in its centre. The forces are displayed in Fig. 4 where panel (a) shows the case of a microscopic crystal with $N = 10^3$ and $\lambda = 10$, whereas in panel (b) the case of a macroscopic crystal with $N = 10^{10}$ and $\lambda = 10^5$ is considered. If we insert a typical lattice constant of $h = 10^{-10}\,\mathrm{m}$, then the crystal in (b) has a length of two metres, where the exaggerated size has been chosen in order to further demonstrate the numerical performance of our method. We compare the case where the sum is approximated by an integral only (black line) to the first

[2]`https://github.com/andreasbuchheit/singular_euler_maclaurin`

order SEM (red line) and to the exact forces (blue dots). We find in (a) that the integral approximation shows a significant error, whereas the first order SEM expansion reproduces the forces reliably, both inside the kink as well as at the edges of the chain. The maximum absolute error for the SEM is always smaller than 3×10^{-7} leading to the precision of 4 digits. In (b), we extend both the crystal and the kink to macroscopic size. Here the computation of the exact forces is impractical due to the large number of particles. Even at this scale, there is a significant difference between the SEM expansion and the integral approximation. The maximum force acting in the centre of the kink scales as $\log(\lambda)/\lambda^2$, whereas the first order SEM contribution scales as λ^{-2}. In the centre of the chain, both are independent of the particle number for $N \gg 1$. The logarithm increases too slowly, such that the integral does not dominate the SEM contribution, even on the macro scale. Therefore, the claim that a sufficiently broad distribution of charges allows us to replace a force sum by the corresponding integral (see e.g. [5, Eq. (5.3)]) is not correct in the case of the 3D Coulomb interaction in one-dimension. Therefore, even in the thermodynamic limit, the SEM contribution remains relevant.

We then investigate the error in the maximum norm over a chain of $N = 200$ particles as a function of the kink width λ for different order ℓ of the SEM expansion and display the results in Fig. 5. We find that the error in the integral approximation does not depend on the kink width λ. Its maximum value is reached at the edges of the crystal, whereas in the centre, it scales as λ^{-2}. If we include the zero order SEM correction, the error at the edges is already compensated and the maximum error occurs in the chain centre. For $\ell = 1$, the error scales approximately as λ^{-4}. For higher orders ℓ, the scaling coefficient equals approximately $\ell + 3$ for odd orders ℓ. The precise scaling coefficients obtained from a fit of the last 5 data points are given in Fig. 5. For the case $\ell = 7$, the SEM expansion yields a maximum error smaller than 10^{-17} corresponding to 13 digits of precision.

The analysis of the error scaling shows that an inclusion of the SEM correction is important for the correct prediction of long-range forces, even more so if finite chains with edges are considered, where the integral approximation yields a large error independent of the choice of λ. A very regular scaling of the error with λ is observed, with the first order SEM already offering a λ^{-4} scaling. We have thus established that the new expansion yields precise and fast approximations to the singular sum with an error that decays exponentially with the expansion order and with a runtime that is independent of the particle number. The integral approximation on the other hand is unreliable for the system under consideration and yields uncontrolled and typically significant errors.

4. Main derivation

In this section, we derive the SEM expansion and prove the theorems of this chapter. The proofs of technical lemmas can be found in the next section. Before deriving the zero order SEM expansion, we gather properties of the function $\mathcal{C}$.

LEMMA 1.16. *Let $s \in S$. For fixed $y > 0$, the function*

$$\mathcal{C}(y,\cdot) : (0,\infty) \to \mathbb{C}$$

is infinitely differentiable,

$$\partial_\beta^\ell \mathcal{C}(y,\beta) = (-1)^\ell \left(\sum_{n=\lceil y \rceil}^{\infty} n^\ell s(n) e^{-\beta n} - \int_y^\infty z^\ell s(z) e^{-\beta z} \,\mathrm{d}z, \right), \ \ell \in \mathbb{N}_0, \ \beta > 0,$$

and all derivatives decay exponentially for $|y| \to \infty$. Furthermore, all derivatives have a continuous extension for $\beta = 0$, i.e for $y > 0$ fixed the limit

$$\lim_{\beta \searrow 0} \partial_\beta^\ell \mathcal{C}(y,\beta)$$

exists for all $\ell \in \mathbb{N}_0$.

LEMMA 1.17. *Let $s \in S$ and $\ell \in \mathbb{N}_0$, $\beta > 0$. The function*

$$\partial_\beta^\ell \mathcal{C}(\cdot,\beta) : (0,\infty) \to \mathbb{C}$$

is infinitely differentiable on $\mathbb{R}_+ \setminus \mathbb{N}$ and obeys the jump relation

$$\lim_{y \nearrow n} \partial_\beta^\ell \mathcal{C}(y,\beta) - \lim_{y \searrow n} \partial_\beta^\ell \mathcal{C}(y,\beta) = (-1)^\ell n^\ell s_\beta(n)$$

for all $n \in \mathbb{N}$. The results remain valid in the limit $\beta \searrow 0$.

With the above two lemmas, we prove the zero order SEM expansion.

PROPOSITION 1.18. *Let $x, a, b \in \mathbb{Z}$ with $x \le a < b$ and $\delta \in (0,1]$. Let f factor into*

$$f(y) = s(y-x) g(y),$$

with $s \in S$ and $g \in C^1[a+\delta, b+\delta]$. Then,

$$\sum_{n=a+1}^{b} f(n) - \int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y \tag{1.23}$$

$$= -\lim_{\beta \searrow 0} \mathcal{C}(y-x,\beta) g(y) \Big|_{y=a+\delta}^{y=b+\delta} + \lim_{\beta \searrow 0} \int_{a+\delta}^{b+\delta} \mathcal{C}(y-x,\beta) g'(y)\,\mathrm{d}y.$$

Proof. The function $\mathcal{C}(\cdot,\beta)$ exhibits discontinuities at $n\in\mathbb{N}$ and is smooth on $\mathbb{R}_+\setminus\mathbb{N}$. Both the size of the jump at the positive integers as well as the derivative of the function on $\mathbb{R}_+\setminus\mathbb{N}$ yield the shielded interaction s_β at the respective point, namely

$$\lim_{\epsilon\searrow 0}\Big(\mathcal{C}(n-\epsilon,\beta)-\mathcal{C}(n+\epsilon,\beta)\Big)=s_\beta(n),\quad n\in\mathbb{N}, \tag{1.24}$$

and

$$\partial_y\mathcal{C}(y,\beta)=s_\beta(y),\quad \text{for } y\in\mathbb{R}_+\setminus\mathbb{N}. \tag{1.25}$$

By the jump condition (1.24), we replace the weighted interaction in the sum on the left hand side of (1.23)

$$\sum_{n=a+1}^{b} f(n)=\lim_{\beta\searrow 0}\sum_{n=a+1}^{b}\lim_{\epsilon\searrow 0}\Big(\mathcal{C}(n-x-\epsilon,\beta)-\mathcal{C}(n-x+\epsilon,\beta)\Big)g(n), \tag{1.26}$$

and subsequently remove the shielding of s through the limit $\beta\searrow 0$. We then split (1.26) into two separate sums. After performing an index shift in the sum that includes the term $\mathcal{C}(n-x-\epsilon,\beta)$, we obtain

$$\begin{aligned}&\sum_{n=a+1}^{b} f(n)\\ &=\lim_{\beta\searrow 0}\Big(\lim_{\epsilon\searrow 0}\sum_{n=a}^{b-1}\mathcal{C}(n+1-x-\epsilon,\beta)g(n+1)-\lim_{\epsilon\searrow 0}\sum_{n=a+1}^{b}\mathcal{C}(n-x+\epsilon,\beta)g(n)\Big).\end{aligned}$$

Recombining the two sums yields

$$\begin{aligned}&\sum_{n=a+1}^{b} f(n)\\ &\quad=\lim_{\beta\searrow 0}\lim_{\epsilon\searrow 0}\left(\sum_{n=a+1}^{b}\mathcal{C}(y-x,\beta)g(y)\Big|_{y=n+\epsilon}^{y=n+1-\epsilon}-\mathcal{C}(y-x,\beta)g(y)\Bigg|_{y=a+1-\epsilon}^{y=b+1-\epsilon}\right),\end{aligned} \tag{1.27}$$

where the last term results from a correction of the differing summation intervals.

Now we transform the integral on the left hand side of (1.23) by replacing the shielded interaction by derivatives of $\mathcal{C}(\cdot,\beta)$ as in (1.25)

$$\begin{aligned}\int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y=\lim_{\beta\searrow 0}\lim_{\epsilon\searrow 0}\Bigg(&\sum_{n=a+1}^{b}\int_{n+\epsilon}^{n+1-\epsilon}\partial_y\mathcal{C}(y-x,\beta)\,g(y)\,\mathrm{d}y\\ &+\int_{a+\delta-\epsilon}^{a+1-\epsilon}\partial_y\mathcal{C}(y-x,\beta)g(y)\,\mathrm{d}y-\int_{b+\delta-\epsilon}^{b+1-\epsilon}\partial_y\mathcal{C}(y-x,\beta)g(y)\,\mathrm{d}y\Bigg).\end{aligned}$$

We remove all derivatives of $\mathcal{C}(\cdot,\beta)$ through integration by parts, and obtain the expression

$$\begin{aligned}(1.28)\quad &\int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y\\ &= \lim_{\beta\searrow 0}\lim_{\epsilon\searrow 0}\Bigg(\sum_{n=a+1}^{b}\mathcal{C}(y-x,\beta)g(y)\Big|_{y=n+\epsilon}^{y=n+1-\epsilon}+\mathcal{C}(y-x,\beta)g(y)\Big|_{y=a+\delta-\epsilon}^{y=a+1-\epsilon}\\ &\qquad -\mathcal{C}(y-x,\beta)g(y)\Big|_{y=b+\delta-\epsilon}^{y=b+1-\epsilon}\Bigg)-\lim_{\beta\searrow 0}\int_{a+\delta}^{b+\delta}\mathcal{C}(y-x,\beta)g'(y)\,\mathrm{d}y,\end{aligned}$$

where we have combined the separate integrals into a single one. After subtracting (1.28) from (1.27), we get

$$\begin{aligned}(1.29)\quad &\sum_{n=a+1}^{b} f(n)-\int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y\\ &= -\lim_{\beta\searrow 0}\lim_{\epsilon\searrow 0}\mathcal{C}(y-x,\beta)g(y)\Big|_{y=a+\delta-\epsilon}^{y=b+\delta-\epsilon}+\lim_{\beta\searrow 0}\int_{a+\delta}^{b+\delta}\mathcal{C}(y-x,\beta)g'(y)\,\mathrm{d}y.\end{aligned}$$

Note that $\mathcal{C}(\cdot,\beta)$ is left continuous as $\lceil\cdot\rceil$ is left continuous. Therefore, the limit $\epsilon\searrow 0$ in (1.29) yields (1.23).

□

Before we continue our derivation of the SEM expansion, we need to collect additional properties of the function $\mathcal{C}$. We begin by studying derivatives of $\mathcal{C}$ with respect to the shielding parameter β. These derivatives are then put into connection with antiderivatives of $\mathcal{C}$ with respect to y.

Definition 1.19. For $s\in S$, we define the consecutive antiderivatives of $\mathcal{C}(\cdot,\beta)$,

$$\begin{aligned}\mathcal{C}_0(y,\beta)&=\mathcal{C}(y,\beta),\\ \mathcal{C}_{\ell+1}(y,\beta)&=-\int_y^{\infty}\mathcal{C}_\ell(z,\beta)\,\mathrm{d}z,\quad \ell\in\mathbb{N}_0,\end{aligned}$$

for $y>0$ and $\beta>0$.

The well-definedness of above definition follows from Lemma 1.16, as the function $\mathcal{C}(\cdot,\beta)$ is integrable on $[\varepsilon,\infty)$ for any $\varepsilon>0$ and $\beta>0$.

We now show that the antiderivatives $(\mathcal{C}_\ell)_{\ell\in\mathbb{N}_0}$ can be written in terms of derivatives with respect to β. Furthermore, the limit $\beta\searrow 0$

exists for all antiderivatives, thus we can extend them to the case where the shielding of the interaction has been removed.

LEMMA 1.20. *Let $s \in S$ and $\ell \in \mathbb{N}_0$. The function $\mathcal{C}_\ell$ admits the explicit form*

$$\mathcal{C}_\ell(y,\beta) = \frac{1}{\ell!}\sum_{k=0}^{\ell}\binom{\ell}{k} y^{\ell-k}\,\partial_\beta^k \mathcal{C}(y,\beta), \quad y>0, \quad \beta>0. \tag{1.30}$$

In addition, $\mathcal{C}_\ell(\cdot,\beta) \in C^{\ell-1}(0,\infty)$ for all $\beta > 0$. Relation (1.30) can be formally written as

$$\mathcal{C}_\ell(y,\beta) = \frac{1}{\ell!}\Big(y+\partial_\beta\Big)^\ell \mathcal{C}(y,\beta), \quad y>0,\ \beta>0. \tag{1.31}$$

The above relations remain valid in the limit $\beta \searrow 0$.

With the above lemma, we can compute bounds on $(\mathcal{C}_\ell)_{\ell\in\mathbb{N}_0}$. These bounds are needed for a proof of Theorem 1.12 in order to take the expansion order to infinity.

LEMMA 1.21. *Let $s \in S_\alpha$ for $\alpha \in \mathbb{R}$ with constants $c, c_0, \gamma \geq 1$. Set $\ell_\alpha = \max\{0, \lceil\alpha\rceil\} + 1$. Then*

$$\Big|\mathcal{C}_\ell(y,\beta)\Big| \leq \mathcal{M}_\ell(y), \tag{1.32}$$

with $\mathcal{M}_\ell : \mathbb{R}_+ \to \mathbb{R}$ and

$$\mathcal{M}_\ell(y) = c_s\Bigg((\ell_\alpha+1+\ell)^{\ell_\alpha+1}\,\tau^{-\ell}e^{\tau}\Big(\lceil y\rceil^\alpha + \lceil y\rceil^{-1}\Big) + \frac{1}{(\ell+1)!}\max(y^\alpha, \lceil y\rceil^\alpha)\Bigg), \tag{1.33}$$

for all $\ell \in \mathbb{N}_0$, and $y, \beta > 0$, with $c_s > 0$ only depending on s and

$$\tau = \frac{2\pi}{\gamma+1}. \tag{1.34}$$

The estimate holds in particular in the limit $\beta \searrow 0$.

From Lemmas 1.20 and 1.21, we obtain:

LEMMA 1.22. *Let $s \in S_\alpha$, $\alpha \in \mathbb{R}$, and $\ell \in \mathbb{N}_0$. The function*

$$\tilde{\mathcal{A}}_\ell : (0,\infty) \to \mathbb{C},\ \tilde{\mathcal{A}}_\ell(y) = \ell!\lim_{\beta\searrow 0}\mathcal{C}_\ell(y,\beta)$$

lies in in $C^{\ell-1}(0,\infty)$ and is estimated by

$$\big|\tilde{\mathcal{A}}_\ell(y)\big| \leq \ell!\mathcal{M}_\ell(y),$$

for $y > 0$. Here, the bound $\mathcal{M}_\ell$ is the same as in Lemma 1.21.

LEMMA 1.23. *The functions* $(\tilde{\mathcal{A}}_\ell)_{\ell\in\mathbb{N}_0}$ *from Lemma 1.22 coincide with the Bernoulli-*$\mathcal{A}$ *functions* $(\mathcal{A}_\ell)_{\ell\in\mathbb{N}_0}$ *from Definition 1.7,*

$$\tilde{\mathcal{A}}_\ell = \mathcal{A}_\ell, \quad \ell \in \mathbb{N}_0.$$

PROOF. We prove equality of the functions $(\tilde{\mathcal{A}}_\ell)_{\ell\in\mathbb{N}_0}$ and $(\mathcal{A}_\ell)_{\ell\in\mathbb{N}_0}$ by showing that they have the same exponential generating function. Let $\xi, \beta > 0$ and $\ell \in \mathbb{N}_0$. Then

$$\begin{aligned}\tilde{\mathcal{A}}_\ell(\xi) &= \lim_{\beta\searrow 0}(\xi + \partial_\beta)^\ell \mathcal{C}(\xi,\beta) = \lim_{\beta\searrow 0}\sum_{k=0}^{\ell}\binom{\ell}{k}\xi^{\ell-k}\,\partial_\beta^k \mathcal{C}(\xi,\beta)\\ &= \lim_{\beta\searrow 0} e^{-\beta\xi}\partial_\beta^\ell\Big(e^{\beta\xi}\mathcal{C}(\xi,\beta)\Big) = \lim_{\beta\searrow 0}\partial_\beta^\ell\Big(e^{\beta\xi}\mathcal{C}(\xi,\beta)\Big),\end{aligned}$$

and thus

$$e^{\beta\xi}\mathcal{C}(\xi,\beta) = \sum_{\ell=0}^{\infty}\tilde{\mathcal{A}}_\ell(\xi)\frac{\beta^\ell}{\ell!}.$$

□

After having collected all necessary information about the functions $(\mathcal{C}_\ell)_{\ell\in\mathbb{N}_0}$ and $(\mathcal{A}_\ell)_{\ell\in\mathbb{N}_0}$, we now prove the SEM expansion as given in Theorems 1.10 and 1.12.

PROOF OF THEOREM 1.10. Choose $x, a, b \in \mathbb{Z}$, $x \le a < b$ and $\delta \in (0,1]$. Let $f : [a+\delta, b+\delta] \to \mathbb{C}$ factor into

$$f(y) = s(y-x)g(y), \quad y \in [a+\delta, b+\delta],$$

with $s \in S$ and $g \in C^{\ell+1}[a+\delta, b+\delta]$. First, we prove that

$$\begin{aligned}\sum_{n=a+1}^{b} f(n) - \int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y = -\lim_{\beta\searrow 0}\Bigg(&\sum_{k=0}^{\ell}(-1)^k\mathcal{C}_k(y-x,\beta)g^{(k)}(y)\Big|_{y=a+\delta}^{y=b+\delta}\\ &+\int_{a+\delta}^{b+\delta}(-1)^\ell\mathcal{C}_\ell(y-x,\beta)g^{(\ell+1)}(y)\,\mathrm{d}y\Bigg),\end{aligned}$$

for $\ell \in \mathbb{N}_0$. The case $\ell = 0$ follows from Proposition 1.18. For $\ell \ge 1$, we begin with Proposition 1.18 and repeatedly integrate by parts computing antiderivatives of $\mathcal{C}(\cdot,\beta)$, which are given by $(\mathcal{C}_k)_{k\in\mathbb{N}_0}$. We can take the limit $\beta \searrow 0$, as the functions $\mathcal{C}_k(\cdot,\beta)$ are uniformly bounded in $\beta > 0$ for $k \in \mathbb{N}_0$, which follows from Lemma 1.21. Now as the function $g^{(\ell+1)}$ is continuous and thus bounded on the interval $[a+\delta, b+\delta]$, the integrand is uniformly bounded in β. Hence, we can apply the dominated convergence theorem, yielding

$$\sum_{n=a+1}^{b} f(n) - \int_{a+\delta}^{b+\delta} f(y)\,\mathrm{d}y =$$

$$- \sum_{k=0}^{\ell} \frac{(-1)^k}{k!} \mathcal{A}_k(y-x) g^{(k)}(y) \Big|_{y=a+\delta}^{y=b+\delta} + \frac{(-1)^\ell}{\ell!} \int_{a+\delta}^{b+\delta} \mathcal{A}_\ell(y-x) g^{(\ell+1)}(y)\,\mathrm{d}y,$$

where, by Lemma 1.23, we have inserted the Bernoulli–$\mathcal{A}$ functions

$$\mathcal{A}_k(\xi) = k! \lim_{\beta \searrow 0} \mathcal{C}_k(\xi, \beta), \quad \xi > 0.$$

□

Proof of Theorem 1.12. We prove that the expansion order ℓ in Theorem 1.10 can be taken to infinity, if $g \in E_\sigma$ and $\sigma < \tau$ where τ is a constant that only depends on $s \in S$ with

$$\tau = \frac{2\pi}{1+\gamma}. \tag{1.35}$$

First consider the remainder integral, which we define as

$$R_{\ell+1} = \frac{(-1)^\ell}{\ell!} \int_{a+\delta}^{b+\delta} \mathcal{A}_\ell(y-x) g^{(\ell+1)}(y)\,\mathrm{d}y. \tag{1.36}$$

By Lemma 1.22, we have

$$\sup_{y \in [a+\delta, b+\delta]} \left| \frac{1}{k!} \mathcal{A}_k(y-x) \right| = \mathcal{O}\Big(\tau^{-k}\Big), \quad k \to \infty, \tag{1.37}$$

for all $k \in \mathbb{N}_0$. Moreover, as $g \in E_\sigma$, we find that for all $\varepsilon > 0$

$$\sup_{y \in [a+\delta, b+\delta]} \left| g^{(k)}(y) \right| = \mathcal{O}\Big((\sigma+\varepsilon)^k\Big), \quad k \to \infty. \tag{1.38}$$

Thus

$$R_{\ell+1} = \mathcal{O}\left(\left(\frac{\tau}{\sigma+\varepsilon} \right)^{-\ell} \right), \quad \ell \to \infty. \tag{1.39}$$

From the estimates above, we can conclude that the series

$$\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \mathcal{A}_k(y-x) g^{(k)}(y) \tag{1.40}$$

converges uniformly on the interval $[a+\delta, b+\delta]$. Therefore, the limit $\ell \to \infty$ is well-defined, which implies Theorem 1.12.

□

Derivation of Example 1.15. Let $y, \beta > 0$ and $s(y) = |y|^{-\nu}$ with $\nu \in \mathbb{C}$. Then

$$\begin{aligned}\mathcal{C}(y,\beta) &= \sum_{n=\lceil y\rceil}^{\infty} e^{-\beta n} n^{-\nu} - \int_y^\infty e^{-\beta z} z^{-\nu}\,\mathrm{d}z \\ &= e^{-\beta\lceil y\rceil}\sum_{n=0}^{\infty}\frac{1}{(n+\lceil y\rceil)^\nu}e^{-\beta n} - \beta^{\nu-1}\Gamma(1-\nu,\beta y),\end{aligned}$$

with $\Gamma(\cdot,\cdot)$ the incomplete gamma function

$$\Gamma(q,z) = \int_z^\infty t^{q-1}e^{-t}\,\mathrm{d}t, \quad z>0,\ q>0,$$

which can be continued to a meromorphic function on $\mathbb{C}\times\mathbb{C}$, see e.g. [22, Chap. IX]. In the case $\nu \in \mathbb{R}\setminus\mathbb{N}_0$, the series is expanded as

$$e^{-\beta\lceil y\rceil}\sum_{n=0}^{\infty}\frac{1}{(n+\lceil y\rceil)^\nu}e^{-\beta n} = \Gamma(1-\nu,0)\beta^{\nu-1} + \sum_{n=0}^{\infty}(-1)^n\zeta(\nu-n,\lceil y\rceil)\frac{\beta^n}{n!},$$

which holds for $\beta \in (0,2\pi)$ [21, Sec. 1.11, Eq. (8)]. We then use the power series representation of the incomplete gamma function for $\beta > 0$ [21, Sec. 9.2, Eq. (5)],

$$\beta^{\nu-1}\Gamma(1-\nu,\beta y) = \beta^{\nu-1}\Gamma(1-\nu,0) - y^{-(\nu-1)}\sum_{n=0}^{\infty}(-1)^n\frac{y^n}{n+1-\nu}\frac{\beta^n}{n!}.$$

We subtract both terms, after which the singularities cancel. We then find

$$\mathcal{C}(y,\beta) = \sum_{n=0}^{\infty}(-1)^n\left[\zeta(\nu-n,\lceil y\rceil) - \frac{y^{-(\nu-n-1)}}{\nu-n-1}\right]\frac{\beta^n}{n!}.$$

It follows that the radius of convergence of the series equals 2π. We now obtain the generating function of the Bernoulli–$\mathcal{A}$ functions by computing $e^{\beta y}\mathcal{C}(y,\beta)$ by means of the Cauchy product,

$$e^{\beta y}\mathcal{C}(y,\beta) = \sum_{\ell=0}^{\infty}\left[\sum_{k=0}^{\ell}(-1)^k\binom{\ell}{k}y^{\ell-k}\left(\zeta(\nu-k,\lceil y\rceil) - \frac{y^{-(\nu-k-1)}}{\nu-k-1}\right)\right]\frac{\beta^\ell}{\ell!}.$$

Hence, we have proven the form of the SEM operator coefficients for $\nu \in \mathbb{R}\setminus\mathbb{N}_0$. In the case $\nu \in \mathbb{N}_0$, the above expression exhibits a removable singularity. For $k \in \mathbb{N}_0$, we have

$$\zeta(\nu-k,\lceil y\rceil) - \frac{y^{-(\nu-k-1)}}{\nu-k-1} = \zeta(\nu-k,\lceil y\rceil) - \frac{1}{\nu-k-1} - \frac{y^{-(\nu-k-1)}-1}{\nu-k-1}.$$

From [21, Sec. 1.10, Eq. (9)] follows that the first two terms tend to

$$\lim_{\nu\to k+1}\left(\zeta(\nu-k,\lceil y\rceil)-\frac{1}{\nu-k-1}\right)=-\psi(y),$$

with the digamma function ψ [21, Sec. 1.7]. The remaining term is the differential quotient of the function $h_y:\mathbb{R}\to\mathbb{R}$, $y>0$, with

$$h_y(\nu)=y^{-\nu-k-1},$$

which is evaluated at $\nu=k+1$. Thus, the limit equals $-\log y$. Combining the above results, we find that

$$\lim_{\nu\to k+1}\left(\zeta(\nu-k,\lceil y\rceil)-\frac{y^{-(\nu-k-1)}}{\nu-k-1}\right)=-\psi(\lceil y\rceil)-\log y.$$

Finally, we can rewrite the last term as follows [21, Sec. 1.7.1, Eq. (9)],

$$-\psi(\lceil y\rceil)-\log y=\gamma_e-H_{\lceil y\rceil-1}-\log y,$$

with γ_e the Euler–Mascheroni constant and where H_k is the kth harmonic number,

$$H_k=\sum_{j=1}^{k}\frac{1}{j},\quad k\in\mathbb{N}_0.$$

□

5. Technical lemmas

We first prove the two remarks from Section 2 and then proceed with the proofs of the remaining lemmas from Section 4.

Proof of Remark 1.2. Consider $s\in C^\infty(\mathbb{R}\setminus\{0\})$ with

$$s(y)=|y|^{-\nu},\quad \nu\in\mathbb{R}.$$

We first compute the ℓth derivative of s

$$s^{(\ell)}(y)=\left(\prod_{k=1}^{\ell}(k-1+\nu)\right)\frac{(-1)^\ell}{y^\ell}\,|y|^{-\nu},\quad y\in\mathbb{R}\setminus\{0\}.$$

The above product can be written as

$$\prod_{k=1}^{\ell}(k-1+\nu)=\frac{\Gamma(\nu+\ell)}{\Gamma(\nu)},$$

with Γ the gamma function [21, Chap. I]. From the Stirling formula [21, Sec. 1.18], we know that

$$\Gamma(z)\sim\sqrt{\frac{2\pi}{z}}z^ze^{-z},\quad z\to\infty,$$

with ~ meaning that the quotient of both sides tends to 1 in the limit $z \to \infty$. After applying this relation in the limit $\ell \to \infty$, we find

$$\begin{aligned}\frac{\Gamma(\nu+\ell)}{\Gamma(\nu)\ell!} &= \frac{\Gamma(\nu+\ell)}{\Gamma(\nu)\,\ell\Gamma(\ell)} \\ &\sim \frac{1}{\ell\,\Gamma(\nu)}\frac{\ell}{\sqrt{\ell(\ell+\nu)}}e^{-\nu}\left(1+\frac{\nu}{\ell}\right)^{\ell}\left(1+\frac{\nu}{\ell}\right)^{\nu}\ell^{\nu} \\ &\sim \frac{1}{\Gamma(\nu)}\ell^{-(1-\nu)}, \quad \ell \to \infty,\end{aligned}$$

which is bounded for $\nu \le 1$ and constant for $\nu = 1$. If $\nu > 1$, the above expression diverges algebraically, which implies

$$\frac{\Gamma(\nu+\ell)}{\Gamma(\nu)\ell!}\frac{1}{(1+\varepsilon)^{\ell}} \to 0, \quad \ell \to \infty$$

for all $\varepsilon > 0$. In total, we have proven that

$$\begin{aligned}\left|s^{(\ell)}(y)\right| &= \frac{|\Gamma(\nu+\ell)|}{|\Gamma(\nu)|}|y|^{-\ell}|s(y)| \\ &\le c\,\ell!\,(1+\varepsilon)^{\ell}|y|^{-\ell}|s(y)|, \quad y \in \mathbb{R}\setminus\{0\},\end{aligned}$$

with $c > 0$ only depending on the choice of ν and $\varepsilon > 0$. In the case $\nu \le 1$, we can set $\varepsilon = 0$ in the above estimate.

□

Proof of Remark 1.4. Let $s \in S$. Then there exist $c > 0$ and $\gamma \ge 1$ such that

$$|s'(y)| \le c\,\gamma\,|y|^{-1}|s(y)|, \quad y \in \mathbb{R}\setminus\{0\}.$$

Consider $y > 1$. Then

$$|s(y)| \le |s(1)| + \int_1^y |s'(z)|\,\mathrm{d}z \le |s(1)| + \int_1^y c\gamma z^{-1}|s(z)|\,\mathrm{d}z,$$

and after applying Grönwall's inequality [30, Cor. 6.6], we find that

$$|s(y)| \le |s(1)|\exp\left(c\gamma\int_1^y z^{-1}\,\mathrm{d}z\right) = |s(1)|y^{\alpha},$$

with $\alpha = c\gamma$. In the case $y < -1$, we set $\tilde{y} = -y$, thereby extending the estimate to $\mathbb{R}\setminus[-1,1]$.

□

The function $\mathcal{C}$ is a priori not well-defined for $\beta = 0$, the case where the shielding of the interaction has been removed. However, we can show that an extension to $\beta = 0$ is possible. The following estimate plays an important role for this extension.

Lemma 1.24. *Let $s \in S$ with constants $c > 0, \gamma \geq 1$. Then we have*

$$\left|s_\beta^{(\ell)}(y)\right| \leq c\,\ell!\,\gamma^\ell\,|y|^{-\ell}\,|s(y)|$$

for all $y \in \mathbb{R} \setminus \{0\}$, $\ell \in \mathbb{N}_0$ and $\beta > 0$.

Proof. Let $\ell \in \mathbb{N}_0$ and $y > 0$. We find that

$$\begin{aligned}
|s_\beta^{(\ell)}(y)| &\leq \sum_{k=0}^{\ell} \binom{\ell}{k} |s^{(k)}(y)|\,\beta^{\ell-k}\,e^{-\beta y} \\
&\leq c\,\ell!\,\gamma^\ell\,y^{-\ell}|s(y)| \left(\sum_{k=0}^{\ell} \frac{1}{(\ell-k)!} y^{\ell-k}\beta^{\ell-k} \right) e^{-\beta y} \\
&\leq c\,\ell!\,\gamma^\ell\,y^{-\ell}|s(y)|e^{\beta y}e^{-\beta y} \\
&= c\,\ell!\,\gamma^\ell\,y^{-\ell}|s(y)|.
\end{aligned}$$

We can extend the result to $y \in \mathbb{R} \setminus \{0\}$ by replacing y by $-y$ in the above estimates.

□

In the following, we analyse the behaviour of the function $\mathcal{C}$ in both its variables.

Proof of Lemma 1.16. Let $s \in S$ and $y > 0$ fixed. In order to prove differentiability of the function

$$\mathcal{C}(y,\cdot) : (0,\infty) \to \mathbb{C},\ \mathcal{C}(y,\beta) = \sum_{n=\lceil y \rceil}^{\infty} s(n)e^{-\beta n} - \int_y^\infty s(z)e^{-\beta z}\,\mathrm{d}z,$$

it is enough to show that it is differentiable on intervals $[\beta_1, \beta_2]$, with $\beta_1, \beta_2 \in \mathbb{R}_+$ and $\beta_1 < \beta_2$. First, the integrand

$$h : [y,\infty) \times [\beta_1,\beta_2] \to \mathbb{C},\ (z,\beta) \mapsto s(z)e^{-\beta z}$$

is smooth in both variables. The partial derivative with respect to β reads

$$\partial_\beta h(z,\beta) = -zs(z)e^{-\beta z}, \quad \beta \in [\beta_1,\beta_2],\ z \geq y.$$

Now as $s \in S$, the interaction may only grow polynomially, which is a consequence of Remark 1.4. Therefore, there exists $c > 0$ such that

$$|zs(z)|e^{-\beta_1 z} \leq \frac{c}{1+z^2}, \quad z \geq y,$$

from which we obtain

$$|\partial_\beta h(z,\beta)| \leq |zs(z)|e^{-\beta_1} \leq \frac{c}{1+z^2}, \quad \beta \in [\beta_1,\beta_2],\ z \geq y.$$

As the majorant is independent of the choice of $\beta \in [\beta_1, \beta_2]$ and is both summable and integrable on $[y, \infty)$, we conclude that $\mathcal{C}(y, \cdot)$ is differentiable. The derivative is given by

$$\partial_\beta \mathcal{C}(y,\beta) = -\sum_{n=\lceil y\rceil}^{\infty} n s(n) e^{-\beta n} + \int_y^\infty z s(z) e^{-\beta z}\,\mathrm{d}z, \quad \beta > 0.$$

As $s \in S$, also $\tilde{s} \in C^\infty(\mathbb{R} \setminus \{0\})$ with

$$\tilde{s}_\ell(z) = (-1)^\ell z^\ell s(z), \quad z \in \mathbb{R} \setminus \{0\},$$

is an asymptotically smooth function for $\ell \in \mathbb{N}_0$. Since moreover $\tilde{s}_\ell(z)e^{-\beta z}$ equals $\partial_\beta^\ell h(z,\beta)$ for $z > 0$ and $\beta > 0$, we conclude by induction that $\mathcal{C}$ is infinitely differentiable with respect to β. It is sufficient to prove the rest of the lemma for $\ell = 0$.

Choose $\beta > 0$. As s is asymptotically smooth, there exist $\alpha \in \mathbb{R}$ and $c_0 > 0$ such that

$$|s(z)| \le c_0 z^\alpha, \quad z \ge 1,$$

and $c_{\alpha,\beta} > 0$ with

$$e^{-\beta z} \le \frac{c_{\alpha,\beta}}{(1+z)^{\alpha+2}}, \quad z \ge 1.$$

In total, we obtain

$$\begin{aligned}
\sum_{n=\lceil y\rceil}^{\infty} |s(n)| e^{-\beta n} &= e^{-\beta\lceil y\rceil} \sum_{n=0}^{\infty} |s(n+\lceil y\rceil)| e^{-\beta n} \\
&\le c_0\, c_{\alpha,\beta}\, e^{-\beta\lceil y\rceil} \sum_{n=0}^{\infty} \left(\frac{n+\lceil y\rceil}{n+1}\right)^\alpha \frac{1}{(n+1)^2} \\
&\le \frac{\pi^2}{6} c_0\, c_{\alpha,\beta}\, e^{-\beta y} \begin{cases} 1, & \alpha < 0, \\ (1+\lceil y\rceil)^\alpha, & \alpha \ge 0, \end{cases}
\end{aligned}$$

for $y > 0$. The above estimates show that the integral term decays exponentially in y.

We now prove that the limit $\beta \searrow 0$ is well-defined. We begin by applying the EM expansion up to order $\ell \in \mathbb{N}_0$ to the definition of the function $\mathcal{C}$, which yields

$$\mathcal{C}(y,\beta) = -\int_y^{\lceil y\rceil} s_\beta(y)\,\mathrm{d}y + \sum_{k=0}^{\ell} \frac{(-1)^k}{k!} \frac{B_{k+1}(1)}{k+1} s_\beta^{(k)}(\lceil y\rceil) + R_\ell(y,\beta), \tag{1.41}$$

where we have defined the remainder integral as

$$R_\ell(y,\beta) = \frac{(-1)^\ell}{\ell!} \int_{\lceil y\rceil}^\infty \frac{B_{\ell+1}(1+z-\lceil z\rceil)}{\ell+1} s_\beta^{(\ell+1)}(z)\,\mathrm{d}z.$$

In the limit $\beta \searrow 0$, the first two terms in (1.41) converge to

$$-\int_y^{\lceil y\rceil} s(y)\,\mathrm{d}y + \sum_{k=0}^{\ell} \frac{(-1)^k}{k!}\frac{B_{k+1}(1)}{k+1} s^{(k)}(\lceil y\rceil),$$

leaving only R_ℓ to be examined.

From Remark 1.4 follows that for every $s \in S$ there exists an $\alpha \in \mathbb{R}$ such that $s \in S_\alpha$. Together with the estimate (1.4), we find that the function $s^{(\ell+1)}$ is integrable on $[\varepsilon, \infty)$, $\varepsilon > 0$, for all $\ell \in \mathbb{N}_0$ larger than or equal to $\ell_\alpha = \max\{0, \lceil\alpha\rceil\} + 1$. Using Lemma 1.24, we find that the absolute value of the integrand in R_{ℓ_α} can be estimated by

$$c\gamma^{\ell_\alpha}\frac{|B_{\ell_\alpha+1}(1+z-\lceil z\rceil)|}{\ell_\alpha+1} z^{-2}$$

for $z \geq 1$. The bound is integrable on $[1, \infty)$, as it is a product of a bounded and an integrable function. The dominated convergence theorem yields

$$\lim_{\beta\searrow 0} \mathcal{C}(y,\beta) = -\int_y^{\lceil y\rceil} s(z)\,\mathrm{d}z + \sum_{k=0}^{\ell_\alpha} \frac{(-1)^k}{k!}\frac{B_{k+1}(1)}{k+1} s^{(k)}(\lceil y\rceil) + \frac{(-1)^{\ell_\alpha}}{\ell_\alpha!}\int_{\lceil y\rceil}^{\infty} \frac{B_{\ell_\alpha+1}(1+z-\lceil z\rceil)}{\ell_\alpha+1} s^{(\ell_\alpha+1)}(z)\,\mathrm{d}z. \tag{1.42}$$

□

Proof of Lemma 1.17. Let $s \in S$, $\ell \in \mathbb{N}_0$, and $y, \beta > 0$. From Lemma 1.16 then follows that

$$\partial_\beta^\ell \mathcal{C}(y,\beta) = (-1)^\ell \left(\sum_{n=\lceil y\rceil}^{\infty} n^\ell s(n) e^{-\beta n} - \int_y^{\infty} z^\ell s(z) e^{-\beta z}\,\mathrm{d}z \right).$$

By (1.41), we then find

$$\partial_\beta^\ell \mathcal{C}(y,\beta) = -\int_y^{\lceil y\rceil} (-1)^\ell z^\ell s_\beta(z)\,\mathrm{d}z + \sum_{k=0}^{\ell_\alpha} \frac{(-1)^k}{k!}\frac{B_{k+1}(1)}{k+1} (-1)^\ell \lceil y\rceil^\ell s_\beta^{(k)}(\lceil y\rceil) + \frac{(-1)^{\ell_\alpha}}{\ell_\alpha!}\int_{\lceil y\rceil}^{\infty} \frac{B_{\ell_\alpha+1}(1+z-\lceil z\rceil)}{\ell_\alpha+1} (-1)^\ell z^\ell s_\beta^{(\ell_\alpha+1)}(z)\,\mathrm{d}z. \tag{1.43}$$

Here we have chosen $\ell_\alpha = \max\{0, \lceil\alpha\rceil\} + \ell + 1$ with $\alpha \in \mathbb{R}$ such that $s \in S_\alpha$ as in the proof of Lemma 1.16. From (1.42), we can conclude that the above equation holds also for $\beta \searrow 0$. Consider an interval

$(n, n+1)$, $n \in \mathbb{N}_0$. From (1.43), we find that $\partial_\beta^\ell \mathcal{C}$ is an antiderivative of a smooth function,

$$\partial_\beta^\ell \mathcal{C}(y,\beta) = c_n - \int_y^{n+1} (-1)^\ell z^\ell s_\beta(z)\,\mathrm{d}z, \quad y \in (n, n+1),$$

where c_n only depends on s and on n. Thus $\partial_\beta^\ell \mathcal{C}$ is smooth in y on $\mathbb{R}_+ \setminus \mathbb{N}$.

We now prove the jump relation. First take $n \in \mathbb{N}$. Then for $\varepsilon_1, \varepsilon_2 \in (0,1)$, we compute

$$\begin{aligned}\partial_\beta^\ell \mathcal{C}(n-\varepsilon_1,\beta) - \partial_\beta^\ell \mathcal{C}(n+\varepsilon_2,\beta) = \\ &- \int_{n-\varepsilon_1}^{n+\varepsilon_2} (-1)^\ell z^\ell s_\beta(z)\,\mathrm{d}z + \int_n^{n+1} (-1)^\ell z^\ell s_\beta(z)\,\mathrm{d}z \\ &+ \sum_{k=0}^{\ell_\alpha} \frac{(-1)^k}{k!} \frac{B_{k+1}(1)}{k+1} (-1)^\ell \lceil z \rceil^\ell s_\beta^{(k)}(\lceil z \rceil) \Big|_{z=n+\varepsilon_2}^{n-\varepsilon_1} \\ &+ \frac{(-1)^{\ell_\alpha}}{\ell_\alpha!} \int_n^{n+1} \frac{B_{\ell_\alpha+1}(1+z-\lceil z \rceil)}{\ell_\alpha+1} (-1)^\ell z^\ell s_\beta^{(\ell_\alpha+1)}(z)\,\mathrm{d}z.\end{aligned}$$

After performing the limits $\varepsilon_1, \varepsilon_2 \searrow 0$, we find for the right hand side of (1.43)

$$\begin{aligned}&\int_n^{n+1} (-1)^\ell z^\ell s_\beta(z)\,\mathrm{d}z + \sum_{k=1}^{\ell_\alpha} \frac{(-1)^k}{k!} \frac{B_{k+1}(1)}{k+1} (-1)^\ell z^\ell s_\beta^{(k)}(z) \Big|_{z=n+1}^{n} \\ &\quad + \frac{(-1)^{\ell_\alpha}}{\ell_\alpha!} \int_n^{n+1} \frac{B_{\ell_\alpha+1}(1+z-\lceil z \rceil)}{\ell_\alpha+1} (-1)^\ell z^\ell s_\beta^{(\ell_\alpha+1)}(z)\,\mathrm{d}z \\ &\qquad = (-1)^\ell n^\ell s_\beta(n).\end{aligned}$$

In the last equality, we have applied the EM expansion (1.1) with the parameters $a = n-1$, $b = n$ and $\delta = 1$ up to order ℓ_α.

□

Using the jump relations, we can now prove the alternative representation of the functions $(\mathcal{C}_\ell)_{\ell \in \mathbb{N}_0}$ in terms of derivatives of $\mathcal{C}$ with respect to β.

Proof of Lemma 1.20. Let $s \in S$ and $y, \beta > 0$. We prove the relation by induction. The case $\ell = 0$ holds by definition. Take now

$\ell \in \mathbb{N}_0$ and assume that the form (1.30) holds for ℓ,

$$\mathcal{C}_\ell(y,\beta) = \frac{1}{\ell!}\sum_{k=0}^{\ell}\binom{\ell}{k} y^{\ell-k}\,\partial_\beta^k \mathcal{C}(y,\beta), \qquad y>0, \quad \beta>0. \tag{1.44}$$

We now prove that it then holds for $\ell+1$. Subsequently, we can extend the definition of $\mathcal{C}_\ell$ to $\beta = 0$ by Lemma 1.16.

First recall the jump relation

$$\lim_{y\nearrow n}\partial_\beta^k\mathcal{C}(y,\beta) - \lim_{y\searrow n}\partial_\beta^k\mathcal{C}(y,\beta) = (-n)^k s_\beta(n)$$

for $n\in\mathbb{N}$, $k\in\mathbb{N}_0$, as well as the derivative formula

$$\partial_y\partial_\beta^k\mathcal{C}(y,\beta) = (-y)^k s_\beta(y),$$

which holds for $y\in\mathbb{R}_+\setminus\mathbb{N}$. Both relations are valid for $\beta\geq 0$.

For $\beta>0$, the derivative of the function

$$\tilde{\mathcal{C}}_{\ell+1}(\cdot,\beta):\mathbb{R}_+\to\mathbb{C},\ \tilde{\mathcal{C}}_{\ell+1}(y,\beta) = \frac{1}{(\ell+1)!}\sum_{k=0}^{\ell+1}\binom{\ell+1}{k} y^{\ell+1-k}\,\partial_\beta^k\mathcal{C}(y,\beta),$$

at $y\in\mathbb{R}_+\setminus\mathbb{N}$ takes the form

$$\begin{aligned}
&\frac{1}{(\ell+1)!}\sum_{k=0}^{\ell}\binom{\ell+1}{k}\Big((\ell+1-k)y^{\ell-k}\partial_\beta^k\mathcal{C}(y,\beta) + y^{\ell+1-k}(-y)^k s_\beta(y)\Big)\\
=&\frac{1}{\ell!}\sum_{k=0}^{\ell}\binom{\ell}{k} y^{\ell-k}\,\partial_\beta^k\,\mathcal{C}(y,\beta) + \frac{1}{(\ell+1)!}\sum_{k=0}^{\ell+1}\binom{\ell+1}{k}(-1)^k\,y^{\ell+1}s_\beta(y)\\
=&\mathcal{C}_\ell(y,\beta) + \frac{y^{\ell+1}s_\beta(y)}{(\ell+1)!}(1-1)^{\ell+1} = \mathcal{C}_\ell(y,\beta).
\end{aligned}$$

In order to prove that $\tilde{\mathcal{C}}_{\ell+1}$ and $\mathcal{C}_{\ell+1}$ differ at most by a constant, we have to show that both are continuous. The function $\mathcal{C}_\ell(\cdot,\beta)$ is from $C^{\ell-1}$, therefore its antiderivative $\mathcal{C}_{\ell+1}(\cdot,\beta)$ is in C^ℓ, and thus continuous. We have already shown that $\tilde{\mathcal{C}}_{\ell+1}(\cdot,\beta)$ is smooth on $\mathbb{R}_+\setminus\mathbb{N}$. In order to prove that it is also continuous on $\mathbb{R}_+$, we need to investigate the behaviour at the positive integers. Let $n\in\mathbb{N}$, then from the jump relation follows

$$\begin{aligned}
\lim_{y\nearrow n}\tilde{\mathcal{C}}_{\ell+1}(y,\beta) - \lim_{y\searrow n}\tilde{\mathcal{C}}_{\ell+1}(y,\beta) =& \frac{1}{(\ell+1)!}\sum_{k=0}^{\ell+1}\binom{\ell+1}{k} n^{\ell+1-k}(-n)^k s_\beta(n)\\
=&\frac{n^{\ell+1}s_\beta(n)}{(\ell+1)!}\sum_{k=0}^{\ell+1}\binom{\ell+1}{k}(-1)^k = 0,
\end{aligned}$$

proving continuity. Thus, the function can only differ from $\mathcal{C}_{\ell+1}(\cdot,\beta)$ by an additive constant. This constant is zero as both functions vanish in the limit $y \to \infty$ by Lemma 1.16. We remember that the jump relation also holds for $\beta = 0$. Together with the induction hypothesis

$$\lim_{\beta \searrow 0} \mathcal{C}_\ell(\cdot, \beta) \in C^{\ell-1}(0,\infty),$$

we find that

$$\lim_{\beta \searrow 0} \mathcal{C}_{\ell+1}(\cdot, \beta) \in C^{\ell}(0,\infty).$$

□

NOTATION 1.25. Let $s \in S$, $\ell \in \mathbb{N}_0$, $\xi \in \mathbb{R}$, and $y \in \mathbb{R} \setminus \{0\}$. We then write

$$s_{\xi,\ell,\beta}(y) = \frac{1}{\ell!}(y-\xi)^\ell s_\beta(y). \tag{1.45}$$

LEMMA 1.26. *Let $s \in S$ and $\ell \in \mathbb{N}_0$. The function $\mathcal{C}_\ell(\cdot,\cdot)$ takes the form*

$$\mathcal{C}_\ell(y,\beta) = \sum_{n=\lceil y \rceil}^{\infty} s_{y,\ell,\beta}(n) - \int_y^\infty s_{y,\ell,\beta}(z)\,\mathrm{d}z, \quad y > 0, \quad \beta > 0. \tag{1.46}$$

PROOF. From Lemma 1.16, we find that

$$\partial_\beta^k \mathcal{C}(y,\beta) = \sum_{n=\lceil y \rceil}^{\infty} (-1)^k n^k s_\beta(n) - \int_y^\infty (-1)^k z^k s_\beta(z)\,\mathrm{d}z$$

for $y > 0$, $\beta > 0$. Together with the representation of the functions $(C_\ell)_{\ell \in \mathbb{N}_0}$ from Lemma 1.20,

$$\mathcal{C}_\ell(y,\beta) = \frac{1}{\ell!}\sum_{k=0}^{\ell}\binom{\ell}{k} y^{\ell-k}\,\partial_\beta^k \mathcal{C}(y,\beta)$$

the lemma follows from an application of the binomial theorem.

□

LEMMA 1.27. *Let $s \in S$ with constants $c > 0, \gamma \geq 1$. For $y > 0$, $\xi \geq 0$ and $y > \xi$, we have*

$$\left|s^{(k)}_{\xi,\ell,\beta}(y)\right| \leq c\,\frac{k!}{\ell!}\,\gamma^{k-\ell}\Big(\gamma(1-\xi/y)+1\Big)^\ell |y|^{\ell-k}\,|s(y)| \tag{1.47}$$

for $y \in \mathbb{R} \setminus \{0\}$, $k, \ell \in \mathbb{N}_0$ with $k > \ell$, and $\beta > 0$. For $\xi = y$, we have

$$\left|s^{(k)}_{y,\ell,\beta}(y)\right| \leq \begin{cases} c\,\dfrac{k!}{\ell!}\,\gamma^{k-\ell}\,|y|^{\ell-k}\,|s(y)|, & k \geq \ell, \\ 0, & k < \ell. \end{cases} \tag{1.48}$$

PROOF. Take $y > 0$. Then

$$s^{(k)}_{\xi,\ell,\beta}(y) = \frac{1}{\ell!}\sum_{j=0}^{k} j!\binom{k}{j}\binom{\ell}{j}(y-\xi)^{\ell-j} s^{(k-j)}_{\beta}(y).$$

For $\xi = y$, we get (1.48) from Lemma 1.24. Otherwise

$$s^{(k)}_{\xi,\ell,\beta}(y) = \frac{k!}{\ell!}\, y^{\ell}(1-\xi/y)^{\ell}\sum_{j=0}^{\ell}\binom{\ell}{j}(y-\xi)^{-j}\frac{s^{(k-j)}_{\beta}(y)}{(k-j)!}.$$

For $s \in S$ we obtain by Definition 1.1

$$\begin{aligned}\left|s^{(k)}_{\xi,\ell,\beta}(y)\right| &\le c\,\frac{k!}{\ell!}\,\gamma^{k}\,|y|^{\ell-k}\,|s(y)|\,(1-\xi/y)^{\ell}\sum_{j=0}^{\ell}\binom{\ell}{j}(1-\xi/y)^{-j}\gamma^{-j}\\ &= c\,k!/\ell!\,\gamma^{k}\Big(1-\xi/y+\gamma^{-1}\Big)^{\ell}\,|y|^{\ell-k}\,|s(y)|.\end{aligned}$$

□

PROOF OF LEMMA 1.21. Take $s \in S_\alpha$ with parameters $\alpha \in \mathbb{R}$, $c > 0$ and $\gamma \ge 1$. In the following proof, $c_s > 0$ shall denote a generic constant that depends only s and can change between different equations. Let $\ell \in \mathbb{N}_0$, $\xi > 0$ and $\beta \ge 0$. Then the function

$$s_{\xi,\ell,\beta} : \mathbb{R}\setminus\{0\} \to \mathbb{C},\ \ s_{\xi,\ell,\beta}(y) = \frac{1}{\ell!}(y-\xi)^{\ell} s_{\beta}(y),$$

is asymptotically smooth and belongs to $S_{\alpha+\ell}$. This also holds for $\beta = 0$. Using the representation of $\mathcal{C}_\ell(\cdot,\beta)$ from Lemma 1.26, we have

$$\mathcal{C}_\ell(y,\beta) = \sum_{n=\lceil y\rceil}^{\infty} s_{y,\ell,\beta}(n) - \int_{y}^{\infty} s_{y,\ell,\beta}(z)\,\mathrm{d}z.$$

Subsequently, we apply the EM expansion to the right hand side up to order $k_\alpha = \ell_\alpha + \ell$ with $\ell_\alpha = \max\{0,\lceil\alpha\rceil\} + 1$, and obtain

$$\begin{aligned}\mathcal{C}_\ell(y,\beta) = &-\int_{y}^{\lceil y\rceil} s_{y,\ell,\beta}(z)\,\mathrm{d}z + \sum_{k=0}^{k_\alpha}\frac{(-1)^k}{k!}\frac{B_{k+1}(1)}{k+1}s^{(k)}_{y,\ell,\beta}(\lceil y\rceil)\\ &+\frac{(-1)^{k_\alpha}}{k_\alpha!}\int_{\lceil y\rceil}^{\infty}\frac{B_{k_\alpha+1}(1+z-\lceil z\rceil)}{k_\alpha+1}s^{(k_\alpha+1)}_{y,\ell,\beta}(z)\,\mathrm{d}z.\end{aligned}$$

We then derive bounds for $\mathcal{C}_\ell(y,\beta)$ that are uniform in β. We apply the following strategy: First, we consider $\lceil y\rceil \in \mathbb{N}$. Then the result is extended to $y \in \mathbb{R}_+$ by means of the Taylor expansion. We find that

$$|\mathcal{C}_\ell(\lceil y\rceil,\beta)| \le \sum_{k=0}^{k_\alpha} \left|\frac{B_{k+1}(1)}{(k+1)!}\right| \left|s^{(k)}_{\lceil y\rceil,\ell,\beta}(\lceil y\rceil)\right| + \int_{\lceil y\rceil}^{\infty} \left|\frac{B_{k_\alpha+1}(1+z-\lceil z\rceil)}{(k_\alpha+1)!}\right| \left|s^{(k_\alpha+1)}_{\lceil y\rceil,\ell,\beta}(z)\right| \,\mathrm{d}z. \tag{1.49}$$

We apply the estimate from Lemma 1.27,

$$\left|s^{(k)}_{y,\ell,\beta}(y)\right| \le \begin{cases} c\,\dfrac{k!}{\ell!}\,\gamma^{k-\ell}\,|y|^{\ell-k}\,|s(y)|, & k \ge \ell,\\ 0, & k < \ell,\end{cases}$$

and use

$$\frac{k!}{\ell!} \le k^{k-\ell}, \quad \ell \in \mathbb{N}_0.$$

The Bernoulli polynomials are bounded as follows, see Eq. (19) and discussion in [36],

$$\max_{y\in[0,1]} \left|\frac{B_k(y)}{k!}\right| \le \frac{4}{(2\pi)^k}, \quad k \in \mathbb{N}_0.$$

In total, we find the following bound for the first term on the right hand side of (1.49)

$$4c\,(\ell_\alpha+\ell)^{\ell_\alpha} |s(\lceil y\rceil)| \sum_{k=\ell}^{\ell_\alpha+\ell} \frac{1}{(2\pi)^{k+1}} \left(\frac{\gamma}{\lceil y\rceil}\right)^{k-\ell}.$$

The sum yields

$$\sum_{k=\ell}^{\ell_\alpha+\ell} \frac{1}{(2\pi)^{k+1}} \left(\frac{\gamma}{\lceil y\rceil}\right)^{k-\ell} \le (\ell_\alpha+1)\gamma^{\ell_\alpha}(2\pi)^{-\ell}, \tag{1.50}$$

and thus

$$\sum_{k=0}^{k_\alpha} \left|\frac{B_{k+1}(1)}{(k+1)!}\right| \left|s^{(k)}_{\lceil y\rceil,\ell,\beta}(\lceil y\rceil)\right| \le c_s \lceil y\rceil^{\alpha} (\ell_\alpha+\ell)^{\ell_\alpha} (2\pi)^{-\ell}.$$

We proceed by an investigation of the remainder integral in (1.49). From Lemma 1.27 follows that

$$\left|s^{(k)}_{\xi,\ell,\beta}(z)\right| \le c\,\frac{k!}{\ell!}\,\gamma^{k-\ell} \big(\gamma(1-\xi/z)+1\big)^{\ell} |z|^{\ell-k} |s(z)|,$$

with $z \ge \xi$ and $k = \ell_\alpha + \ell + 1$. We insert ℓ_α and, as $s \in S$, we find that the integrand is bounded by

$$c_s(\ell_\alpha+1+\ell)^{\ell_\alpha+1} \left(\frac{\gamma+1}{2\pi}\right)^{\ell} z^{-2}.$$

We therefore obtain for the integral

$$\int_{\lceil y\rceil}^{\infty}\left|\frac{B_{k_\alpha+1}(1+z-\lceil z\rceil)}{(k_\alpha+1)!}\right|\left|s^{(k_\alpha+1)}_{\lceil y\rceil,\ell,\beta}(z)\right|\mathrm{d}z \le c_s(\ell_\alpha+1+\ell)^{\ell_\alpha+1}\left(\frac{\gamma+1}{2\pi}\right)^{\ell}\lceil y\rceil^{-1}.$$

Combining the above estimates, we find that

$$|\mathcal{C}_\ell(\lceil y\rceil,\beta)| \le c_s(\ell_\alpha+1+\ell)^{\ell_\alpha+1}\,\tau^{-\ell}\left(\lceil y\rceil^{\alpha}+\lceil y\rceil^{-1}\right), \tag{1.51}$$

where $\tau = 2\pi/(\gamma+1)$. Now take $y\in\mathbb{R}_+\smallsetminus\mathbb{N}$. We expand $\mathcal{C}_\ell(\cdot,\beta)$ around $\lceil y\rceil$. Let $\ell,k\in\mathbb{N}_0$ and $k\le\ell$, then

$$\partial_y^k\mathcal{C}_\ell(y,\beta) = \mathcal{C}_{\ell-k}(y,\beta),$$

and thus

$$\mathcal{C}_\ell(y,\beta) = \sum_{k=0}^{\ell}\frac{1}{k!}\mathcal{C}_{\ell-k}(\lceil y\rceil,\beta)\,(y-\lceil y\rceil)^k + \frac{1}{(\ell+1)!}s_\beta(\xi)\,(y-\lceil y\rceil)^{\ell+1},$$

with $\xi\in(y,\lceil y\rceil)$. By (1.51), the absolute value is bounded as follows

$$\begin{aligned}&|\mathcal{C}_\ell(y,\beta)|\\ &\le c_s(\lceil y\rceil^{\alpha}+\lceil y\rceil^{-1})\sum_{k=0}^{\ell}\frac{1}{k!}(\ell_\alpha+1+\ell-k)^{\ell_\alpha+1}\,\tau^{-(\ell-k)} + \frac{c_s\max(y^\alpha,\lceil y\rceil^\alpha)}{(\ell+1)!}.\end{aligned}$$

The sum yields

$$\begin{aligned}&\sum_{k=0}^{\ell}\frac{1}{k!}(\ell_\alpha+1+\ell-k)^{\ell_\alpha+1}\,\tau^{-(\ell-k)}\\ &\le(\ell_\alpha+1+\ell)^{\ell_\alpha+1}\tau^{-\ell}\sum_{k=0}^{\ell}\frac{1}{k!}\tau^k\\ &\le(\ell_\alpha+1+\ell)^{\ell_\alpha+1}\tau^{-\ell}e^{\tau}.\end{aligned}$$

In total, we find the uniform bound in $\beta\ge0$,

$$\left|\mathcal{C}_\ell(y,\beta)\right| \le c_s\left((\ell_\alpha+1+\ell)^{\ell_\alpha+1}\,\tau^{-\ell}\left(\lceil y\rceil^{\alpha}+\lceil y\rceil^{-1}\right)+\frac{\max(y^\alpha,\lceil y\rceil^\alpha)}{(\ell+1)!}\right),$$

concluding the proof.

□

6. Conclusions

The SEM expansion allows us to efficiently compute macroscopically large sums, even if the summand function includes a singularity. It solves the convergence problems of the standard EM expansion and makes it applicable to functions that are highly relevant in practice. The approximation error is found to decrease polynomially in the width of the function and exponentially in the expansion order, if the summand function is of sufficiently small exponential type. This opens the door to realistic numerical simulations of one-dimensional condensed matter systems.

Our new method so far is restricted to one dimension. In the next chapters, we generalise the Euler–Maclaurin expansion and subsequently its singular extension to lattices in higher dimensions.

CHAPTER 2

Multidimensional Euler–Maclaurin expansion

1. Introduction

In the previous chapter, we have introduced the singular Euler–Maclaurin (SEM) expansion, thereby extending the classical Euler–Maclaurin (EM) summation formula to physically relevant functions that may include singularities. However, both the EM and SEM expansion are only applicable to sums in one dimension, whereas many realistic applications, for instance in condensed matter, usually appear as higher-dimensional problems. It is therefore our goal to extend the SEM expansion to lattices in spaces of arbitrary dimension.

When approaching the generalisation of the SEM expansion to higher dimensions, one does encounter the problem that one needs to quantify differences between high-dimensional sums and related integrals. In the previous chapter, we have used to the classical EM expansion in order to define and estimate such differences, proving the SEM by using the EM expansion. Similar to that, we need a generalisation of the EM expansion to higher dimensions in order to prove a higher dimensional analogue of the SEM. In this chapter, we generalise the EM expansion to lattices in spaces of arbitrary dimension. While useful both for analytical and numerical purposes on its own right, this generalised EM expansion is then used in the next chapter as a stepping stone for proving the SEM expansion in higher dimensions.

There exist previous attempts for generalising the EM expansion to higher dimensions. The approach most often found in practice is based on a tensorisation of the one-dimensional expansion using so called Todd operators. Tensorised expansions have the benefit of being simple, yet they are restrictive in the set of geometries and functions that they can be applied to. A tensorised multidimensional EM expansion for simple lattice polytopes has been presented by Karhson [34]. There exist only few attempts at generalising the EM expansion to higher dimensions that do not rely on a repeated application of the one-dimensional summation formula. Among the most notable examples is the work by Müller [41] that offers a generalisation of the expansion to two dimensions. In

This chapter is based on [7, Sections 1–3].

[23], Freeden provides an abstract extension of the result by Müller to higher dimensions, yet without giving error estimates. All of above attempts offer different advantages and disadvantages. The works that are based on tensorisation are easy to use in practice, yet have to be constructed for particular geometries. The works that aim at a more general extension of the traditional expansion, while being applicable to more general geometries and function sets, on the other hand are theoretical and do not consider error estimates, convergence properties, and, in general, applicability in numerical practice.

In this chapter, we set out to derive a natural generalisation of the EM expansion to multidimensional lattice sums, while avoiding a tensorisation of the traditional expansion. We cast the difference between a lattice sum and a related integral in terms of surface integrals over derivatives of the summand function. The coefficients of the associated differential operator are formed by a generalisation of the periodised Bernoulli functions from Section 1.1 to higher dimensions. We derive their properties, formulate the EM expansion on multidimensional lattices and provide sharp error estimates for the remainder.

This chapter is structured as follows. In Section 2, we introduce necessary notation and provide a condensed overview on distribution theory and regularity theory of elliptic partial differential operators. The multidimensional EM expansion is then derived and presented in Section 3.

2. Preliminaries

The following overview on distribution theory and elliptic regularity is based on Hörmander [31, 32]. For explicit expressions for many distributions and an extensive introduction to the Fourier transform, see the reference work by Gel'fand [25]. An accessible introduction to elliptic regularity can furthermore be found in the book by Trèves [49].

2.1. Distributions. We first review some basic notation. Let in the following $\Omega \subseteq \mathbb{R}^d$ be open and $k \in \mathbb{N}_0$ or $k = \infty$. We denote by $C^k(\Omega)$ the set of k-times continuously differentiable functions $f : \Omega \to \mathbb{C}$. We now briefly review convergence of sequences of functions in the space $C^k(\Omega)$. We say that a sequence $(u_n)_{n\in\mathbb{N}}$ converges to $u \in C^k(\Omega)$ in $C^k(\Omega)$ if all derivatives of order smaller or equal k converge compactly on Ω. This means that for every $K \subset \Omega$ compact and $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ with $|\boldsymbol{\alpha}| \le k$, we have

$$\lim_{n\to\infty} \sup_{\boldsymbol{x}\in K} \left| D^{\boldsymbol{\alpha}} u_n(\boldsymbol{x}) - D^{\boldsymbol{\alpha}} u(\boldsymbol{x}) \right| = 0.$$

The set $C_0^k(\Omega)$ describes the subset of functions $u \in C^k(\Omega)$ whose support

$$\operatorname{supp} u = \overline{\{\boldsymbol{x} \in \Omega : u(\boldsymbol{x}) \neq 0\}}$$

is included in a compact subset of Ω.

The space of test functions $\mathscr{D}(\Omega) = C_0^\infty(\Omega)$, consisting of smooth, compactly supported functions, serves as a basic object of study in distribution theory[1]. Its dual space consists of linear continuous functionals acting on test functions. It is called the space of distributions on Ω, which we denote by $\mathscr{D}'(\Omega)$. As a typical example, we now introduce the Dirac delta distribution $\delta_{\boldsymbol{x}_0}$ at $\boldsymbol{x}_0 \in \Omega$ that maps a test function to its value at $\boldsymbol{x}_0$,

$$\langle \delta_{\boldsymbol{x}_0}, \psi \rangle = \psi(\boldsymbol{x}_0), \quad \psi \in \mathscr{D}(\Omega).$$

We move on to a discussion of p-integrable functions. For $p \in [1, \infty]$, we define $L^p(\Omega)$ as the space of all measurable functions $v : \Omega \to \mathbb{C}$ with finite p-norm,

$$\|v\|_{p,\Omega}^p = \int_\Omega |v(\boldsymbol{x})|^p \, \mathrm{d}\boldsymbol{x} < \infty,$$

in case that $p < \infty$ and

$$\|v\|_{\infty,\Omega} = \operatorname*{ess\,sup}_{\boldsymbol{x} \in \Omega} |v(\boldsymbol{x})| < \infty,$$

for $p = \infty$. The space of locally p-integrable functions $L^p_{\mathrm{loc}}(\Omega)$ is given by

$$L^p_{\mathrm{loc}}(\Omega) = \{v : \Omega \to \mathbb{C} \text{ measurable }, v|_K \in L^p(K) \; \forall K \subset \Omega \text{ compact}\}.$$

Any function $v \in L^1_{\mathrm{loc}}(\Omega)$ induces a distribution by means of

$$\langle v, \cdot \rangle : \mathscr{D}(\Omega) \to \mathbb{C}, \; \langle v, \psi \rangle = \int_\Omega v(\boldsymbol{x}) \psi(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}.$$

In the following, we will in particular consider the homogeneous function $s_\nu : \mathbb{R}^d \setminus \{\mathbf{0}\} \to \mathbb{C}$,

$$s_\nu(\boldsymbol{x}) = \frac{1}{|\boldsymbol{x}|^\nu}, \tag{2.1}$$

with $\nu \in \mathbb{C}$. It is clear that s_ν can be understood as a distribution on $\mathbb{R}^d \setminus \{\mathbf{0}\}$. This distribution can subsequently be extended to $\mathbb{R}^d$ by means of the following theorem, which is a special case of [31, Theorems 3.2.3 and 3.2.4].

[1] This space is equipped with a stronger topology than the one inherited from $C^\infty(\Omega)$.

THEOREM 2.1. *The function s_ν, $\nu \in \mathbb{C}$, can be extended to a distribution on $\mathbb{R}^d$. In case that $\nu \neq d+2k$, $k \in \mathbb{N}_0$, this extension is unique. Otherwise, for $\nu = d+2k$, there exist infinitely many extensions where two of them differ by a linear combination of derivatives of order k of $\delta_{\mathbf{0}}$.*

We now discuss the convolution of a distribution $u \in \mathscr{D}'(\mathbb{R}^d)$ with a smooth function φ under the assumption that one of the two has compact support. The convolution reads $u * \varphi \in C^\infty(\mathbb{R}^d)$ and is defined via

$$(u * \varphi)(\boldsymbol{x}) = \big\langle u, \varphi(\boldsymbol{x} - \boldsymbol{\cdot})\big\rangle, \quad \boldsymbol{x} \in \mathbb{R}^d.$$

We move on to a discussion of the Fourier transform. For a function $v \in L^1(\mathbb{R}^d)$, we define its Fourier transform $\hat{v} = \mathcal{F}v$ as

$$\hat{v}(\boldsymbol{\xi}) = \mathcal{F}v(\boldsymbol{\xi}) = \int_{\mathbb{R}^d} e^{-2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}, \quad \boldsymbol{\xi} \in \mathbb{R}^d.$$

We then review the Schwartz space $S(\mathbb{R}^d)$ of rapidly decaying smooth functions,

$$S(\mathbb{R}^d) = \Big\{ u \in C^\infty(\mathbb{R}^d) : \sup_{\boldsymbol{x} \in \mathbb{R}^d} |\boldsymbol{x}^{\boldsymbol{\beta}} D^{\boldsymbol{\alpha}} u(\boldsymbol{x})| < \infty \ \forall \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^d \Big\}.$$

The Fourier transform of a Schwartz function is again a Schwartz function. Hence, $\mathcal{F}$ defines an isomorphism on $S(\mathbb{R}^d)$. The definition of the Fourier transform $\mathcal{F}$ extends by duality to its dual space $S'(\mathbb{R}^d)$. Elements of $S'(\mathbb{R}^d)$ are called tempered distributions. We now discuss the Fourier transform of the homogeneous distribution s_ν in (2.1). A proof of the following theorem can be found in [25, Chapter 3.3].

THEOREM 2.2. *Let $\nu \in \mathbb{C}$. Any extension of s_ν to a distribution on $\mathbb{R}^d$ is a tempered distribution. Its Fourier transform can be identified as a C^∞-function on $\mathbb{R}^d \setminus \{\mathbf{0}\}$. For $\nu \neq (d+2k)$, $k \in \mathbb{N}_0$, the Fourier transform takes the explicit form*

$$\hat{s}_\nu(\boldsymbol{\xi}) = \pi^{\nu - \frac{d}{2}} \frac{\Gamma\left(\frac{d-\nu}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} |\boldsymbol{\xi}|^{-d+\nu}, \quad \boldsymbol{\xi} \in \mathbb{R}^d \setminus \{\mathbf{0}\},$$

where Γ denotes the Gamma function.

2.2. Elliptic regularity. Let $P : \mathbb{R}^d \to \mathbb{C}$ be a polynomial of degree $m \in \mathbb{N}_0$ with

$$P(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d} a_{\boldsymbol{\alpha}} \boldsymbol{\xi}^{\boldsymbol{\alpha}}, \quad \boldsymbol{\xi} \in \mathbb{R}^d, \quad |\boldsymbol{\alpha}| \leq m.$$

We call the polynomial elliptic if

$$P_m(\boldsymbol{\xi}) = \sum_{|\boldsymbol{\alpha}|=m} a_{\boldsymbol{\alpha}} \boldsymbol{\xi}^{\boldsymbol{\alpha}}, \quad \boldsymbol{\xi} \in \mathbb{R}^d,$$

vanishes only for $\boldsymbol{\xi} = 0$. A differential operator with constant coefficients is called elliptic if its associated polynomial is elliptic.

We now summarise results on the regularity of elliptic differential operators with constant coefficients. The following theorem is a standard result, see e.g. [32, Theorem 11.1.10].

Theorem 2.3. *An elliptic differential operator $\mathcal{L}$ with constant coefficients is hypoelliptic. This means that $\mathcal{L}u \in C^\infty(\Omega)$ for $u \in \mathscr{D}'(\Omega)$ already implies that $u \in C^\infty(\Omega)$.*

We can replace smoothness by analyticity in Theorem 2.3, see for instance [32, Corollary 11.4.13].

Theorem 2.4. *An elliptic differential operator $\mathcal{L}$ with constant coefficients is analytic-hypoelliptic, which means that if $\mathcal{L}u$ is analytic on Ω for $u \in \mathscr{D}'(\Omega)$, then u is already an analytic function on Ω.*

The following theorem constitutes a generalisation of the result in [31, Theorem 4.4.2].

Theorem 2.5. *Let $(u_j)_{j\in\mathbb{N}}$ be a sequence in $\mathscr{D}'(\Omega)$ that converges to $u \in \mathscr{D}'(\Omega)$,*

$$\lim_{j\to\infty} \langle u_j, \psi\rangle = \langle u, \psi\rangle, \quad \psi \in \mathscr{D}(\Omega).$$

Furthermore, let $\mathcal{L}$ be an elliptic differential operator with constant coefficients. If we have $\mathcal{L}u_j \in C^\infty(\Omega)$ for all $j \in \mathbb{N}$ and if the sequence $(\mathcal{L}u_j)_{j\in\mathbb{N}}$ converges in $C^\infty(\Omega)$ to $v \in C^\infty(\Omega)$, then $(u_j)_{j\in\mathbb{N}}$ and u are C^∞-functions and $(u_j)_{j\in\mathbb{N}}$ converges to u in $C^\infty(\Omega)$, that is compactly on Ω in all derivatives.

Proof. As $\mathcal{L}u_j \in C^\infty(\Omega)$ for all $j \in \mathbb{N}$ and as

$$\mathcal{L}u = \lim_{j\to\infty} \mathcal{L}u_j = v \text{ in } \mathscr{D}'(\Omega),$$

we find from Theorem 2.3 that already $u_j \in C^\infty(\Omega)$ and $u \in C^\infty(\Omega)$. In the following, we show that

$$\lim_{j\to\infty} u_j = u \text{ in } C^\infty(\Omega).$$

First choose an open neighbourhood $Y \subseteq \Omega$ of the compact set K such that there exists $\chi \in \mathscr{D}(\Omega)$ with $\chi = 1$ on Y. As $\mathcal{L}$ is an elliptic operator with constant coefficients, there exists a fundamental solution $E \in \mathscr{D}'(\Omega)$ by [31, Theorem 7.3.10]. After setting $f_j = \mathcal{L}u_j$ and $f = \mathcal{L}u$, we obtain

$$u_j - u = \big(u_j - E * (\chi f_j)\big) - \big(u - E * (\chi f)\big) + E * \big(\chi \cdot (f_j - f)\big).$$

We find on Y that

$$\mathcal{L}\big(u_j - E * (\chi f_j)\big) = f_j - \chi f_j = 0.$$

Due to continuity of the convolution [48, Theorem 27.3]

$$E * \cdot : \mathscr{D}(\Omega) \to C^\infty(\Omega),$$

we have that

$$\lim_{j\to\infty} \big(u_j - E * (\chi f_j)\big) = u - E * (\chi f) \text{ in } \mathscr{D}'(Y).$$

Now by [31, Theorem 4.4.2], the above limit also holds in $C^\infty(Y)$. As the convolution is continuous, we hence find that

$$\lim_{j\to\infty} E * \big(\chi \cdot (f_j - f)\big) = 0 \text{ in } C^\infty(Y).$$

Thus, for all $\boldsymbol{\alpha} \in \mathbb{N}_0^d$,

$$D^{\boldsymbol{\alpha}}(u_j - u) = D^{\boldsymbol{\alpha}}\big(u_j - E*(\chi f_j)\big) - D^{\boldsymbol{\alpha}}\big(u - E*(\chi f)\big) + E * D^{\boldsymbol{\alpha}}\big(\chi\cdot(f_j - f)\big) \to 0$$

uniformly on K for $j \to \infty$.

□

2.3. Band-limited functions.

Definition 2.6 (Band-limited function). Let $f : \mathbb{R}^d \to \mathbb{C}$. Then f is called band-limited with bandwidth $\sigma > 0$ if it is the Fourier transform of a function $h \in C_0\big(B_\sigma\big)$,

$$f = \hat{h} = \mathcal{F}h.$$

Here, B_σ denotes the Euclidean ball of radius $\sigma > 0$. We denote the vector space of all band-limited functions with bandwidth σ by E_σ.

We need the next lemma in the derivation of error estimates for the EM expansion in higher dimensions.

Lemma 2.7. *Let $f \in E_\sigma$ with $\sigma > 0$ and $f = \hat{h}$ and let $\Omega \subset \mathbb{R}^d$ be open and bounded. Then*

$$\|\Delta^\ell f\|_{1,\Omega} \le (2\pi\sigma)^{2\ell} \mathrm{vol}(\Omega) \|f\|_1,$$

where Δ denotes the d-dimensional Laplace operator and where $\mathrm{vol}(\Omega)$ *is the Lebesgue measure of Ω.*

Proof. As $\Delta^\ell f$ is continuous and hence bounded on the compact set $\bar{\Omega}$, we have

$$\|\Delta^\ell f\|_{1,\Omega} \le \mathrm{vol}(\Omega) \|\Delta^\ell f\|_\infty.$$

A straightforward application of the calculation rules of the Fourier transform yields

$$\Delta^\ell f = \mathcal{F}\Big(|2\pi\,\boldsymbol{\cdot}\,|^{2\ell} h\Big),$$

and thus by the standard integral estimate

$$\|\Delta^\ell f\|_\infty \leq \Big\||2\pi\,\boldsymbol{\cdot}\,|^{2\ell} h\Big\|_1.$$

From $\operatorname{supp} h \subseteq \bar{B}_\sigma$ then follows

$$\Big\|\,|2\pi\,\boldsymbol{\cdot}\,|^{2\ell} h\,\Big\|_1 = \Big\|\,|2\pi\,\boldsymbol{\cdot}\,|^{2\ell} h\,\Big\|_{1,\bar{B}_\sigma} \leq (2\pi\sigma)^{2\ell}\|h\|_1.$$

□

3. Derivation

We now set out to derive the EM expansion on lattices in $d \in \mathbb{N}$ dimensions and start by introducing necessary definitions and notations. First, we review the concept of multidimensional lattices.

Definition 2.8 (Lattices and related properties). We call $\Lambda \subseteq \mathbb{R}^d$ a lattice if there exists $M_\Lambda \in \mathbb{R}^{d\times d}$ with $\det(M_\Lambda) \neq 0$ such that

$$\Lambda = M_\Lambda \mathbb{Z}^d.$$

The set of all lattices in $\mathbb{R}^d$ is denoted by $\mathfrak{L}(\mathbb{R}^d)$. We furthermore define the elementary lattice cell E_Λ as

$$E_\Lambda = M_\Lambda [0,1]^d,$$

whose volume is called the covolume V_Λ of the lattice,

$$V_\Lambda = \operatorname{vol}(E_\Lambda) = \big|\det(M_\Lambda)\big|.$$

We set $a_\Lambda > 0$ as the smallest distance between non-equal lattice points,

$$a_\Lambda = \min_{\boldsymbol{x}\in\Lambda\setminus\{\boldsymbol{0}\}} |\boldsymbol{x}|.$$

The dual, or reciprocal, lattice Λ^* is defined as

$$\Lambda^* = M_{\Lambda^*}\mathbb{Z}^d,$$

where

$$M_{\Lambda^*} = M_\Lambda^{-\top},$$

with $M_\Lambda^{-\top} = \left(M_\Lambda^{-1}\right)^\top$. Then

$$\langle \boldsymbol{y}, \boldsymbol{x}\rangle \in \mathbb{Z} \quad \forall \boldsymbol{x} \in \Lambda,\, \boldsymbol{y} \in \Lambda^*.$$

Finally, $n_\Lambda \in \mathbb{N}$ is the number of elements of Λ with norm a_Λ.

We now review the Poisson summation formula that relates sums on a lattice Λ to sums on the reciprocal lattice Λ^*.

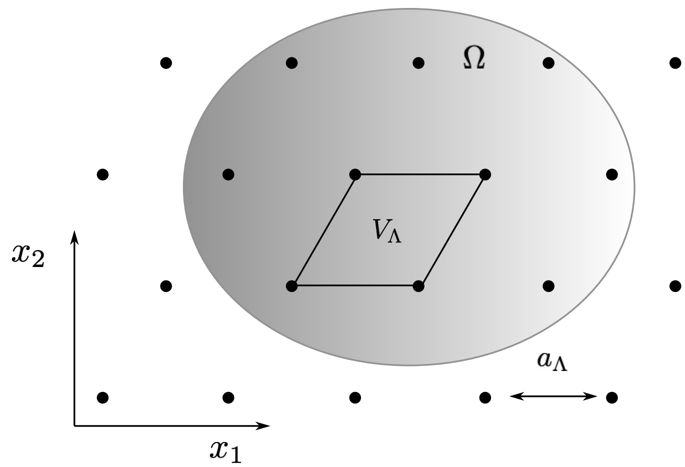

FIGURE 1. Lattice for $d = 2$. The shaded area shows a domain Ω for which $\partial\Omega \cap \Lambda = \varnothing$.

LEMMA 2.9 (Poisson summation formula). *Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and let $f \in L^1(\mathbb{R}^d)$. If there exist $C, \varepsilon > 0$ such that*

$$\big|f(\boldsymbol{z})\big| + \big|\hat{f}(\boldsymbol{z})\big| \le C\big(1 + |\boldsymbol{z}|\big)^{-(d+\varepsilon)}, \quad \boldsymbol{z} \in \mathbb{R}^d,$$

then

$$V_\Lambda \sum_{\boldsymbol{z}\in\Lambda} f(\boldsymbol{z}) e^{-2\pi i \langle \boldsymbol{z}, \boldsymbol{y}\rangle} = \sum_{\boldsymbol{z}\in\Lambda^*} \hat{f}(\boldsymbol{z} + \boldsymbol{y}), \qquad \boldsymbol{y} \in \mathbb{R}^d.$$

PROOF. The identity is a well known result in case that $\Lambda = \mathbb{Z}^d$, see [47, Chapter VII, Corollary 2.6] or [31, Section 7.2]. It is readily generalised to a lattice Λ by observing that for $f \in L^1(\mathbb{R}^d)$,

$$\mathcal{F}\big(f(M_\Lambda \,\cdot)\big) = \frac{1}{|\det M_\Lambda|} \hat{f}(M_\Lambda^{-\top} \,\cdot) = \frac{1}{V_\Lambda} \hat{f}(M_{\Lambda^*} \,\cdot).$$

□

The EM expansion is going to rely on surface integrals of derivatives of the summand function over the boundary of a domain Ω. We now specify the term domain.

NOTATION 2.10 (Domain). From now on, a domain $\Omega \subseteq \mathbb{R}^d$ shall denote a non-empty and connected open set with Lipschitz boundary $\partial\Omega$.

In Fig. 1, a hexagonal lattice (black dots) is displayed. The grey area shows a domain whose boundary does not intersect any lattice point.

In the next step, we introduce a new mathematical operator

$$\sum\!\!\!\!\!\!\int$$

that quantifies the difference between lattice sums and related integrals.

Notation 2.11 (Sum-integral). Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\Omega \subseteq \mathbb{R}^d$ measurable. For $f \in L^1(\Omega)$ summable on $\Omega \cap \Lambda$, we denote the difference between the sum of f over all lattice points in Ω and the integral of f over Ω per lattice covolume as

$$\mathop{\sum\!\!\!\!\!\!\int}_{\Omega,\Lambda} f = \sum_{\boldsymbol{y}\in\Omega\cap\Lambda} f(\boldsymbol{y}) - \frac{1}{V_\Lambda} \int_\Omega f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

In case that the sum-integral is applied to longer expressions, we explicitly state the variable with respect to which summation and integration are executed,

$$\mathop{\sum\!\!\!\!\!\!\int}_{\boldsymbol{y}\in\Omega,\Lambda} f(\boldsymbol{y}) = \mathop{\sum\!\!\!\!\!\!\int}_{\Omega,\Lambda} f.$$

For sufficiently regular functions f and regions Ω, we want to find a representation of the difference between lattice sum and integral, i.e.

$$\mathop{\sum\!\!\!\!\!\!\int}_{\Omega,\Lambda} f$$

in terms of a surface integral over derivatives of f and a remainder integral. In order to arrive at this goal, we define a generalisation of the periodised Bernoulli functions to higher dimensional lattices. As the sums that will appear in their definition do not converge a priori, we have to include a regularisation factor, which we call smooth cutoff that forces convergence.

Definition 2.12 (Mollifiers and smooth cutoff functions). Choose $\chi \in \mathscr{D}(B_1)$ rotationally invariant with $\chi \geq 0$ that integrates to 1 over $\mathbb{R}^d$. For $\beta > 0$, set

$$\chi_\beta = \beta^{-d}\chi(\,\cdot\,/\beta)$$

with $\operatorname{supp}\chi_\beta \subseteq \bar{B}_\beta$. We call χ_β a mollifier and its Fourier transform $\hat{\chi}_\beta$ a smooth cutoff function.

The following lemma is a standard result that quantifies the convergence of convolutions with a mollifier.

Lemma 2.13. *Let $\Omega \subseteq \mathbb{R}^d$ open and $u \in C^k(\Omega)$, $k \in \mathbb{N}_0 \cup \{\infty\}$. The convolution of u with the mollifier χ_β results in the smooth function*

$u_\beta : \Omega_\beta \to \mathbb{C}$,

$$u_\beta(\boldsymbol{x}) = \chi_\beta * u(\boldsymbol{x}) = \int_{B_1} \chi(\boldsymbol{y}) u(\boldsymbol{x} - \beta \boldsymbol{y})\, d\boldsymbol{y},$$

with $\Omega_\beta = \{\boldsymbol{x} \in \Omega : \operatorname{dist}(\boldsymbol{x}, \partial\Omega) > \beta\}$. *Then for every* $\beta_0 > 0$ *we have that* $u_\beta \to u$ *as* $\beta \to 0$ *in* $C^k(\Omega_{\beta_0})$.

The subsequent lemma shows that the limit of smooth cutoff functions in β is compact in all derivatives.

LEMMA 2.14. *Let* $\hat{\chi}_\beta$, $\beta > 0$, *be a family of smooth cutoff functions. Then*

$$\hat{\chi}_\beta \to \hat{\chi}_\beta(\mathbf{0}) = 1,\ \ \beta \to 0,\ \text{ in } C^\infty(\mathbb{R}^d).$$

PROOF. First take $R > 0$ such that $\operatorname{supp} \chi \subseteq B_R$. For any compact set $K \subset \mathbb{R}^d$ and $\boldsymbol{\xi} \in K$, we find

$$\begin{aligned}\hat{\chi}_\beta(\boldsymbol{\xi}) - 1 &= \int_{B_{\beta R}} \chi_\beta(\boldsymbol{x}) \Big(e^{-2\pi i \langle \boldsymbol{x}, \boldsymbol{\xi} \rangle} - 1 \Big)\, \mathrm{d}\boldsymbol{x} \\ &= \int_{B_R} \chi(\boldsymbol{x}) \int_0^\beta (-2\pi i t \langle \boldsymbol{x}, \boldsymbol{\xi} \rangle) e^{-2\pi i t \langle \boldsymbol{x}, \boldsymbol{\xi} \rangle}\, \mathrm{d}t\, \mathrm{d}\boldsymbol{x}\end{aligned}$$

due to

$$\chi_\beta = \beta^{-d} \chi(\cdot/\beta).$$

Now as $\chi \geq 0$ and $\hat{\chi}(0) = 1$, we obtain

$$\begin{aligned}|\hat{\chi}_\beta(\boldsymbol{\xi}) - 1| &\leq \int_{B_R} \chi(\boldsymbol{x}) \int_0^\beta \Big| 2\pi i t \langle \boldsymbol{x}, \boldsymbol{\xi} \rangle \Big|\, \mathrm{d}t\, \mathrm{d}\boldsymbol{x} \\ &\leq 2\pi\beta |\boldsymbol{\xi}| R \to 0, \quad \beta \to 0,\end{aligned}$$

uniformly on K. For $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ with $|\boldsymbol{\alpha}| \geq 1$ and $\boldsymbol{\xi} \in \mathbb{R}^d$, it holds that

$$\begin{aligned}|D^{\boldsymbol{\alpha}} \hat{\chi}_\beta(\boldsymbol{\xi})| &= \left| \int_{B_R} \chi(\boldsymbol{x}) (-2\pi i \beta \boldsymbol{x})^{\boldsymbol{\alpha}} e^{-2\pi i \beta \langle \boldsymbol{x}, \boldsymbol{\xi} \rangle}\, \mathrm{d}\boldsymbol{x} \right| \\ &\leq (2\pi\beta R)^{|\boldsymbol{\alpha}|} \to 0, \quad \beta \to 0,\end{aligned}$$

uniformly on $\mathbb{R}^d$.

□

LEMMA 2.15. *Let* $\hat{\chi}_\beta$, $\beta \in (0,1)$, *be a family of smooth cutoff functions. For all* $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ *there exists a constant* $C > 0$ *with*

$$\sup_{\beta \in (0,1)} \Big| D^{\boldsymbol{\alpha}} \hat{\chi}_\beta(\boldsymbol{\xi}) \Big| \leq C \Big(1 + |\boldsymbol{\xi}| \Big)^{-|\boldsymbol{\alpha}|}, \quad \boldsymbol{\xi} \in \mathbb{R}^d.$$

PROOF. Remembering that $\chi_\beta = \beta^{-d}\chi(\,\cdot\,/\beta)$, we have

$$D^{\boldsymbol{\alpha}}\hat{\chi}_\beta(\boldsymbol{\xi}) = \mathcal{F}\Big((-2\pi i\,\cdot\,)^{\boldsymbol{\alpha}}\chi_\beta\Big)(\boldsymbol{\xi}) = \beta^{|\boldsymbol{\alpha}|}\mathcal{F}\Big((-2\pi i\,\cdot\,)^{\boldsymbol{\alpha}}\chi\Big)(\beta\boldsymbol{\xi}), \quad \boldsymbol{\xi}\in\mathbb{R}^d.$$

After setting $h_{\boldsymbol{\alpha}}(\boldsymbol{x}) = (-2\pi i\boldsymbol{x})^{\boldsymbol{\alpha}}\chi(\boldsymbol{x})$, $\boldsymbol{x}\in\mathbb{R}^d$, we obtain for $\boldsymbol{\gamma}\in\mathbb{N}_0^d$ and $\boldsymbol{\xi}\in\mathbb{R}^d$

$$(2\pi i\beta\boldsymbol{\xi})^{\boldsymbol{\gamma}} D^{\boldsymbol{\alpha}}\hat{\chi}_\beta(\boldsymbol{\xi}) = \beta^{|\boldsymbol{\alpha}|}\mathcal{F}\big(D^{\boldsymbol{\gamma}} h_{\boldsymbol{\alpha}}\big)(\beta\boldsymbol{\xi}).$$

As $\beta\in(0,1)$, it follows that

$$\big|\boldsymbol{\xi}^{\boldsymbol{\gamma}}\big|\cdot\big|D^{\boldsymbol{\alpha}}\hat{\chi}_\beta(\boldsymbol{\xi})\big| \le |2\pi|^{-|\boldsymbol{\gamma}|}\cdot\big\|D^{\boldsymbol{\gamma}} h_{\boldsymbol{\alpha}}\big\|_1,$$

where the right hand side does not depend on $\boldsymbol{\xi}$ and β. The desired estimate is found from

$$\big(1+|\boldsymbol{\xi}|\big)^{|\boldsymbol{\alpha}|}\big|D^{\boldsymbol{\alpha}}\hat{\chi}_\beta(\boldsymbol{\xi})\big| \le \left(1+\sum_{k=1}^{d}|\xi_k|\right)^{|\boldsymbol{\alpha}|}\big|D^{\boldsymbol{\alpha}}\hat{\chi}_\beta(\boldsymbol{\xi})\big|, \quad \boldsymbol{\xi}\in\mathbb{R}^d,$$

as, after expanding the polynomial on the right hand side by the binomial theorem, the above consideration yields a uniform bound in $\boldsymbol{\xi}$ and β.

□

Equipped with the concept of smooth cutoff functions, we are now in the position to define lattice sums over the function $s_\nu = |\cdot|^{-\nu}$ in (2.1). The behaviour of these sums is subsequently analysed in the limit $\beta\to 0$, removing the regularisation. With this technique, we now present the fundamental theorem of this chapter, from which the multidimensional Bernoulli functions and the multidimensional EM expansion are derived.

THEOREM 2.16. *Let $\Lambda\in\mathfrak{L}(\mathbb{R}^d)$ and $\nu\in\mathbb{C}$. We set $\mathcal{Z}_{\Lambda,\nu}:\mathbb{R}^d\setminus\Lambda\to\mathbb{C}$,*

$$\mathcal{Z}_{\Lambda,\nu}(\boldsymbol{y}) = V_{\Lambda^*}\lim_{\beta\to 0}\sum_{\boldsymbol{z}\in\Lambda^*}{}' \hat{\chi}_\beta(\boldsymbol{z})\frac{e^{-2\pi i\langle\boldsymbol{z},\boldsymbol{y}\rangle}}{|\boldsymbol{z}|^\nu},$$

where the primed sum excludes $\boldsymbol{z}=0$. The function $\mathcal{Z}_{\Lambda,\nu}$ is well-defined, i.e. the limit exists for all $\boldsymbol{y}\in\mathbb{R}^d\setminus\Lambda$, and is independent of the chosen regularisation. The function $\mathcal{Z}_{\Lambda,\nu}$ can be extended to a tempered distribution on $\mathbb{R}^d$ by virtue of

$$\langle\mathcal{Z}_{\Lambda,\nu},\psi\rangle = V_{\Lambda^*}\sum_{\boldsymbol{z}\in\Lambda^*}{}'\frac{\hat{\psi}(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}, \quad \psi\in S(\mathbb{R}^d).$$

Furthermore, the function $\mathcal{Z}_{\Lambda,\nu}$ is analytic and the limit $\beta\to 0$ is compact in all derivatives.

In order to prove above theorem, we need two lemmas.

LEMMA 2.17. *$\mathcal{Z}_{\Lambda,\nu}$ as in Theorem 2.16 defines a tempered distribution.*

PROOF. We first choose $\beta > 0$ and define the auxiliary function

$$\mathcal{Z}_{\Lambda,\nu,\beta} : \mathbb{R}^d \to \mathbb{C},\ \mathcal{Z}_{\Lambda,\nu,\beta}(\boldsymbol{y}) = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \hat{\chi}_\beta(\boldsymbol{z}) \frac{e^{-2\pi i \langle \boldsymbol{z},\boldsymbol{y}\rangle}}{|\boldsymbol{z}|^\nu}.$$

Above Dirichlet series is well-defined due to the superpolynomial decay of the Schwartz function $\hat{\chi}_\beta$. As $\mathcal{Z}_{\Lambda,\nu,\beta}$ is bounded, it defines a tempered distribution via

$$\langle \mathcal{Z}_{\Lambda,\nu,\beta}, \psi \rangle = \int_{\mathbb{R}^d} \mathcal{Z}_{\Lambda,\nu,\beta}(\boldsymbol{y})\, \psi(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y} = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \hat{\chi}_\beta(\boldsymbol{z}) \frac{\hat{\psi}(\boldsymbol{z})}{|\boldsymbol{z}|^\nu},$$

for $\psi \in S(\mathbb{R}^d)$. Now due to $|\hat{\chi}_\beta| \le 1$ and $\hat{\chi}_\beta \to 1$ as $\beta \to 0$, the dominated convergence theorem yields

$$\lim_{\beta\to 0} \langle \mathcal{Z}_{\Lambda,\nu,\beta}, \psi \rangle = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \frac{\hat{\psi}(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} = \langle \mathcal{Z}_{\Lambda,\nu}, \psi \rangle,$$

establishing that also $\mathcal{Z}_{\Lambda,\nu}$ is a tempered distribution.

□

In the next lemma, we discuss the convergence of Dirichlet series that arise in the proof of Theorem 2.16 after applying the Poisson summation formula to the auxiliary functions.

LEMMA 2.18. *Let $\Lambda \in \mathcal{L}(\mathbb{R}^d)$ and $\nu \in \mathbb{C}$ with $\mathrm{Re}(\nu) > d$. For a family of mollifiers χ_β, $\beta > 0$, the functions $h_\beta : \mathbb{R}^d \setminus \Lambda_\beta \to \mathbb{C}$,*

$$h_\beta(\boldsymbol{y}) = \sum_{\boldsymbol{z}\in\Lambda} \chi_\beta * s_\nu(\boldsymbol{z} + \boldsymbol{y}),$$

with $\Lambda_\beta = \Lambda + \bar{B}_\beta$, belong to $C^\infty(\mathbb{R}^d \setminus \Lambda_\beta)$ and converge to $h : \mathbb{R}^d \setminus \Lambda \to \mathbb{C}$,

$$h(\boldsymbol{y}) = \sum_{\boldsymbol{z}\in\Lambda} |\boldsymbol{z} + \boldsymbol{y}|^{-\nu}.$$

in $C^\infty(\mathbb{R}^d \setminus \Lambda_{\beta_0})$ as $\beta \to 0$ for any $\beta_0 > 0$. All statements remain true if Λ is replaced by a subset Λ' of the lattice.

PROOF. We begin by noticing that function s_ν can be extended to holomorphic function $\tilde{s}_\nu$ on a conic[2] complex neighbourhood U of $\mathbb{R}^d \setminus \{\boldsymbol{0}\}$. Due to the restriction $\mathrm{Re}(\nu) > d$, the Dirichlet series

$$\sum_{\boldsymbol{z}\in\Lambda} \tilde{s}_\nu(\boldsymbol{z} + \boldsymbol{y})$$

converges compactly in $\boldsymbol{y}$ on $U \setminus \Lambda$. This is found from the Weierstraß M-test, where the majorant is established via

$$|\tilde{s}_\nu(\boldsymbol{z} + \boldsymbol{y})| \le |\boldsymbol{z}/2|^{-\mathrm{Re}(\nu)}$$

[2]A set $U \subseteq \mathbb{C}^d$ is conic if $U = tU$, $t > 0$.

for $\boldsymbol{z} \in \Lambda$ sufficiently large. Now h is analytic on $\mathbb{R}^d \setminus \Lambda$ as the compact limit of analytic functions. After writing h_β in the form

$$h_\beta(\boldsymbol{y}) = \chi_\beta * h(\boldsymbol{y}), \quad \boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda_\beta,$$

we find by Lemma 2.13 that $h_\beta \to h$ in $C^\infty(\mathbb{R}^d \setminus \Lambda_{\beta_0})$ as $\beta \to 0$ for all $\beta_0 > 0$. Finally, note that all above arguments remain applicable if Λ is replaced by an arbitrary subset Λ' of the lattice.

□

With above two lemmas, we show the fundamental theorem of the multidimensional EM expansion.

Proof of Theorem 2.16. We have established in Lemma 2.17 that $\mathcal{Z}_{\Lambda,\nu}$ defines a tempered distribution. Now, we show that this distribution already defines an analytic function on $\mathbb{R}^d \setminus \Lambda$. We begin with our auxiliary functions $\mathcal{Z}_{\Lambda,\nu,\beta}$, $\beta > 0$, from Lemma 2.17,

$$\mathcal{Z}_{\Lambda,\nu,\beta}(\boldsymbol{y}) = V_{\Lambda^*} \sideset{}{'}\sum_{\boldsymbol{z} \in \Lambda^*} f_\beta(\boldsymbol{z}) e^{-2\pi i \langle \boldsymbol{y}, \boldsymbol{z} \rangle}, \quad \boldsymbol{y} \in \mathbb{R}^d,$$

where $f_\beta = \hat{\chi}_\beta s_\nu$. The Dirichlet series over the dual lattice is now replaced by a sum over Λ by means of the Poisson summation formula. In consideration of this goal, we first assume that

$$\operatorname{Re}(\nu) < -(d+1).$$

Under this restriction, f_β can be extended to a function in $C^{d+1}(\mathbb{R}^d)$ where $f_\beta(\boldsymbol{0}) = 0$. Hence, we can include $\boldsymbol{z} = \boldsymbol{0}$ in above Dirichlet series. Poisson summation can now be applied as, first, f_β decays superpolynomially due to the smooth cutoff function $\hat{\chi}_\beta$, and, second, as

$$|\mathcal{F} f_\beta(\boldsymbol{z})| \le C\big(1 + |\boldsymbol{z}|\big)^{-(d+1)}, \quad \boldsymbol{z} \in \mathbb{R}^d,$$

due to $f_\beta \in C^{d+1}(\mathbb{R}^d)$. The Poisson summation formula thus yields

$$\mathcal{Z}_{\Lambda,\nu,\beta}(\boldsymbol{y}) = \sum_{\boldsymbol{z} \in \Lambda} \hat{f}_\beta(\boldsymbol{z} + \boldsymbol{y}), \quad \boldsymbol{y} \in \mathbb{R}^d.$$

For $\boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda_\beta$ with $\Lambda_\beta = \Lambda + \bar{B}_\beta$, above formula can be brought in the form that we have investigated in Lemma 2.18,

$$\mathcal{Z}_{\Lambda,\nu,\beta}(\boldsymbol{y}) = \sum_{\boldsymbol{z} \in \Lambda} \chi_\beta * \hat{s}_\nu(\boldsymbol{z} + \boldsymbol{y}) = c_{\nu,d} \sum_{\boldsymbol{z} \in \Lambda} \chi_\beta * s_{d-\nu}(\boldsymbol{z} + \boldsymbol{y}),$$

with $c_{\nu,d} \in \mathbb{C}$ as given in Theorem 2.2. The assumption on ν now yields $\operatorname{Re}(d - \nu) > d$ and by Lemma 2.18

$$\lim_{\beta \to 0} \mathcal{Z}_{\Lambda,\nu,\beta} = \mathcal{Z}_{\Lambda,\nu} \text{ in } C^\infty(\mathbb{R}^d \setminus \Lambda).$$

Here we have used that for every $K \subset \mathbb{R}^d \setminus \Lambda$ compact there exists $\beta_0 > 0$ such that $K \subset \mathbb{R}^d \setminus \Lambda_\beta$ for all $\beta < \beta_0$. In addition, the lemma shows that the function $\mathcal{Z}_{\Lambda,\nu}$ is not only smooth, but also analytic.

Finally, we employ elliptic regularity in order to extend the result to all $\nu \in \mathbb{C}$. Observe that for $\ell \in \mathbb{N}_0$,

$$\Delta^\ell \mathcal{Z}_{\Lambda,\nu,\beta} = (2\pi i)^{2\ell} \mathcal{Z}_{\Lambda,\nu-2\ell,\beta}. \tag{2.2}$$

We thus only need to choose ℓ sufficiently large such that

$$\mathrm{Re}(\nu - 2\ell) < -(d+1).$$

Our previous investigation then shows that the right hand side of (2.2) converges in $C^\infty(\mathbb{R}^d \setminus \Lambda)$ as $\beta \to 0$. By elliptic regularity in the form of Theorem 2.5, we find that $\mathcal{Z}_{\Lambda,\nu,\beta}$, which a priori only converges weakly to a distribution, also converges in $C^\infty(\mathbb{R}^d \setminus \Lambda)$ for $\beta \to 0$. Theorem 2.4 shows analyticity of $\mathcal{Z}_{\Lambda,\nu}$.

□

From the function $\mathcal{Z}_{\Lambda,\nu}$, we can construct the Bernoulli functions for multidimensional lattices.

Definition 2.19 (Bernoulli functions). Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\ell \in \mathbb{N}_0$. We define the Bernoulli functions $\mathcal{B}_\Lambda^{(\ell)} : \mathbb{R}^d \setminus \Lambda \to \mathbb{R}$ as

$$\mathcal{B}_\Lambda^{(\ell)}(\boldsymbol{y}) = \frac{\mathcal{Z}_{\Lambda,2(\ell+1)}(\boldsymbol{y})}{(2\pi i)^{2(\ell+1)}}.$$

In analogy to $\mathcal{Z}_{\Lambda,\nu}$, they define tempered distributions via

$$\langle \mathcal{B}_\Lambda^{(\ell)}, \psi \rangle = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \frac{\hat{\psi}(\boldsymbol{z})}{\big(2\pi i|\boldsymbol{z}|\big)^{2(\ell+1)}},$$

for $\psi \in S(\mathbb{R}^d)$.

Remark 2.20. From inspecting the scalar product in the exponential, we find that the functions $\mathcal{B}_\Lambda^{(\ell)}$ are Λ-periodic,

$$\mathcal{B}_\Lambda^{(\ell)}(\,\cdot\, + \boldsymbol{x}) = \mathcal{B}_\Lambda^{(\ell)}, \qquad \boldsymbol{x} \in \Lambda.$$

We emphasise the central distributional property of the Bernoulli functions, on which the multidimensional EM expansion is based.

Proposition 2.21 (Sum-integral property of $\mathcal{B}_\Lambda^{(\ell)}$). *Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\ell \in \mathbb{N}_0$. Then for $\psi \in S(\mathbb{R}^d)$,*

$$\left\langle \Delta^{\ell+1}\mathcal{B}_\Lambda^{(\ell)}, \psi \right\rangle = \left\langle \text{Ш}_\Lambda - V_\Lambda^{-1}, \psi \right\rangle = \sum\!\!\!\!\!\!\int_{\mathbb{R}^d,\Lambda} \psi,$$

where $Ш_\Lambda$ *is the Dirac comb for the lattice* Λ,

$$Ш_\Lambda = \sum_{\boldsymbol{z}\in\Lambda} \delta_{\boldsymbol{z}},$$

and where $\delta_{\boldsymbol{z}}$ *is the Dirac delta distribution.*

Proof. For $\ell \in \mathbb{N}_0$, the action of the distribution $\mathcal{B}_\Lambda^{(\ell)}$ on $\psi \in S(\mathbb{R}^d)$ yields

$$\langle \mathcal{B}_\Lambda^{(\ell)}, \psi\rangle = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \frac{\hat{\psi}(\boldsymbol{z})}{(2\pi i|\boldsymbol{z}|)^{2(\ell+1)}}.$$

By duality, the distributional poly-Laplacian $\Delta^{\ell+1}\mathcal{B}_\Lambda^{(\ell)}$ reads

$$\langle \Delta^{\ell+1}\mathcal{B}_\Lambda^{(\ell)}, \psi\rangle = \langle \mathcal{B}_\Lambda^{(\ell)}, \Delta^{\ell+1}\psi\rangle = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \hat{\psi}(\boldsymbol{z}) = V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*} \hat{\psi}(\boldsymbol{z}) - V_{\Lambda^*}\hat{\psi}(\boldsymbol{0}).$$

We apply Poisson summation,

$$V_{\Lambda^*} \sum_{\boldsymbol{z}\in\Lambda^*} \hat{\psi}(\boldsymbol{z}) - V_{\Lambda^*}\hat{\psi}(\boldsymbol{0}) = \sum_{\boldsymbol{z}\in\Lambda} \psi(\boldsymbol{z}) - V_{\Lambda^*}\int_{\mathbb{R}^d} \psi(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z},$$

and find, as $V_{\Lambda^*} = V_\Lambda^{-1}$, that

$$\left\langle \Delta^{\ell+1}\mathcal{B}_\Lambda^{(\ell)}, \psi\right\rangle = \left\langle Ш_\Lambda - V_\Lambda^{-1}, \psi\right\rangle = \sum\!\!\!\!\!\!\int_{\mathbb{R}^d,\Lambda} \psi.$$

□

We subsequently investigate the maximum norm of the Bernoulli functions of sufficiently high order ℓ, which enters in the error scaling of the expansion.

Corollary 2.22 (Maximum norm of $\mathcal{B}_\Lambda^{(\ell)}$). *Let* $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ *and* $\ell \in \mathbb{N}_0$. *For* $2(\ell+1) > d$, *the functions* $B_\Lambda^{(\ell)}$ *can be continuously extended to* $\mathbb{R}^d$ *with maximum norm*

$$\|\mathcal{B}_\Lambda^{(\ell)}\|_\infty = \frac{1}{V_\Lambda} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \frac{1}{|2\pi\boldsymbol{z}|^{2(\ell+1)}}.$$

The scaling as $\ell \to \infty$ *is determined by* a_{Λ^*},

$$\lim_{\ell\to\infty} (2\pi a_{\Lambda^*})^{2(\ell+1)} \|\mathcal{B}_\Lambda^{(\ell)}\|_\infty = \frac{n_{\Lambda^*}}{V_\Lambda},$$

with n_{Λ^*} *the number of elements of* Λ^* *with norm* a_{Λ^*}.

Proof. Let $k = 2(\ell+1) - d > 0$ such that the Dirichlet series in Definition 2.19 converges absolutely without β-regularisation on $\mathbb{R}^d$. Clearly, the maximum norm is bounded by

$$\left\|\mathcal{B}_\Lambda^{(\ell)}\right\|_\infty \le \frac{1}{V_\Lambda} \sum_{\boldsymbol{z}\in\Lambda^*}{}' \frac{1}{|2\pi\boldsymbol{z}|^{2(\ell+1)}},$$

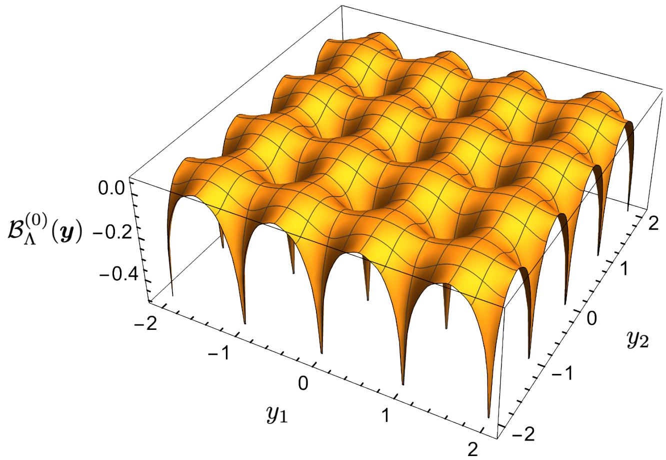

Figure 2. Multidimensional Bernoulli function $\mathcal{B}_\Lambda^{(0)}$ for $d = 2$ and $\Lambda = \mathbb{Z}^2$.

and the inequality sign can be replaced by an equality sign as the upper bound is reached on Λ. For the scaling as $\ell \to \infty$, we note that

$$\lim_{\ell\to\infty}(2\pi a_{\Lambda^*})^{2(\ell+1)}\|\mathcal{B}_\Lambda^{(\ell)}\|_\infty = \frac{1}{V_\Lambda}\lim_{\ell\to\infty}\sum_{\boldsymbol{z}\in\Lambda^*}{}' \left(\frac{a_{\Lambda^*}}{|\boldsymbol{z}|}\right)^{2(\ell+1)} = \frac{n_{\Lambda^*}}{V_\Lambda},$$

by the monotone convergence theorem.

□

In Fig. 2, we show the Bernoulli function $\mathcal{B}_\Lambda^{(0)}$ for a two-dimensional square lattice $\Lambda = \mathbb{Z}^2$. The logarithmic singularities at the lattice points originate from the fundamental solution to the two-dimensional Laplace operator.

The Bernoulli functions and their derivatives describe the coefficients of the differential operator of the multidimensional EM expansion.

Definition 2.23 (EM operator). Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\ell \in \mathbb{N}_0$. For $\boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda$, we define the ℓth order EM operator $\boldsymbol{\mathcal{D}}_{\Lambda,0,\boldsymbol{y}}^{(\ell)}$ as

$$\boldsymbol{\mathcal{D}}_{\Lambda,0,\boldsymbol{y}}^{(\ell)} = \sum_{k=0}^{\ell}\Big(\nabla\Delta^{\ell-k}\mathcal{B}_\Lambda^{(\ell)}(\boldsymbol{y}) - \Delta^{\ell-k}\mathcal{B}_\Lambda^{(\ell)}(\boldsymbol{y})\nabla\Big)\Delta^k.$$

With $\boldsymbol{\mathcal{D}}_{\Lambda,0,\boldsymbol{y}}$, we denote the infinite order EM operator obtained by setting $\ell = \infty$ in above definition.

We will prove at a later point that the infinite order operator is well-defined for band-limited functions with bandwidth $\sigma < a_{\Lambda^*}$.

The function $\mathcal{B}_\Lambda^{(\ell)}$ can be identified as an infinite linear combination of parametrices for the poly-Laplace operator. A parametrix for $\Delta^{\ell+1}$ is a distribution $E \in \mathscr{D}'\big(\mathbb{R}^d\big)$ with

$$\Delta^{\ell+1} E = \delta_{\mathbf{0}} - \psi$$

where ψ is a smooth function [31, Definition 7.1.21]. Green's third identity, also called representation formula, is also applicable, with a small modification, if we replace the fundamental solution by a parametrix, see [33, p. 235, Eq. (20.1.6)]. We only give the result for $\ell = 0$, where the case of general ℓ readily follows after repeated application of Green's second identity.

Lemma 2.24. *Let E be a parametrix for the Laplace operator, such that $\Delta E = \delta_{\mathbf{0}} - \psi$, $\psi \in C^\infty\big(\mathbb{R}^d\big)$. Then $E \in C^\infty\big(\mathbb{R}^d \setminus \{\mathbf{0}\}\big)$ and for $f \in C^2\big(\bar{\Omega}\big)$, a domain $\Omega \subseteq \mathbb{R}^d$, and $\boldsymbol{x} \in \Omega$, we find that*

$$f(\boldsymbol{x}) - \int\limits_{\Omega} \psi(\boldsymbol{x}-\boldsymbol{y}) f(\boldsymbol{y})\, d\boldsymbol{y}$$

$$= \int\limits_{\partial\Omega} \Big(\partial_{\boldsymbol{n}_{\boldsymbol{y}}} E(\boldsymbol{x}-\boldsymbol{y}) f(\boldsymbol{y}) - E(\boldsymbol{x}-\boldsymbol{y}) \partial_{\boldsymbol{n}_{\boldsymbol{y}}} f(\boldsymbol{y})\Big)\, dS_{\boldsymbol{y}} + \int\limits_{\Omega} E(\boldsymbol{x}-\boldsymbol{y}) \Delta f(\boldsymbol{y})\, d\boldsymbol{y},$$

where $\partial_{\boldsymbol{n}_{\boldsymbol{y}}} = \langle \nabla_{\boldsymbol{y}}, \boldsymbol{n}_{\boldsymbol{y}} \rangle$ denotes the normal derivative and $\boldsymbol{n}_{\boldsymbol{y}}$ is the unit outward normal vector to Ω at $\boldsymbol{y} \in \partial\Omega$. Furthermore, f is assumed to have compact support in $\bar{\Omega}$ if Ω is unbounded.

We finally arrive at the EM expansion on multidimensional lattices.

Theorem 2.25 (Multidimensional EM expansion). *Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\Omega \subseteq \mathbb{R}^d$ a domain such that $\partial\Omega \cap \Lambda = \varnothing$. If $f \in C^{2(\ell+1)}(\bar{\Omega})$, $\ell \in \mathbb{N}_0$, with compact support in $\bar{\Omega}$ in case of an unbounded domain, then the sum-integral of f over (Ω, Λ) has the representation*

$$\sum\!\!\!\!\!\!\int\limits_{\Omega,\Lambda} f = \int\limits_{\partial\Omega} \Big\langle \boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,0,\boldsymbol{y}} f(\boldsymbol{y}), \boldsymbol{n}_{\boldsymbol{y}} \Big\rangle\, \mathrm{d}S_{\boldsymbol{y}} + \int\limits_{\Omega} \mathcal{B}^{(\ell)}_{\Lambda}(\boldsymbol{y}) \Delta^{\ell+1} f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}.$$

If Ω is bounded and $f \in E_\sigma$ with $\sigma < a_{\Lambda^*}$, then

$$\sum\!\!\!\!\!\!\int\limits_{\Omega,\Lambda} f = \int\limits_{\partial\Omega} \langle \boldsymbol{\mathcal{D}}_{\Lambda,0,\boldsymbol{y}} f(\boldsymbol{y}), \boldsymbol{n}_{\boldsymbol{y}} \rangle\, \mathrm{d}S_{\boldsymbol{y}}.$$

Proof. Corollary 2.22 yields that the poly-Laplacian of $\mathcal{B}^{(\ell)}_{\Lambda}$ describes a tempered distribution,

$$\Delta^{\ell+1} \mathcal{B}^{(\ell)}_{\Lambda} = \text{Ш}_{\Lambda} - V_{\Lambda}^{-1} = \Delta\big(\Delta^{\ell} \mathcal{B}^{(\ell)}_{\Lambda}\big).$$

Then, by assumption on Ω and f,

$$\sum_{\Omega \cap \Lambda} f$$

only exhibits a finite number of non-zero addends. Hence Lemma 2.24 can be applied to the sum-integral, from which we obtain

$$\sum\!\!\!\!\!\!\int_{\Omega,\Lambda} f = \int_{\partial\Omega} \Big(\partial_{\boldsymbol{n}_{\boldsymbol{y}}} \Delta^{\ell} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) - \Delta^{\ell} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) \partial_{\boldsymbol{n}_{\boldsymbol{y}}}\Big) f(\boldsymbol{y})\, \mathrm{d}S_{\boldsymbol{y}} + \int_{\Omega} \Delta^{\ell} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) \Delta f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y},$$

having used that $\Delta^{\ell-k}\mathcal{B}_{\Lambda}^{(\ell)}$ is both Λ-periodic and symmetric,

$$\Delta^{\ell-k}\mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{z}-\boldsymbol{y}) = \Delta^{\ell-k}\mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}), \quad \boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda,\ \boldsymbol{z} \in \Lambda.$$

We subsequently apply Green's second identity ℓ times to the right hand side, yielding

$$\sum\!\!\!\!\!\!\int_{\Omega,\Lambda} f = \int_{\partial\Omega} \sum_{k=0}^{\ell} \Big(\partial_{\boldsymbol{n}_{\boldsymbol{y}}} \Delta^{\ell-k} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) - \Delta^{\ell-k} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) \partial_{\boldsymbol{n}_{\boldsymbol{y}}}\Big) \Delta^k f(\boldsymbol{y})\, \mathrm{d}S_{\boldsymbol{y}} + \int_{\Omega} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) \Delta^{\ell+1} f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}.$$

Now for a bounded domain Ω, $f \in E_\sigma$, and $2(\ell+1) > d$, we seek an estimate for the remainder

$$\mathcal{R}_{\Lambda}^{(\ell)} = \int_{\Omega} \mathcal{B}_{\Lambda}^{(\ell)}(\boldsymbol{y}) \Delta^{\ell+1} f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}.$$

We know from Corollary 2.22 that, by assumption on ℓ, $\mathcal{B}_{\Lambda}^{(\ell)}$ is continuous and bounded. Hence

$$\big|\mathcal{R}_{\Lambda}^{(\ell)}\big| \le \|\mathcal{B}_{\Lambda}^{(\ell)}\|_\infty \|\Delta^{\ell+1} f\|_{1,\Omega}.$$

As $f \in E_\sigma$, with $f = \hat{h}$, we find by Lemma 2.7 that

$$\|\Delta^{\ell+1} f\|_{1,\Omega} \le (2\pi\sigma)^{2(\ell+1)} \mathrm{vol}(\Omega) \|h\|_1.$$

We insert the asymptotic scaling of the Bernoulli functions from Corollary 2.22, which results in the estimate

$$\lim_{\ell\to\infty} \big(\sigma/a_{\Lambda^*}\big)^{-2(\ell+1)} \big|\mathcal{R}_{\Lambda}^{(\ell)}\big| \le \frac{n_{\Lambda^*} \mathrm{vol}(\Omega)}{V_\Lambda} \|h\|_1.$$

Thus,

$$\big|\mathcal{R}_{\Lambda}^{(\ell)}\big| \sim \big(\sigma/a_{\Lambda^*}\big)^{2(\ell+1)},$$

and the remainder integral vanishes in the limit $\ell \to \infty$ in case that $\sigma < a_{\Lambda^*}$.

□

In the following, we show that the expansion is also applicable for functions on unbounded domains if they exhibit a sufficiently fast asymptotic decay at infinity.

Corollary 2.26 (EM expansion on unbounded domains). *The EM expansion of order $\ell \in \mathbb{N}_0$ extends to unbounded domains $\Omega \subseteq \mathbb{R}^d$ with $\partial\Omega \cap \Lambda = \varnothing$ and functions $f \in C^{2(\ell+1)}(\bar{\Omega})$ for which there exist $C, \varepsilon > 0$ such that*

$$|\langle \boldsymbol{t}, \nabla\rangle^k f(\boldsymbol{y})| \le C\big(1 + |\boldsymbol{y}|\big)^{-(d+\varepsilon)}, \quad \boldsymbol{y} \in \bar{\Omega},$$

for all $\boldsymbol{t} \in \partial B_1$ and $k \le 2(\ell+1)$.

Proof. Choose $\eta \in \mathscr{D}(\mathbb{R}^d)$ with $\eta(\boldsymbol{0}) = 1$. Then for $n \in \mathbb{N}$, set $\eta_n = \eta(\cdot/n)$. As $f_n = \eta_n f$ is compactly supported, the sum-integral can be expanded as follows

$$\sum\!\!\!\!\!\!\int_{\Omega,\Lambda} f_n = \int_{\partial\Omega} \Big\langle \boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,0,\boldsymbol{y}} f_n(\boldsymbol{y}), \boldsymbol{n}_{\boldsymbol{y}} \Big\rangle \, \mathrm{d}S_{\boldsymbol{y}} + \int_{\Omega} \mathcal{B}^{(\ell)}_{\Lambda}(\boldsymbol{y}) \Delta^{\ell+1} f_n(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y},$$

for all $n \in \mathbb{N}$. Now there exists bounds to the derivatives of η_n that are independent of n,

$$\|D^{\boldsymbol{\alpha}} \eta_n\|_\infty \le \frac{1}{n^{|\boldsymbol{\alpha}|}} \|D^{\boldsymbol{\alpha}} \eta\|_\infty \le \|D^{\boldsymbol{\alpha}} \eta\|_\infty.$$

The bounds on the derivatives of f_n on $\bar{\Omega}$ yield a majorant that is both integrable and summable. The EM expansion for f then follows from the dominated convergence theorem.

□

The error of the EM expansion is controlled by the remainder

$$\mathcal{R}^{(\ell)}_{\Lambda} = \int_{\Omega} \mathcal{B}^{(\ell)}_{\Lambda}(\boldsymbol{y}) \Delta^{\ell+1} f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}.$$

The expansion from Theorem 2.25 can now be used in two different ways. The first option is to apply the EM expansion as a quadrature rule that approximates an integral by a discrete sum. The error under grid refinement, $\Lambda_h = h\Lambda$ for $h > 0$, of the integral approximation is then given by

$$V_{\Lambda_h} |\mathcal{R}^{(\ell)}_{\Lambda_h}| \le h^{2(\ell+1)} V_\Lambda \|\mathcal{B}^{(\ell)}_{\Lambda}\|_\infty \|\Delta^{\ell+1} f\|_{1,\Omega},$$

for $2(\ell+1) > d$. Here the bound for the maximum norm of $\mathcal{B}^{(\ell)}_{\Lambda}$ follows from Corollary 2.22. The second option is to approximate a discrete lattice sum by an integral. Here, if we dilate the argument of the function f and set $f_\lambda(\boldsymbol{x}) = f(\boldsymbol{x}/\lambda)$, with $\lambda > 0$, we find that

$$|\mathcal{R}^{(\ell)}_{\Lambda}| \le \lambda^{-2(\ell+1)} \|\mathcal{B}^{(\ell)}_{\Lambda}\|_\infty \|\Delta^{\ell+1} f\|_{1,\Omega}.$$

This option will be further explored in the numerical application in Chapter 4.4. Let us now consider the scaling of the remainder $\mathcal{R}_\Lambda^{(\ell)}$ in the limit $\ell \to \infty$. In the proof of the expansion, we have shown that if the functions f is band-limited, $f = \mathcal{F}h$, with bandwidth σ, then the approximation error decays exponentially with the expansion order if $\sigma < a_{\Lambda^*}$,

$$|\mathcal{R}_\Lambda^{(\ell)}| \leq C_{\Lambda,\Omega} \|h\|_1 \left(\frac{a_{\Lambda^*}}{\sigma}\right)^{-2(\ell+1)},$$

where $C_{\Lambda,\Omega} > 0$ only depends on Λ and Ω. The EM expansion is however not useful if f includes an algebraic singularity. Then f cannot be well-approximated by a band-limited function and the expansion error is typically large and uncontrolled. In this challenging, yet highly relevant case, we need a more advanced version of the multidimensional EM expansion. We develop this singular expansion in the next chapter.

CHAPTER 3

Singular Euler–Maclaurin expansion on multidimensional lattices

1. Introduction

Let us choose a lattice $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, a bounded domain $\Omega \subset \mathbb{R}^d$ with $\partial\Omega \cap \Lambda = \varnothing$, and a lattice point $\boldsymbol{x} \in \Lambda$ that lies outside of $\bar{\Omega}$. Then, for a function $f_{\boldsymbol{x}} : \bar{\Omega} \to \mathbb{C}$ of the form

$$f_{\boldsymbol{x}}(\boldsymbol{y}) = s(\boldsymbol{y} - \boldsymbol{x})g(\boldsymbol{y}),$$

with a function $s \in C^\infty(\mathbb{R}^d \setminus \{\boldsymbol{0}\})$ that has an algebraic singularity at $\boldsymbol{0}$, and for $g \in C^{2(\ell+1)}(\bar{\Omega})$, the EM expansion of order ℓ from Theorem 2.25 of the sum-integral

$$\sumint_{\Omega,\Lambda} f_{\boldsymbol{x}}$$

does not converge in the limit $\ell \to \infty$, even for band-limited functions $g \in E_\sigma$ with $\sigma < a_{\Lambda^*}$. We call s the interaction and g the interpolating function. The lack of convergence arises because of the algebraic singularity of s, due to which $f_{\boldsymbol{x}}$ is not band-limited, which in turn causes the derivatives of $f_{\boldsymbol{x}}$ to increase quickly with the derivative order. This results in an approximation error that is uncontrolled and typically large, even for low expansion orders ℓ. In the following, we consider the physically most relevant interaction function

$$s_\nu = |\cdot|^{-\nu}, \quad \nu \in \mathbb{C}.$$

We have already seen in Chapter 1 that the one-dimensional EM expansion does not converge for functions with singularities and we have overcome this problem by means of the one-dimensional SEM expansion. Now in the same way as the derivation of the SEM expansion for $d = 1$ was based on the traditional EM expansion, we make use of the multidimensional EM expansion in the following in order to show existence of the mathematical objects that appear in the multidimensional SEM expansion.

As we have shown for $d = 1$, we can make the EM expansion applicable to singular summand functions by including the singularity in

This chapter is based on [7, Section 4].

a generalisation of the Bernoulli functions, which we call Bernoulli-$\mathcal{A}$ functions. With these Bernoulli-$\mathcal{A}$ functions, the action of the differential operator is restricted to the the well-behaved function g, thereby avoiding derivatives of the interaction s. This procedure remedies the divergence of the remainder integral and thus leads to an expansion that is useful in practice.

The derivation of the multidimensional SEM expansion is structured as follows. We construct the Bernoulli-$\mathcal{A}$ functions in Section 2. To this end, we first discuss fundamental solutions to the poly-Laplace operator in Section 2.1. We then suitably combine the fundamental solutions with the interaction in Section 2.2 to a function that we call Bernoulli symbol, as it shares properties with symbols that arise in the study of pseudo-differential operators. The Bernoulli-$\mathcal{A}$ functions then follow as regularised sum-integrals of the Bernoulli symbol in Section 2.3. In Section 3, we then introduce the SEM operator, whose coefficient functions are determined by the Bernoulli-$\mathcal{A}$ functions and subsequently present the SEM expansion for an exterior singularity, which lies outside of the region Ω. Section 4 finally extends the expansion to singularities inside Ω, which gives rise to an additional local SEM operator.

2. Derivation

2.1. Fundamental solutions to the poly-Laplace operator. The Bernoulli-$\mathcal{A}$ functions are based on fundamental solutions to poly-Laplace operators.

Notation 3.1 (Rotationally symmetric fundamental solutions of $\Delta^{\ell+1}$). Let $\ell \in \mathbb{N}_0$. We denote by $\phi_\ell \in S'(\mathbb{R}^d)$ a rotationally symmetric fundamental solution to $\Delta^{\ell+1}$, where

$$\Delta^{\ell+1}\phi_\ell = \delta_{\mathbf{0}}.$$

Remark 3.2. The representation of the poly-Laplace operator in spherical coordinates shows that the choice of ϕ_ℓ is only unique up to a rotationally invariant polynomial of order 2ℓ.

Lemma 3.3. *Every fundamental solution ϕ_ℓ can be identified as a C^∞-function on $\mathbb{R}^d \setminus \{\mathbf{0}\}$. One possible choice is*

$$\phi_\ell(\boldsymbol{x}) = C_{\ell,d}\,|\boldsymbol{x}|^{2(\ell+1)-d}, \quad \ell \in \mathbb{N}_0 \text{ and } d \text{ odd},$$

$$\begin{cases} \phi_\ell(\boldsymbol{x}) = C_{\ell,d}\,|\boldsymbol{x}|^{2(\ell+1)-d}, & \ell = 1,\dots,m-1, \\ \phi_\ell(\boldsymbol{x}) = C^{(1)}_{\ell,d}\,|\boldsymbol{x}|^{2(\ell+1)-d} - C^{(2)}_{\ell,d}\,|\boldsymbol{x}|^{2(\ell+1)-d}\ln|\boldsymbol{x}|, & \ell \geq m \text{ for } d = 2m, \end{cases}$$

for $m \in \mathbb{N}$ and with constants $C_{\ell,d}, C^{(1)}_{\ell,d}, C^{(2)}_{\ell,d} \in \mathbb{R}$.

The explicit form of above constants is given in [2, Chapter I.2]. We furthermore require the following estimate on the derivatives of the fundamental solutions [2, Proposition 3.3].

LEMMA 3.4. *For ϕ_ℓ as in Lemma 3.3 and $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ there exists a constant $C > 0$ such that for all $\boldsymbol{x} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$*

$$|D^{\boldsymbol{\alpha}} \phi_\ell(\boldsymbol{x})| \le C |\boldsymbol{x}|^{2(\ell+1)-d-|\boldsymbol{\alpha}|} \Big(\big| \ln |\boldsymbol{x}| \big| + 1 + \ln(\ell+1) \Big).$$

The representation formula in the following lemma is a direct consequence of Green's second and third identity.

LEMMA 3.5. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain. For $\ell \in \mathbb{N}_0$ and for $g \in C^{2(\ell+1)}(\bar{\Omega})$, we can express $g(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega$, by the representation formula,*

$$g(\boldsymbol{x}) = \sum_{k=0}^{\ell} \int_{\partial\Omega} \Big(\partial_{\boldsymbol{n_y}} \Delta^{\ell-k} \phi_\ell(\boldsymbol{x}-\boldsymbol{y}) - \Delta^{\ell-k} \phi_\ell(\boldsymbol{x}-\boldsymbol{y}) \partial_{\boldsymbol{n_y}} \Big) \Delta^k g(\boldsymbol{y}) \, dS_{\boldsymbol{y}} + \int_{\Omega} \phi_\ell(\boldsymbol{x}-\boldsymbol{y}) \Delta^{\ell+1} g(\boldsymbol{y}) \, d\boldsymbol{y}.$$

The next lemma immediately follows from the estimates for the derivatives of the fundamental solutions. A proof in case of the Laplace operator, $\ell = 0$, can be found in [27, Lemma 4.1].

LEMMA 3.6. *Let $\Omega \subset \mathbb{R}^d$ open and bounded. For $g \in C(\bar{\Omega})$ and $\ell \in \mathbb{N}_0$, the Newton potential*

$$f(\boldsymbol{x}) = \int_{\Omega} \phi_\ell(\boldsymbol{x}-\boldsymbol{y}) g(\boldsymbol{y}) \, d\boldsymbol{y}, \quad \boldsymbol{x} \in \Omega,$$

defines a $C^{2\ell+1}$-function on Ω. The derivatives up to order $2\ell+1$ are given by

$$D^{\boldsymbol{\alpha}} f(\boldsymbol{x}) = \int_{\Omega} D^{\boldsymbol{\alpha}} \phi_\ell(\boldsymbol{x}-\boldsymbol{y}) g(\boldsymbol{y}) \, d\boldsymbol{y}, \quad \boldsymbol{x} \in \Omega,$$

for $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ with $|\boldsymbol{\alpha}| \le 2\ell+1$.

We now discuss a representation of the poly-Laplace operator in terms of surface integrals over directional derivatives that will appear at several key points in our considerations[1]. It allows us to uncover geometric meaning in otherwise seemingly complicated expressions.

[1]The representation can be considered as a special case of Pizetti's formula, see e.g. [25, p. 74].

Proposition 3.7 (Integral representation of the poly-Laplace operator). *Let $\boldsymbol{y} \in \mathbb{R}^d$ and $\ell \in \mathbb{N}_0$. For $g \in C^{2\ell}(U)$ on some open neighbourhood U of $\boldsymbol{y}$, it holds*

$$\Delta^\ell g(\boldsymbol{y}) = \frac{p_{\ell,d}}{\omega_d} \int_{\partial B_1} \langle \boldsymbol{z}, \nabla \rangle^{2\ell} g(\boldsymbol{y}) \, \mathrm{d}S_{\boldsymbol{z}},$$

with ω_d the surface area of the unit sphere and where the prefactor is given by

$$p_{\ell,d} = \frac{(d/2)_\ell}{(1/2)_\ell}.$$

Here, $(x)_\ell = x(x+1)\cdots(x+\ell-1)$ denotes the Pochhammer symbol.

Proof. From an application of the Fourier transform follows that the assertion is equivalent to

$$\frac{1}{\omega_d} \int_{\partial B_1} \langle \boldsymbol{z}, \boldsymbol{\xi} \rangle^{2\ell} \, \mathrm{d}S_{\boldsymbol{z}} = \frac{1}{p_{\ell,d}} = \frac{(1/2)_\ell}{(d/2)_\ell}, \quad \boldsymbol{\xi} \in \partial B_1.$$

We now apply the Funk–Hecke theorem [28, Theorem 3.4.1] for the constant spherical harmonic, and transform the integral over the sphere into a one-dimensional integral,

$$\frac{1}{\omega_d} \int_{\partial B_1} \langle \boldsymbol{z}, \boldsymbol{\xi} \rangle^{2\ell} \, \mathrm{d}S_{\boldsymbol{z}} = \frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} t^{2\ell} \big(1 - t^2\big)^{(d-3)/2} \, \mathrm{d}t.$$

The integral is readily evaluated in terms of Gamma functions. We then find, after inserting the surface area of the sphere, that

$$\frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} t^{2\ell} \big(1 - t^2\big)^{(d-3)/2} \, \mathrm{d}t = \frac{1}{\sqrt{\pi}} \frac{\Gamma(d/2)}{\Gamma\big((d-1)/2\big)} \frac{\Gamma\big((d-1)/2\big)\Gamma(\ell + 1/2)}{\Gamma(d/2 + \ell)}.$$

As $\Gamma(1/2) = \sqrt{\pi}$, the above expression reduces to

$$\frac{\Gamma(1/2 + \ell)}{\Gamma(1/2)} \frac{\Gamma(d/2)}{\Gamma(d/2 + \ell)} = \frac{(1/2)_\ell}{(d/2)_\ell} = \frac{1}{p_{\ell,d}}.$$

□

2.2. Bernoulli symbols. We now construct the Bernoulli symbol by combining the interaction with a shifted fundamental solution of $\Delta^{\ell+1}$ from which a Taylor expansion of precisely chosen order has been subtracted.

Definition 3.8 (Bernoulli symbol). Let $\nu \in \mathbb{C}$ and $\ell \in \mathbb{N}_0$. Then for $\boldsymbol{y}, \boldsymbol{z} \in \mathbb{R}^d \smallsetminus \{\boldsymbol{0}\}$, we set

$$a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) = \frac{1}{|\boldsymbol{z}|^\nu}\Big(\phi_\ell(\boldsymbol{y} - \boldsymbol{z}) - \sum_{k=0}^{2\ell+1} \frac{1}{k!}\langle -\boldsymbol{z}, \nabla\rangle^k \phi_\ell(\boldsymbol{y})\Big), \quad \boldsymbol{y} \neq \boldsymbol{z},$$

and call $a_\nu^{(\ell)}$ Bernoulli symbol of order ℓ for the interaction exponent ν.

It is of crucial importance to make the correct choice for the order of the Taylor expansion. If too many derivatives are taken, we loose integrability of the symbol in the second argument. If on the other hand too few derivatives are taken, the Bernoulli symbol will depend on the particular choice of the fundamental solution. The correct choice preserves both properties.

Lemma 3.9. *The Bernoulli symbol does not depend on the choice of the fundamental solution ϕ_ℓ.*

Proof. We show that two arbitrary choices for the rotationally symmetric fundamental solution, which we denote by $\phi_{\ell,1}$ and $\phi_{\ell,2}$, lead to the same resulting Bernoulli symbol. First, by Remark 3.2, the fundamental solutions differ by a polynomial P of order 2ℓ,

$$\phi_{\ell,1} - \phi_{\ell,2} = P.$$

Now, we denote by $a_{\nu,1}^{(\ell)}$ and $a_{\nu,2}^{(\ell)}$ the associated Bernoulli symbols for the two fundamental solutions and show that they are identical. As the polynomial P is equal to its Taylor series of order 2ℓ,

$$a_{\nu,1}^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) - a_{\nu,2}^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) = \frac{1}{|\boldsymbol{z}|^\nu}\Big(P(\boldsymbol{y} - \boldsymbol{z}) - \sum_{k=0}^{2\ell+1} \frac{1}{k!}\langle -\boldsymbol{z}, \nabla\rangle^k P(\boldsymbol{y})\Big) = 0.$$

□

The following lemma shows that certain spherical surface integrals over spheres of the Bernoulli symbol with respect to its second argument vanish. This will become important later, when we show that the resulting Bernoulli-$\mathcal{A}$ functions are uniquely defined.

Lemma 3.10. *Let $\nu \in \mathbb{C}$, and $\ell \in \mathbb{N}_0$. Then for $\boldsymbol{y} \in \mathbb{R}^d \smallsetminus \{\boldsymbol{0}\}$*

$$\int_{\partial B_r} a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) \,\mathrm{d}S_{\boldsymbol{z}} = 0, \quad r < |\boldsymbol{y}|.$$

Proof. For $|\boldsymbol{z}| < |\boldsymbol{y}|$, the shifted fundamental solution inside the Bernoulli symbol can be expanded in a Taylor series in $\boldsymbol{z}$. This then leads to

$$a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) = \frac{1}{|\boldsymbol{z}|^\nu} \sum_{k=2(\ell+1)}^{\infty} \frac{1}{k!}\langle -\boldsymbol{z}, \nabla\rangle^k \phi_\ell(\boldsymbol{y}),$$

where the series converges uniformly in $\boldsymbol{y}$ on B_r for $0 < r < |\boldsymbol{y}|$. We subsequently evaluate the integral of the Bernoulli symbol over a sphere with radius r,

$$\int\limits_{\partial B_r} a_\nu^{(\ell)}(\boldsymbol{y},\boldsymbol{z})\,\mathrm{d}S_{\boldsymbol{z}} = \frac{1}{r^\nu}\sum_{k=\ell+1}^{\infty}\frac{1}{(2k)!}\int\limits_{\partial B_r}\langle \boldsymbol{z},\nabla\rangle^{2k}\,\phi_\ell(\boldsymbol{y})\,\mathrm{d}S_{\boldsymbol{z}},$$

where odd powers of $\boldsymbol{z}$ vanish in the surface integral due to symmetry. From the integral representation of the poly-Laplace operator from Proposition 3.7, we obtain

$$\int\limits_{\partial B_r}\langle \boldsymbol{z},\nabla\rangle^{2k}\,\phi_\ell(\boldsymbol{y})\,\mathrm{d}S_{\boldsymbol{z}} = \frac{\omega_d}{p_{\ell,d}} r^{(d-1+2k)}\Delta^k\phi_\ell(\boldsymbol{y}).$$

Finally, as $k \geq \ell+1$, we have that

$$\Delta^k\phi_\ell(\boldsymbol{y}) = 0, \quad \boldsymbol{y}\in\mathbb{R}^d\setminus\{\boldsymbol{0}\}.$$

Thus above sum vanishes.

□

The following lemma gives estimates on the derivatives of the symbol with respect to its second argument, which are used in the proof of the well-definedness of the Bernoulli-$\mathcal{A}$ functions.

LEMMA 3.11. *Let $\ell\in\mathbb{N}_0$, $\nu\in\mathbb{C}$, $\boldsymbol{\alpha}\in\mathbb{N}_0^d$, and $K\subset\mathbb{R}^d\setminus\{\boldsymbol{0}\}$ compact. Then there exist $R>0$ and $C>0$ such that*

$$\left|D_{\boldsymbol{z}}^{\boldsymbol{\alpha}} a_\nu^{(\ell)}(\boldsymbol{y},\boldsymbol{z})\right| \leq C|\boldsymbol{z}|^{2(\ell+1)-\mathrm{Re}(\nu)-|\boldsymbol{\alpha}|}, \quad |\boldsymbol{z}|>R,\ \boldsymbol{y}\in K,$$

where C only depends on ℓ, ν, $\boldsymbol{\alpha}$, and K.

PROOF. First recall the definition of the symbol,

$$a_\nu^{(\ell)}(\boldsymbol{y},\boldsymbol{z}) = \frac{1}{|\boldsymbol{z}|^\nu}\Big(\phi_\ell(\boldsymbol{y}-\boldsymbol{z}) - \sum_{k=0}^{2\ell+1}\frac{1}{k!}\langle -\boldsymbol{z},\nabla\rangle^k\,\phi_\ell(\boldsymbol{y})\Big).$$

In this proof, we use $C>0$ as a generic constant that depends on ℓ, ν, $\boldsymbol{\alpha}$, K and whose value changes during the proof. We first give an estimate on the derivatives of the terms in brackets. Lemma 3.4 yields

$$\left|D_{\boldsymbol{z}}^{\boldsymbol{\alpha}}\phi_\ell(\boldsymbol{y}-\boldsymbol{z})\right| \leq C|\boldsymbol{y}-\boldsymbol{z}|^{2(\ell+1)+1-d-|\boldsymbol{\alpha}|}, \quad |\boldsymbol{y}-\boldsymbol{z}|>1,$$

where we have increased the exponent by 1 in order to bound the logarithm. For

$$R > 2\max\Big\{1,\sup_{\boldsymbol{y}\in K}|\boldsymbol{y}|\Big\},$$

we find for all $\gamma\in\mathbb{R}$ that

$$|\boldsymbol{y}-\boldsymbol{z}|^\gamma \leq 2^{|\gamma|}|\boldsymbol{z}|^\gamma, \quad |\boldsymbol{z}|>R.$$

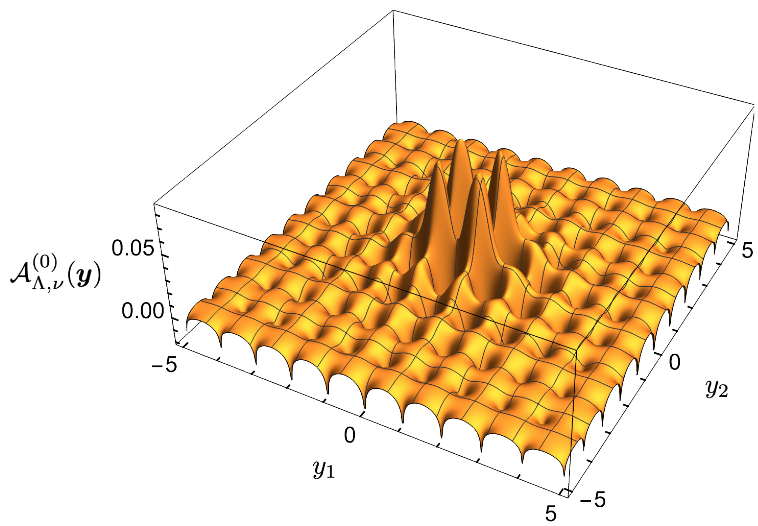

FIGURE 1. Bernoulli-$\mathcal{A}$ function $\mathcal{A}^{(0)}_{\Lambda,\nu}$ for $d = 2$, $\Lambda = \mathbb{Z}^2$, and $\nu = 2.001$.

Hence,

$$\left|D^{\boldsymbol{\alpha}}_{\boldsymbol{z}}\phi_\ell(\boldsymbol{y}-\boldsymbol{z})\right| \le C|\boldsymbol{z}|^{2(\ell+1)+\varepsilon-d-|\boldsymbol{\alpha}|} \le C|\boldsymbol{z}|^{2(\ell+1)-|\boldsymbol{\alpha}|}, \quad |\boldsymbol{z}| > R.$$

We furthermore have that

$$\left|D^{\boldsymbol{\alpha}}_{\boldsymbol{z}}\sum_{k=0}^{2\ell+1}\frac{1}{k!}\langle -\boldsymbol{z},\nabla\rangle^k\,\phi_\ell(\boldsymbol{y})\right| \le C|\boldsymbol{z}|^{2(\ell+1)-|\boldsymbol{\alpha}|}.$$

A bound on the derivatives of the interaction $|\boldsymbol{\cdot}|^{-\nu}$ can be easily established by induction on the multi-index, which reads

$$\left|D^{\boldsymbol{\alpha}}_{\boldsymbol{z}}|\boldsymbol{z}|^{-\nu}\right| \le C|\boldsymbol{z}|^{-\mathrm{Re}(\nu)-|\boldsymbol{\alpha}|}, \quad \boldsymbol{z}\in\mathbb{R}^d\setminus\{\boldsymbol{0}\}.$$

With above results, the Leibniz rule then yields the sought estimate.

□

2.3. Bernoulli-$\mathcal{A}$ functions. We define the Bernoulli-$\mathcal{A}$ functions as regularised sum integrals of the the Bernoulli symbol, which was introduced in the previous section. This procedure allows us to sum over an infinite number of fundamental solutions ϕ_ℓ, while keeping the resulting expressions well defined. These fundamental solutions then provide the required singularities that lead to Dirac delta distributions at lattice points if the poly-Laplace operator is applied.

Definition 3.12 (Bernoulli-$\mathcal{A}$ functions). Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, $\nu \in \mathbb{C}$, and $\ell \in \mathbb{N}_0$. We define $\mathcal{A}_{\Lambda,\nu}^{(\ell)} : \mathbb{R}^d \setminus \Lambda \to \mathbb{C}$ as

$$\mathcal{A}_{\Lambda,\nu}^{(\ell)}(\boldsymbol{y}) = \lim_{\beta \to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_{\delta,\Lambda}} \hat{\chi}_\beta(\boldsymbol{z})\, a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}),$$

for a family of smooth cutoff functions $\hat{\chi}_\beta$, $\beta > 0$, and an arbitrary $\delta \in (0, a_\Lambda)$ such that $\delta < |\boldsymbol{y}|$.

We display the zero order Bernoulli-$\mathcal{A}$ function $\mathcal{A}_{\Lambda,\nu}^{(0)}$ in Fig. 2.3 for a two-dimensional square lattice and an interaction exponent $\nu = 2.001$. The function shows the characteristic logarithmic singularity of the fundamental solution of the Laplace operator for $d = 2$ at all lattice points. It furthermore exhibits a singularity at the origin $\boldsymbol{y} = \boldsymbol{0}$ that depends on the exponent ν and on the order ℓ. The asymptotic decay of the function is determined by the interaction. In the following theorem, we show well-definedness of the Bernoulli-$\mathcal{A}$ functions and present their central properties. Its proof is based on the multidimensional Euler–Maclaurin expansion that has been developed in the previous chapter.

Theorem 3.13 (Fundamental theorem of the SEM expansion). *For $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, $\ell \in \mathbb{N}_0$, and $\nu \in \mathbb{C}$, the function $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$ is well-defined, and independent of the choices for ϕ_ℓ, δ, and χ. Furthermore, $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$ is analytic and the limit $\beta \to 0$ in the definition of $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$ is compact in all derivatives.*

We separate the proof into several propositions and lemmas, for which the conditions on Λ, ℓ, ν, and $\hat{\chi}_\beta$ from Definition 3.12 shall hold. In the first proposition, we discuss the well-definedness of the sum-integral in the Bernoulli-$\mathcal{A}$ functions in case of a finite regularisation parameter β.

Proposition 3.14. *Choose $\beta > 0$. Then the auxiliary function $\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)} : \mathbb{R}^d \setminus \Lambda \to \mathbb{C}$ with*

$$\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}(\boldsymbol{y}) = \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_{\delta,\Lambda}} \hat{\chi}_\beta(\boldsymbol{z})\, a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}), \quad \delta < |\boldsymbol{y}|,\ 0 < \delta < a_\Lambda,$$

is analytic and independent of the choices for δ and ϕ_ℓ.

Proof. As the smooth cutoff function $\hat{\chi}_\beta(\boldsymbol{z})$ decays superpolynomially as $|\boldsymbol{z}| \to \infty$, the sum integral is well-defined. This decay allows furthermore to exchange differentiation with the sum-integral. Hence $\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}$ inherits analyticity from its underlying Bernoulli symbol.

We first show independence of the auxiliary function from the choice of δ. Let $\boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda$ and choose δ_1, δ_2 in $(0, a_\Lambda)$ such that both are smaller than $|\boldsymbol{y}|$. Without loss of generality, we can assume $\delta_2 > \delta_1$. Now the lattice sum is independent of the choice for δ as $\delta < a_\Lambda$, where a_Λ is the minimal distance of two lattice points. Hence, the difference of the sum-integrals for the two choices δ_1 and δ_2 is proportional to the integral

$$\int_{B_{\delta_2} \setminus B_{\delta_1}} \hat{\chi}_\beta(\boldsymbol{z})\, a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z})\, \mathrm{d}\boldsymbol{z}. \tag{3.1}$$

We know from Lemma 3.10 that

$$\int_{\partial B_r} a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z})\, \mathrm{d}S_{\boldsymbol{z}} = 0, \quad r < |\boldsymbol{y}|.$$

As the cut-off function $\hat{\chi}_\beta$ is rotationally invariant, the integral in (3.1) vanishes as well, which proves independence of the auxiliary function from δ. Finally, Lemma 3.9 shows that the Bernoulli symbol and hence also the auxiliary function does not depend on the particular choice of the fundamental solution ϕ_ℓ.

□

Proposition 3.15. *The auxiliary functions* $\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}$, $\beta > 0$, *are locally integrable on* $\mathbb{R}^d \setminus \{\boldsymbol{0}\}$ *with*

$$\int_K \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}(\boldsymbol{y})\, d\boldsymbol{y} = \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_\delta, \Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \int_K a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z})\, d\boldsymbol{y},$$

for $K \subset \mathbb{R}^d \setminus \{\boldsymbol{0}\}$ *compact and* $\delta > 0$ *such that*

$$\delta < \min\big(a_\Lambda, \operatorname{dist}(\boldsymbol{0}, K)\big).$$

They furthermore converge in $L^1_{loc}(\mathbb{R}^d \setminus \{\boldsymbol{0}\})$ *for* $\beta \to 0$ *to the locally integrable function* $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$, *which is independent of the choice of* χ. *In particular,*

$$\int_K \mathcal{A}_{\Lambda,\nu}^{(\ell)}(\boldsymbol{y})\, d\boldsymbol{y} = \lim_{\beta \to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_\delta, \Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \int_K a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z})\, d\boldsymbol{y}.$$

Proof. As $a_\nu^{(\ell)}(\,\cdot\,, \boldsymbol{z}) \in L^1_{loc}(\mathbb{R}^d)$ for $\boldsymbol{z} \in \mathbb{R}^d \setminus \{\boldsymbol{0}\}$, we find together with the superpolynomially decay of $\hat{\chi}_\beta$ that the integral of the auxiliary function over the compact set $K \subset \mathbb{R}^d \setminus \{\boldsymbol{0}\}$ exists. It reads

$$\int_K \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y} = \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_\delta, \Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \int_K a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z})\, \mathrm{d}\boldsymbol{y}.$$

Now choose $R > 0$ large enough such that $K \subset B_R$, $\operatorname{dist}(K, \partial B_R) > \delta$ and such that the estimates from Lemma 3.11 are valid. Furthermore, it shall hold that $\partial B_R \cap \Lambda = \varnothing$. We subsequently divide the auxiliary function into two parts,

$$\mathcal{A}^{(\ell)}_{\Lambda,\nu,\beta}(\boldsymbol{y}) = \sum\!\!\!\!\!\!\int_{B_R \setminus B_\delta, \Lambda} \hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot) + \sum\!\!\!\!\!\!\int_{\mathbb{R}^d \setminus B_R, \Lambda} \hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot), \quad \boldsymbol{y} \in K.$$

The sum-integral over the unbounded domain is then expanded by means of the EM expansion in Corollary 2.26 of yet to be specified order $m \in \mathbb{N}_0$,

$$\sum\!\!\!\!\!\!\int_{\mathbb{R}^d \setminus B_R, \Lambda} \hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot) = -\int_{\partial B_R} \Big\langle \boldsymbol{\mathcal{D}}^{(m)}_{\Lambda,0,\boldsymbol{z}}\Big(\hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot)\Big)(\boldsymbol{z}), \boldsymbol{n}_{\boldsymbol{z}}\Big\rangle \,\mathrm{d}S_{\boldsymbol{z}}$$
$$+ \int_{\mathbb{R}^d \setminus B_R} \mathcal{B}^{(m)}_\Lambda(\boldsymbol{z}) \Delta^{m+1}\big(\hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot)\big)(\boldsymbol{z}) \,\mathrm{d}\boldsymbol{z}.$$

Due to $\operatorname{dist}(\partial B_R, \Lambda) > 0$, the integrand in the surface integral is smooth in a neighbourhood of ∂B_R. From $\hat{\chi}_\beta \to 1$ as $\beta \to 0$ in $C^\infty(\mathbb{R}^d)$, we deduce that both the sum-integral over $B_R \setminus B_\delta$ as well as the surface integral over ∂B_R converge in $L^1(K)$ to the function

$$\sum\!\!\!\!\!\!\int_{B_R \setminus B_\delta, \Lambda} a_\nu^{(\ell)}(\boldsymbol{y}, \cdot) - \int_{\partial B_R} \Big\langle \boldsymbol{\mathcal{D}}^{(m)}_{\Lambda,0,\boldsymbol{z}} a_\nu^{(\ell)}(\boldsymbol{y}, \cdot)(\boldsymbol{z}), \boldsymbol{n}_{\boldsymbol{z}}\Big\rangle \,\mathrm{d}S_{\boldsymbol{z}},$$

which follows from the dominated convergence theorem. Now consider the remainder

$$\mathcal{R}^{(m)}_\beta(\boldsymbol{y}) = \int_{\mathbb{R}^d \setminus B_R} \mathcal{B}^{(m)}_\Lambda(\boldsymbol{z}) \Delta^{m+1}\big(\hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot)\big)(\boldsymbol{z}) \,\mathrm{d}\boldsymbol{z}, \quad \boldsymbol{y} \in K.$$

The integral representation of the poly-Laplace operator in Proposition 3.7 yields

$$\Delta^{m+1}\big(\hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot)\big)$$
$$= \frac{p_{m+1,d}}{\omega_d} \sum_{k=0}^{2(m+1)} \binom{2(m+1)}{k} \int_{\partial B_1} \langle \boldsymbol{t}, \nabla\rangle^{2(m+1)-k} \hat{\chi}_\beta \,\langle \boldsymbol{t}, \nabla\rangle^k a_\nu^{(\ell)}(\boldsymbol{y}, \cdot) \,\mathrm{d}S_{\boldsymbol{t}}.$$

The uniform estimates from Lemma 2.15 for $\hat{\chi}_\beta$ and from Lemma 3.11 for $a_\nu^{(\ell)}$ show that

$$|\Delta^{m+1}\big(\hat{\chi}_\beta a_\nu^{(\ell)}(\boldsymbol{y}, \cdot)\big)(\boldsymbol{z})| \le C \sum_{k=0}^{2(m+1)} \binom{2(m+1)}{k} |\boldsymbol{z}|^{-2(m+1)+k} |\boldsymbol{z}|^{2(\ell+1)-\mathrm{Re}(\nu)-k}$$
$$= 2^{2(m+1)} C |\boldsymbol{z}|^{2(\ell+1)-\mathrm{Re}(\nu)-2(m+1)}$$

for all $\boldsymbol{z} \in \mathbb{R}^d \setminus B_R$ and where the constant $C > 0$ depends only on K, m, ℓ and ν. By choosing m large enough such that

$$2(m+1) > \max\left\{2(\ell+1) - \mathrm{Re}(\nu) + d, 2(\ell+1)\right\}$$

is fulfilled, we then guarantee that the bound for $\left|\Delta^{m+1}\left(\hat{\chi}_\beta a_\nu^{(\ell)}\right)\right|$ is integrable on $K \times (\mathbb{R}^d \setminus B_R)$ and that $B_\Lambda^{(m)}$ is bounded by means of Corollary 2.22. From the dominated convergence theorem then follows that $\mathcal{R}_\beta^{(m)}$ converges in $L^1(K)$ to the function

$$\int\limits_{\mathbb{R}^d \setminus B_R} \mathcal{B}_\Lambda^{(m)}(\boldsymbol{z}) \Delta_{\boldsymbol{z}}^{m+1} a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) \,\mathrm{d}\boldsymbol{z}.$$

Hence, $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$ does not depend on χ and is locally integrable on $\mathbb{R}^d \setminus \{\boldsymbol{0}\}$ as the L^1_{loc}-limit of locally integrable functions.

□

The next proposition shows that the poly-Laplacian of the auxiliary function, as a distribution, results in a sum-integral that includes the β-regularised interaction. On $\mathbb{R}^d \setminus \Lambda$, this distribution can be identified as a smooth function where the limit $\beta \to 0$ converges compactly in all derivatives.

Proposition 3.16 (Sum-integral property). *Let $\beta > 0$. Then*

$$\Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)} = \hat{\chi}_\beta \frac{\mathrm{III}_\Lambda - V_\Lambda^{-1}}{|\cdot|^\nu}$$

as a distribution in $\mathscr{D}'(\mathbb{R}^d \setminus \{\boldsymbol{0}\})$. Furthermore,

$$\lim_{\beta \to 0} \Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta} = -\frac{V_\Lambda^{-1}}{|\cdot|^\nu} \text{ in } C^\infty(\mathbb{R}^d \setminus \Lambda)$$

and

$$\lim_{\beta \to 0} \left\langle \Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}, \psi \right\rangle = \left\langle \frac{\mathrm{III}_\Lambda - V_\Lambda^{-1}}{|\cdot|^\nu}, \psi \right\rangle = \sum\!\!\!\!\!\!\int_{\mathbb{R}^d,\Lambda} \frac{\psi}{|\cdot|^\nu}$$

for all $\psi \in \mathscr{D}(\mathbb{R}^d \setminus \{\boldsymbol{0}\})$.

Proof. Let $\psi \in \mathscr{D}(\mathbb{R}^d \setminus \{\boldsymbol{0}\}$. Then

$$\left\langle \Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}, \psi \right\rangle = \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_\delta, \Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \left\langle \Delta_{\boldsymbol{\xi}}^{\ell+1} a_\nu^{(\ell)}(\boldsymbol{\xi}, \boldsymbol{z}), \psi(\boldsymbol{\xi}) \right\rangle,$$

with $\boldsymbol{\xi}$ a placeholder with respect to which the action of the distribution shall be applied. After inserting the definition of the symbol $a_\nu^{(\ell)}$,

$$a_\nu^{(\ell)}(\boldsymbol{y}, \boldsymbol{z}) = \frac{1}{|\boldsymbol{z}|^\nu} \left(\phi_\ell(\boldsymbol{y} - \boldsymbol{z}) - \sum_{k=0}^{2\ell+1} \frac{1}{k!} \langle -\boldsymbol{z}, \nabla \rangle^k \phi_\ell(\boldsymbol{y}) \right),$$

we find from the defining property of the fundamental solution that

$$\left\langle \Delta_{\boldsymbol{\xi}}^{\ell+1} a_\nu^{(\ell)}(\boldsymbol{\xi},\boldsymbol{z}), \psi(\boldsymbol{\xi}) \right\rangle = \frac{\psi(\boldsymbol{z})}{|\boldsymbol{z}|^\nu},$$

where we use that $\mathbf{0} \notin \operatorname{supp} \psi$. Then

$$\left\langle \Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}, \psi \right\rangle = \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d\setminus B_\delta,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\psi(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} = \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\psi(\boldsymbol{z})}{|\boldsymbol{z}|^\nu},$$

as δ is chosen small enough such that $\psi = 0$ on B_δ. We then find by the dominated convergence theorem that

$$\lim_{\beta\to 0} \left\langle \Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}, \psi \right\rangle = \left\langle \frac{Ш_\Lambda - V_\Lambda^{-1}}{|\,\cdot\,|^\nu}, \psi \right\rangle. \tag{3.2}$$

From above representation, it is evident that the distribution $\Delta^{\ell+1}\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}$ can be identified as a smooth function on $\mathbb{R}^d \setminus \Lambda$, namely

$$\Delta^{\ell+1} \mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)} = -\hat{\chi}_\beta \frac{V_\Lambda^{-1}}{|\,\cdot\,|^\nu}.$$

As $\hat{\chi}_\beta \to 1$ for $\beta \to 0$ in $C^\infty(\mathbb{R}^d)$, see Lemma 2.14, the limit in (3.2) does not only exist in a weak sense but also in $C^\infty(\mathbb{R}^d \setminus \Lambda)$.

□

With Proposition 3.14, 3.15, and 3.16, we are now in the position to prove the fundamental theorem of the SEM expansion.

Proof of Theorem 3.13. We know from Proposition 3.15 that the auxiliary functions $\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}$, $\beta > 0$, converge for $\beta \to 0$ in $L^1_{\mathrm{loc}}(\mathbb{R}^d \setminus \Lambda)$, and hence as distributions, to $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$. Proposition 3.16 then yields that $\Delta^{\ell+1} A_{\Lambda,\nu,\beta}^{(\ell)}$ can be identified as an element of $C^\infty(\mathbb{R}^d \setminus \Lambda)$ for $\beta > 0$ that converges in $C^\infty(\mathbb{R}^d \setminus \Lambda)$ to the analytic function $\Delta^{\ell+1} A_{\Lambda,\nu}^{(\ell)}$. Hence, by virtue of elliptic regularity in the form of Theorem 2.5, $\mathcal{A}_{\Lambda,\nu,\beta}^{(\ell)}$ converges in $C^\infty(\mathbb{R}^d \setminus \Lambda)$ to $A_{\Lambda,\nu}^{(\ell)}$. In addition, Theorem 2.4 yields analyticity of the limit function. Finally, $\mathcal{A}_{\Lambda,\nu}^{(\ell)}$ does not depend on δ or ϕ_ℓ as our auxiliary functions are independent of this choice, see Proposition 3.14, and it is independent of χ by Proposition 3.15.

□

The proof of the fundamental theorem of the SEM expansion immediately yields the following central distributional property, on which the new expansion is based.

COROLLARY 3.17. *Let* $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, $\ell \in \mathbb{N}_0$, *and* $\nu \in \mathbb{C}$. *Then for* $\psi \in \mathscr{D}(\mathbb{R}^d \setminus \{\mathbf{0}\})$, *we have*

$$\left\langle \Delta^{\ell+1} \mathcal{A}^{(\ell)}_{\Lambda,\nu}, \psi \right\rangle = \sum\!\!\!\!\!\!\int_{\mathbb{R}^d,\Lambda} \frac{\psi}{|\cdot|^\nu}.$$

3. Singular Euler–Maclaurin expansion for exterior lattice points

We now introduce the SEM differential operator whose coefficients are determined by the Bernoulli-$\mathcal{A}$ functions and their derivatives.

DEFINITION 3.18 (SEM operator). We define the ℓth order SEM operator $\boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,\nu,\boldsymbol{y}}$ as

$$\boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,\nu,\boldsymbol{y}} = \sum_{k=0}^{\ell} \Big(\nabla \Delta^{\ell-k} \mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y}) - \Delta^{\ell-k} \mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y}) \nabla \Big) \Delta^k.$$

The infinite order operator $\boldsymbol{\mathcal{D}}_{\Lambda,\nu,\boldsymbol{y}}$ is obtained by setting $\ell = \infty$ in above definition.

After having introduced all necessary functions and operators, we now present the multidimensional SEM expansion on bounded domains.

THEOREM 3.19 (SEM expansion). *Let* $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, $\Omega \subset \mathbb{R}^d$ *a bounded domain such that* $\partial\Omega \cap \Lambda = \varnothing$, *and* $\boldsymbol{x} \in \Lambda \setminus \Omega$. *For* $f_{\boldsymbol{x}} : \bar{\Omega} \to \mathbb{C}$,

$$f_{\boldsymbol{x}}(\boldsymbol{y}) = \frac{g(\boldsymbol{y})}{|\boldsymbol{y} - \boldsymbol{x}|^\nu},$$

with $\nu \in \mathbb{C}$ *and* $g \in C^{2(\ell+1)}(\bar{\Omega})$, $\ell \in \mathbb{N}_0$, *the sum-integral of* $f_{\boldsymbol{x}}$ *over* (Ω, Λ) *has the representation*

$$\sum\!\!\!\!\!\!\int_{\Omega,\Lambda} f_{\boldsymbol{x}} = \int_{\partial\Omega} \left\langle \boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,\nu,\boldsymbol{y}-\boldsymbol{x}}\, g(\boldsymbol{y}), \boldsymbol{n}_{\boldsymbol{y}} \right\rangle \mathrm{d}S_{\boldsymbol{y}} + \int_{\Omega} \mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y} - \boldsymbol{x}) \Delta^{\ell+1} g(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}.$$

PROOF. From the sum-integral property in Corollary 3.17 we find with the representation formula for the parametrix in Lemma 2.24 that

$$\sum\!\!\!\!\!\!\int_{\Omega,\Lambda} f_{\boldsymbol{x}} = \int_{\partial\Omega} \Big(\partial_{\boldsymbol{n}_{\boldsymbol{y}}} \Delta^\ell \mathcal{A}_\ell(\boldsymbol{y} - \boldsymbol{x}) - \Delta^\ell \mathcal{A}_\ell(\boldsymbol{y} - \boldsymbol{x}) \partial_{\boldsymbol{n}_{\boldsymbol{y}}} \Big) g(\boldsymbol{y}) \, \mathrm{d}S_{\boldsymbol{y}} + \int_{\Omega} \Delta^\ell \mathcal{A}_\ell(\boldsymbol{y} - \boldsymbol{x}) \Delta g(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}.$$

The theorem then follows after repeated application of Green's second theorem.

□

Similar as for $d = 1$, the SEM differential operator acts only on the sufficiently regular function g, while derivatives of the interaction are avoided, restoring the convergence properties of the expansion. This is explored in more detail in the numerics section in Chapter 4.4.

4. Singular Euler–Maclaurin expansion for interior lattice points

We have investigated the case of a singularity outside of Ω in the previous section. Now, we move on to the highly relevant case of a singularity at a lattice point $\boldsymbol{x}$ inside the integration region. This situation arises, among others, in the computation of singular long-range interactions in atomic lattices in condensed matter systems. In the following, we show that the multidimensional SEM expansion can be extended to this case by introducing an additional local differential operator. Even more importantly, this operator in general represents the main contribution and remains relevant even in the limit of an infinite system without boundaries. As the operator is local, it can be easily implemented numerically, as soon as its coefficients are known. We now formulate the SEM expansion for interior lattice points.

Theorem 3.20 (SEM expansion for interior lattice points). *Assume the conditions of Theorem 3.19, however with $\boldsymbol{x} \in \Lambda \cap \Omega$. Let in addition $\varepsilon > 0$ with $\varepsilon < a_\Lambda$ small enough such that $\bar{B}_\varepsilon(\boldsymbol{x}) \subset \Omega$. Then*

$$\sum\!\!\!\!\!\!\int_{\Omega \setminus B_\varepsilon(\boldsymbol{x}),\Lambda} f_{\boldsymbol{x}} = \mathcal{D}\!\!\!\!/^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}) + \mathcal{S}^{(\ell)}_{\Lambda,\nu} g(\boldsymbol{x}) + \mathcal{R}^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}),$$

with the local SEM operator $\mathcal{D}\!\!\!\!/^{(\ell)}_{\Lambda,\nu,\varepsilon}$,

$$\mathcal{D}\!\!\!\!/^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}) = \sum_{k=0}^{\ell} \frac{1}{(2k)!} \lim_{\beta \to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus \bar{B}_\varepsilon,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\langle \boldsymbol{z}, \nabla \rangle^{2k}}{|\boldsymbol{z}|^\nu} g(\boldsymbol{x}),$$

a surface integral over derivatives of g of up to order $2\ell + 1$,

$$\mathcal{S}^{(\ell)}_{\Lambda,\nu} g(\boldsymbol{x}) = \int_{\partial\Omega} \Big\langle \boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,\nu,\boldsymbol{y}-\boldsymbol{x}}\, g(\boldsymbol{y}), \boldsymbol{n}_{\boldsymbol{y}} \Big\rangle \,\mathrm{d}S_{\boldsymbol{y}},$$

and a remainder

$$\mathcal{R}^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}) = \sum\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus \bar{B}_\varepsilon,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \int_{\Omega} a^{(\ell)}_\nu(\boldsymbol{y} - \boldsymbol{x}, \boldsymbol{z}) \Delta^{\ell+1} g(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}.$$

For the proof of above theorem, we need the following lemma, which is a direct consequence of the representation formula for the poly-Laplace operator in Lemma 3.5 and of the regularity of the associated Newton potential discussed in Lemma 3.6.

Lemma 3.21. *Let $\ell \in \mathbb{N}_0$, $\boldsymbol{x} \in \mathbb{R}^d$, and $g \in C^{2(\ell+1)}\big(B_\delta(\boldsymbol{x})\big)$ for $\delta > 0$. Then for every linear differential operator with constant coefficients $\mathcal{P}$ of order smaller or equal $2\ell+1$, we have for $\varepsilon < \delta$*

$$\mathcal{P}g(\boldsymbol{x}) = \int\limits_{\partial B_\varepsilon} \sum_{m=0}^{\ell} \Big(\mathcal{P}\partial_{\boldsymbol{n_y}}\Delta^{\ell-m}\phi_\ell(\boldsymbol{y}) - \mathcal{P}\Delta^{\ell-m}\phi_\ell(\boldsymbol{y})\partial_{\boldsymbol{n_y}}\Big)\Delta^m g(\boldsymbol{y}+\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{y}} + \int\limits_{B_\varepsilon} \mathcal{P}\phi_\ell(\boldsymbol{y})\Delta^{\ell+1}g(\boldsymbol{x}+\boldsymbol{y})\,d\boldsymbol{y}.$$

The volume term vanishes in the limit $\varepsilon \to 0$.

Proof of Theorem 3.20. As Ω is open and as $\boldsymbol{x} \in \Omega$, there exists $\varepsilon > 0$ such that $\bar{B}_\varepsilon(\boldsymbol{x}) \in \Omega$. Now apply the SEM expansion in Theorem 3.19 to the sum-integral of $f_{\boldsymbol{x}}$ over the set $(\Omega \setminus B_\varepsilon(\boldsymbol{x}), \Lambda)$. We then treat the surface integral over the inner and the outer surface separately and subsequently group the terms that depend on ε on the right hand side. This yields

$$\sum\!\!\!\!\!\!\!\int\limits_{\Omega\setminus B_\varepsilon(\boldsymbol{x}),\Lambda} f_{\boldsymbol{x}} = \int\limits_{\partial\Omega} \Big\langle \boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,\nu,\boldsymbol{y}-\boldsymbol{x}}\, g(\boldsymbol{y}), \boldsymbol{n_y}\Big\rangle\,\mathrm{d}S_{\boldsymbol{y}} - S_\varepsilon + \mathcal{R}^{(1)}_\varepsilon,$$

with the surface integral over the ε-sphere

$$S_\varepsilon = \int\limits_{\partial B_\varepsilon(\boldsymbol{x})} \Big\langle \boldsymbol{\mathcal{D}}^{(\ell)}_{\Lambda,\nu,\boldsymbol{y}-\boldsymbol{x}}\, g(\boldsymbol{y}), \boldsymbol{n_y}\Big\rangle\,\mathrm{d}S_{\boldsymbol{y}},$$

and with the remainder

$$\mathcal{R}^{(1)}_\varepsilon = \int\limits_{\Omega\setminus B_\varepsilon(\boldsymbol{x})} \mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y}-\boldsymbol{x})\Delta^{\ell+1}g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

After inserting the SEM operator in S_ε,

$$\mathcal{S}_\varepsilon = \int\limits_{\partial B_\varepsilon} \sum_{m=0}^{\ell} \Big(\partial_{\boldsymbol{n_y}}\Delta_{\boldsymbol{y}}^{\ell-m}\mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y}) - \Delta_{\boldsymbol{y}}^{\ell-m}\mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y})\partial_{\boldsymbol{n_y}}\Big)\Delta^m g(\boldsymbol{x}+\boldsymbol{y})\,\mathrm{d}S_{\boldsymbol{y}},$$

it becomes clear that the surface integral crucially depends on the behaviour of $\mathcal{A}^{(\ell)}_{\Lambda,\nu}$ around the origin. For $0 < \delta < \min\{\varepsilon, a_\Lambda\}$, have

$$\mathcal{A}^{(\ell)}_{\Lambda,\nu}(\boldsymbol{y}) = \lim_{\beta\to 0} \sum\!\!\!\!\!\!\!\int\limits_{\boldsymbol{z}\in\mathbb{R}^d\setminus B_\delta,\Lambda} \hat{\chi}_\beta(\boldsymbol{z})a^{(\ell)}_\nu(\boldsymbol{y},\boldsymbol{z}).$$

Note that the symbol $a^{(\ell)}_\nu(\boldsymbol{y},\cdot)$ is locally integrable on $\mathbb{R}^d \setminus \{\boldsymbol{0}\}$, and that $\mathcal{A}^{(\ell)}_{\Lambda,\nu}$ does not depend on the particular choice for δ as long as $\delta < \min\{|\boldsymbol{y}|, a_\Lambda\}$. We are hence able to replace $\mathbb{R}^d \setminus B_\delta$ by $\mathbb{R}^d \setminus \bar{B}_\varepsilon$ in above sum-integral if $|\boldsymbol{y}| < a_\Lambda$.

We now recall from the fundamental Theorem 3.13 that the limit $\beta \to 0$ converges in $C^\infty(\mathbb{R}^d \setminus \Lambda)$. Thus, it is possible to interchange the surface integral in the term $\mathcal{S}_\varepsilon$ together with all derivatives with the limit in β and with the sum-integral. We now insert the definition of the Bernoulli symbol,

$$a_\nu^{(\ell)}(\boldsymbol{y},\boldsymbol{z}) = \frac{1}{|\boldsymbol{z}|^\nu}\Big(\phi_\ell(\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{z}) - \sum_{k=0}^{2\ell+1}\frac{1}{k!}\langle -\boldsymbol{z},\nabla\rangle^k \phi_\ell(\boldsymbol{y}-\boldsymbol{x})\Big),$$

where the odd derivatives cancel in the sum-integral due to symmetry. With these considerations, the term $\mathcal{S}_\varepsilon$ takes the form

$$\mathcal{S}_\varepsilon = -\lim_{\beta\to 0} \sum\!\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d\setminus\bar{B}_\varepsilon,\Lambda} \frac{\hat{\chi}_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\Big(T_{\varepsilon,\boldsymbol{z}}^{(1)} + T_{\varepsilon,\boldsymbol{z}}^{(2)}\Big),$$

with

$$T_{\varepsilon,\boldsymbol{z}}^{(1)} = \sum_{k=0}^{\ell}\frac{1}{(2k)!}\int_{\partial B_\varepsilon}\sum_{m=0}^{\ell}\Big(\langle\nabla,\boldsymbol{z}\rangle^{2k}\partial_{\boldsymbol{n_y}}\Delta^{\ell-m}\phi_\ell(\boldsymbol{y}) - \langle\nabla,\boldsymbol{z}\rangle^{2k}\Delta_{\boldsymbol{y}}^{\ell-m}\phi_\ell(\boldsymbol{y})\partial_{\boldsymbol{n_y}}\Big) \times \Delta^m g(\boldsymbol{y}+\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{y}},$$

and where

$$T_{\varepsilon,\boldsymbol{z}}^{(2)} = -\int_{\partial B_\varepsilon}\sum_{m=0}^{\ell}\Big(\partial_{\boldsymbol{n_y}}\Delta^{\ell-m}\phi_\ell(\boldsymbol{y}-\boldsymbol{z}) - \Delta_{\boldsymbol{y}}^{\ell-m}\phi_\ell(\boldsymbol{y}-\boldsymbol{z})\partial_{\boldsymbol{n_y}}\Big)\Delta^m g(\boldsymbol{y}+\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{y}}.$$

First consider $T_{\varepsilon,\boldsymbol{z}}^{(1)}$. By Lemma 3.21, it can be rewritten as

$$T_{\varepsilon,\boldsymbol{z}}^{(1)} = \sum_{k=0}^{\ell}\frac{1}{(2k)!}\left(\langle\nabla,\boldsymbol{z}\rangle^{2k}g(\boldsymbol{x}) - \int_{B_\varepsilon}\langle\nabla,\boldsymbol{z}\rangle^{2k}\phi_\ell(\boldsymbol{y})\Delta^{\ell+1}g(\boldsymbol{y}+\boldsymbol{x})\,\mathrm{d}\boldsymbol{y}\right).$$

Then for $T_{\varepsilon,\boldsymbol{z}}^{(2)}$, a simple application of Green's second identity yields

$$T_{\varepsilon,\boldsymbol{z}}^{(2)} = \int_{B_\varepsilon}\phi_\ell(\boldsymbol{y}-\boldsymbol{z})\Delta^{\ell+1}g(\boldsymbol{y}+\boldsymbol{x})\,\mathrm{d}\boldsymbol{y}, \quad |\boldsymbol{z}| > \varepsilon.$$

After inserting both terms, we find for the surface integral S_ε

$$S_\varepsilon = -\Big(\not{\mathcal{D}}_{\Lambda,\nu,\varepsilon}^{(\ell)} g(\boldsymbol{x}) + \mathcal{R}_\varepsilon^{(2)}\Big),$$

where

$$\mathcal{R}_\varepsilon^{(2)} = \lim_{\beta\to 0}\sum\!\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d\setminus\bar{B}_\varepsilon,\Lambda}\hat{\chi}_\beta(\boldsymbol{z})\int_{B_\varepsilon(\boldsymbol{x})} a_\nu^{(\ell)}(\boldsymbol{y}-\boldsymbol{x},\boldsymbol{z})\Delta^{\ell+1}g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

Proposition 3.15 now implies that the limit $\beta\to 0$ in the Bernoulli-$\mathcal{A}$ functions converges in $L^1_{\mathrm{loc}}(\mathbb{R}^d\setminus\{\boldsymbol{0}\})$. Hence, we can interchange the volume integral in $\mathcal{R}_\varepsilon^{(1)}$ with the limit $\beta \to 0$. We finally merge $\mathcal{R}_\varepsilon^{(1)}$ and $\mathcal{R}_\varepsilon^{(2)}$ into a single remainder term

$$\mathcal{R}_{\Lambda,\nu,\varepsilon}^{(\ell)} g(\boldsymbol{x}) = \mathcal{R}_\varepsilon^{(1)} + \mathcal{R}_\varepsilon^{(2)} = \sum_{\boldsymbol{z}\in\mathbb{R}^d\setminus\bar{B}_\varepsilon,\Lambda}\!\diagup \quad \hat{\chi}_\beta(\boldsymbol{z}) \int_\Omega a_\nu^{(\ell)}(\boldsymbol{y}-\boldsymbol{x},\boldsymbol{z})\Delta^{\ell+1} g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

We have thus reached the desired form for the ε-dependent terms,

$$-S_\varepsilon + \mathcal{R}_\varepsilon^{(1)} = \mathcal{D}\!\!\!\!/_{\Lambda,\nu,\varepsilon}^{(\ell)} g(\boldsymbol{x}) + \mathcal{R}_{\Lambda,\nu,\varepsilon}^{(\ell)} g(\boldsymbol{x}).$$

□

CHAPTER 4

Hypersingular Euler–Maclaurin expansion and connection to analytic number theory

1. Introduction

In the derivation of the SEM expansion for interior lattice points, we have been able to include singularities inside the integration region Ω by introducing a free parameter ε. Often, by removing such parameters, we are able to remove unnecessary complexity, thereby providing a clearer and more unconstrained view on the inner workings of the theory. In this particular case, the removal of ε is going to reveal a deep connection of our method to analytic number theory. This connection proves very useful in the following, as it provides us with efficient methods for the evaluation of the arising operator coefficients.

2. Derivation of the hypersingular Euler–Maclaurin expansion

We now set out to eliminate the parameter ε by performing the limit $\varepsilon \to 0$. However, the interaction is not always locally integrable and hence divergent integrals may arise if ε is taken to zero. For this reason, we now give meaning to such divergent integrals by means of the Hadamard finite-part integral, see e.g. [38, Chapter 5].

DEFINITION 4.1 (Hadamard finite-part integral). Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and $\boldsymbol{x} \in \Omega$. Consider a function $f_{\boldsymbol{x}} : \bar{\Omega} \setminus \{\boldsymbol{x}\} \to \mathbb{C}$ of the form

$$f_{\boldsymbol{x}}(\boldsymbol{y}) = \frac{g(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^{\nu}}$$

with $\nu \in \mathbb{C}$ and $g \in \mathscr{D}(\Omega)$. The Hadamard finite-part integral is then defined as the action of the homogeneous distribution $|\cdot|^{-\nu}$ on the shifted function g,

$$\underset{\Omega}{⨍} f_{\boldsymbol{x}}(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y} = \Big\langle |\cdot|^{-\nu}, g(\boldsymbol{x}+\cdot) \Big\rangle.$$

This chapter is based on [7, Sections 5–7].

If $\nu \neq d+k$, $k \in \mathbb{N}_0$, the Hadamard integral can be uniquely extended to functions $g \in C^\ell(\bar{\Omega})$, $\ell \in \mathbb{N}_0$, with $\ell \geq \ell_{\nu,d}$,

$$\ell_{\nu,d} = \lfloor \mathrm{Re}(\nu) - d \rfloor,$$

and $\lfloor t \rfloor$ the nearest integer smaller than or equal to t. The extension reads

$$\fint_\Omega f_{\boldsymbol{x}}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \lim_{\varepsilon \to 0} \left(\int_{\Omega \setminus B_\varepsilon(\boldsymbol{x})} f_{\boldsymbol{x}}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} - \big(\mathcal{H}_{\nu,\varepsilon} g\big)(\boldsymbol{x}) \right)$$

with

$$\mathcal{H}_{\nu,\varepsilon} = \sum_{k=0}^{\ell_{\nu,d}} \frac{1}{k!} \int_{\mathbb{R}^d \setminus B_\varepsilon} \frac{\langle \boldsymbol{y}, \nabla \rangle^k}{|\boldsymbol{y}|^\nu}\,\mathrm{d}\boldsymbol{y}.$$

If on the other hand $\nu = d+k$, $k \in \mathbb{N}_0$, the Hadamard integral is uniquely defined up to derivatives of g of order $\nu - d$. One possible choice is

$$\mathcal{H}_{\nu,\varepsilon} = \sum_{k=0}^{\ell_{\nu,d}-1} \frac{1}{k!} \int_{\mathbb{R}^d \setminus B_\varepsilon} \frac{\langle \boldsymbol{y}, \nabla \rangle^k}{|\boldsymbol{y}|^\nu}\,\mathrm{d}\boldsymbol{y} + \frac{1}{\ell_{\nu,d}!} \int_{B_1 \setminus B_\varepsilon} \frac{\langle \boldsymbol{y}, \nabla \rangle^{\ell_{\nu,d}}}{|\boldsymbol{y}|^\nu}\,\mathrm{d}\boldsymbol{y}.$$

Due to spherical symmetry of $|\cdot|^{-\nu}$, the non-unique term vanishes if ν is odd. Other choices for the Hadamard integral are obtained by replacing the domain B_1 above by a bounded and open neighbourhood of $\boldsymbol{0}$.

Integrals that involve the Hadamard regularisation are also referred to as hypersingular integrals. As the expansion that we are going to derive in the following relies on the Hadamard finite-part integral, we shall call it the hypersingular Euler–Maclaurin expansion (HSEM).

One important strategy that we have used in the derivation of the SEM expansion is to consider regularised differences between sums and integrals. This procedure gives meaning to otherwise divergent sums, even if the summand function increases at a polynomial rate at infinity and hence is neither integrable nor summable. Moving on from divergences that arise due to an unfavourable asymptotic behaviour at infinity, we consider divergences that occur due to a local non-integrable algebraic singularity. We can extend the sum-integral in a very natural way to summand functions of this sort by excluding the divergent addend in the sum and by making use of the Hadamard regularisation in the integral.

Definition 4.2 (Hadamard sum-integral). Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, $\boldsymbol{x} \in \Lambda$, and $\Omega \subset \mathbb{R}^d$ a bounded domain such that $\partial\Omega \cap \Lambda = \varnothing$. Let $f_{\boldsymbol{x}} : \Omega \to \mathbb{C}$ be of the form

$$f_{\boldsymbol{x}}(\boldsymbol{y}) = \frac{g(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|^\nu},$$

with $\nu \in \mathbb{C}$ and $g \in C^\ell(\Omega)$, $\ell \in \mathbb{N}_0$ such that $\ell \geq \ell_{\nu,d}$. We then define the Hadamard sum-integral as

$$\sum\!\!\!\!\!\!\!\int_{\Omega,\Lambda} f_{\boldsymbol{x}} = {\sum_{\boldsymbol{y}\in\Omega\cap\Lambda}}' f_{\boldsymbol{x}}(\boldsymbol{y}) - \frac{1}{V_\Lambda} \fint_\Omega f_{\boldsymbol{x}}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y},$$

where the primed sum excludes $\boldsymbol{y} = \boldsymbol{x}$.

The local HSEM differential operator is then defined in terms of regularised Hadamard sum-integrals.

Definition 4.3 (Hypersingular Euler–Maclaurin operator). Let $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$, $\nu \in \mathbb{C}$, and $\ell \in \mathbb{N}_0$. We define the ℓth order hypersingular Euler–Maclaurin (HSEM) operator $\mathcal{D}_{\Lambda,\nu}^{(\ell)}$ as

$$\mathcal{D}_{\Lambda,\nu}^{(\ell)} = \sum_{k=0}^{\ell} \frac{1}{(2k)!} \lim_{\beta\to 0} \sum\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\langle \boldsymbol{z}, \nabla\rangle^{2k}}{|\boldsymbol{z}|^\nu}.$$

The infinite order operator $\mathcal{D}_{\Lambda,\nu}$ is obtained by setting $\ell = \infty$ in the above definition.

Theorem 4.4 (Hypersingular Euler–Maclaurin expansion). *Consider $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\Omega \subset \mathbb{R}^d$ a bounded domain such that $\partial\Omega \cap \Lambda = \varnothing$. For $\boldsymbol{x} \in \Lambda \cap \Omega$, let $f_{\boldsymbol{x}} : \bar{\Omega} \to \mathbb{C}$ be of the form*

$$f_{\boldsymbol{x}}(\boldsymbol{y}) = \frac{g(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^\nu},$$

with $\nu \in \mathbb{C}$ and $g \in C^{2m+3}(\bar{\Omega})$, $m \in \mathbb{N}_0$, such that

$$2(m+1) \geq \ell_{\nu,d} = \lfloor \mathrm{Re}(\nu) - d \rfloor.$$

Then for $\ell \in \mathbb{N}_0$ with $\ell \leq m$,

$$\sum\!\!\!\!\!\!\!\int_{\Omega,\Lambda} f_{\boldsymbol{x}} = \mathcal{D}_{\Lambda,\nu}^{(\ell)} g(\boldsymbol{x}) + \mathcal{S}_{\Lambda,\nu}^{(\ell)} g(\boldsymbol{x}) + \mathcal{R}_{\Lambda,\nu}^{(\ell)} g(\boldsymbol{x}).$$

The expansion of the sum-integral consists of the local HSEM operator $\mathcal{D}_{\Lambda,\nu}^{(\ell)}$, of a surface integral over derivatives of g of up to order $2\ell+1$,

$$\mathcal{S}_{\Lambda,\nu}^{(\ell)} g(\boldsymbol{x}) = \int_{\partial\Omega} \left\langle \boldsymbol{\mathcal{D}}_{\Lambda,\nu,\boldsymbol{y}-\boldsymbol{x}}^{(\ell)}\, g(\boldsymbol{y}), \boldsymbol{n}_{\boldsymbol{y}} \right\rangle \mathrm{d}S_{\boldsymbol{y}},$$

and of the remainder

$$\mathcal{R}_{\Lambda,\nu}^{(\ell)} g(\boldsymbol{x}) = \lim_{\beta\to 0} \sum\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \int_\Omega a_\nu^{(\ell)}(\boldsymbol{y}-\boldsymbol{x},\boldsymbol{z}) \Delta^{\ell+1} g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

Proof. We begin with the SEM for interior lattice points in Theorem 3.20,

$$\sum\!\!\!\!\!\!\!\int_{\Omega\setminus B_\varepsilon(\boldsymbol{x}),\Lambda} f_{\boldsymbol{x}} = \mathcal{D}^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}) + \mathcal{R}^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}) + \mathcal{S}^{(\ell)}_{\Lambda,\nu} g(\boldsymbol{x}),$$

and add the Hadamard regularisation per lattice covolume to both sides,

$$\frac{\mathcal{H}_{\varepsilon,\nu} g(\boldsymbol{x})}{V_\Lambda} = \frac{1}{V_\Lambda}\sum_{k=0}^{\ell_{\nu,d}} \frac{1}{k!}\int_{\mathbb{R}^d\setminus B_\varepsilon} \frac{\langle \boldsymbol{y},\nabla\rangle^k}{|\boldsymbol{y}|^\nu} g(\boldsymbol{x})\,\mathrm{d}\boldsymbol{y}.$$

If the case $2k=\nu$ is encountered, then replace $\mathbb{R}^d\setminus B_\varepsilon$ by $B_1\setminus B_\varepsilon$ in the corresponding integral. We now show that the HSEM expansion is found as we take the limit $\varepsilon\to 0$ on both sides of above equation. The left hand side readily follows from the definition of the Hadamard integral,

$$\lim_{\varepsilon\to 0}\left(\sum\!\!\!\!\!\!\!\int_{\Omega\setminus B_\varepsilon(\boldsymbol{x}),\Lambda} f_{\boldsymbol{x}} + \frac{\mathcal{H}_{\varepsilon,\nu} g(\boldsymbol{x})}{V_\Lambda}\right) = \sum\!\!\!\!\!\!\!\int_{\Omega,\Lambda} f_{\boldsymbol{x}}.$$

On the right hand side, we first separate the Hadamard regularisation into two contributions,

$$\mathcal{H}_{\varepsilon,\nu} g(\boldsymbol{x}) = \mathcal{H}^{(1)}_{\varepsilon,\nu} g(\boldsymbol{x}) + \mathcal{H}^{(2)}_{\varepsilon,\nu} g(\boldsymbol{x}).$$

Here $\mathcal{H}^{(1)}_{\varepsilon,\nu} g(\boldsymbol{x})$ consists of the directional derivatives of g of order smaller or equal $2\ell+1$ and $\mathcal{H}^{(2)}_{\varepsilon,\nu} g(\boldsymbol{x})$ includes any remaining higher order derivatives. Note that in the following odd derivatives cancel due to due to the symmetry of the lattice and the interaction. We prove that the first contribution regularises the HSEM operator while the second regularisation is absorbed in the remainder integral. We compute the first limit and obtain

$$\begin{aligned}
&\lim_{\varepsilon\to 0}\left(\mathcal{D}^{(\ell)}_{\Lambda,\nu,\varepsilon} + \frac{\mathcal{H}^{(1)}_{\varepsilon,\nu} g(\boldsymbol{x})}{V_\Lambda}\right)\\
&=\lim_{\varepsilon\to 0}\left(\sum_{k=0}^{\ell}\frac{1}{(2k)!}\lim_{\beta\to 0}\sum\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d\setminus\bar{B}_\varepsilon,\Lambda}\hat{\chi}_\beta(\boldsymbol{z})\frac{\langle\nabla,\boldsymbol{z}\rangle^{2k}}{|\boldsymbol{z}|^\nu}g(\boldsymbol{x}) + \frac{\mathcal{H}^{(1)}_{\varepsilon,\nu} g(\boldsymbol{x})}{V_\Lambda}\right)\\
&=\sum_{k=0}^{\ell}\frac{1}{(2k)!}\lim_{\beta\to 0}\sum\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda}\hat{\chi}_\beta(\boldsymbol{z})\frac{\langle\nabla,\boldsymbol{z}\rangle^{2k}}{|\boldsymbol{z}|^\nu}g(\boldsymbol{x})\\
&=\mathcal{D}^{(\ell)}_{\Lambda,\nu} g(\boldsymbol{x}),
\end{aligned}$$

where we have used that $\hat{\chi}_\beta \to 1$ for $\beta \to 0$ in $C^\infty(\mathbb{R}^d)$. Thus derivatives of $\hat{\chi}_\beta$ do not contribute in the Hadamard integral. Concerning the second limit, we first write the remainder integral as

$$\mathcal{R}^{(\ell)}_{\Lambda,\nu,\varepsilon}(\boldsymbol{x}) = \lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d\setminus\bar{B}_\varepsilon,\Lambda} \frac{\hat{\chi}_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} h_{\boldsymbol{x}}(\boldsymbol{z}),$$

where we have defined the auxiliary function

$$h_{\boldsymbol{x}}(\boldsymbol{z}) = \int_\Omega \Big(\phi_\ell(\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{z}) - \sum_{k=0}^{2\ell+1} \frac{1}{k!}\langle -\boldsymbol{z}, \nabla\rangle^k \phi_\ell(\boldsymbol{y}-\boldsymbol{x})\Big)\Delta^{\ell+1} g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

We show that the appropriate Hadamard regularisation for the sum-integral in the remainder coincides with the second Hadamard regularisation above, namely

$$\mathcal{H}_{\varepsilon,\nu} h_{\boldsymbol{x}}(\boldsymbol{0}) = \mathcal{H}^{(2)}_{\varepsilon,\nu} g(\boldsymbol{x}).$$

We first have that

$$\langle \boldsymbol{z}, \nabla\rangle^k h_{\boldsymbol{z}}(\boldsymbol{0}) = 0, \quad k = 0,\dots,2\ell+1,$$

as a truncated Taylor expansion of order $2\ell+1$ has been subtracted from the shifted fundamental solution. These orders hence need no regularisation. Then by the integral representation of the poly-Laplace operator in Proposition 3.7, we transform the directional derivatives in the second Hadamard regularisation into powers of the Laplace operator,

$$\mathcal{H}^{(2)}_{\varepsilon,\nu} g(\boldsymbol{x}) = \sum_{k=\ell+1}^{\lfloor \ell_{\nu,d}/2\rfloor} \frac{1}{(2k)!} \int_{\mathbb{R}^d\setminus B_\varepsilon} \frac{|\boldsymbol{y}|^{2k-\nu}}{p_{k,d}}\,\mathrm{d}\boldsymbol{y}\ \Delta^k g(\boldsymbol{x}),$$

where we again replace $\mathbb{R}^d \setminus B_\varepsilon$ by $B_1 \setminus B_\varepsilon$ if the case $2k = \nu$ arises. Now as $k \geq \ell+1$ we find by the representation formula for the poly-Laplace operator in Lemma 3.5 that

$$\begin{aligned}
&\Delta^k h_{\boldsymbol{x}}(\boldsymbol{0})\\
&= \Delta^k_{\boldsymbol{z}} \int_\Omega \Big(\phi_\ell(\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{z}) - \sum_{k=0}^{2\ell+1}\frac{1}{k!}\langle -\boldsymbol{z},\nabla\rangle^k \phi_\ell(\boldsymbol{y}-\boldsymbol{x})\Big)\Delta^{\ell+1} g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\Big|_{\boldsymbol{z}=\boldsymbol{0}}\\
&= \Delta^{k-(\ell+1)}_{\boldsymbol{z}} \Delta^{\ell+1}_{\boldsymbol{z}} \int_\Omega \phi_\ell(\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{z})\Delta^{\ell+1} g(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\Big|_{\boldsymbol{z}=\boldsymbol{0}}\\
&= \Delta^{k-(\ell+1)}\Delta^{\ell+1} g(\boldsymbol{x}+\boldsymbol{z})\Big|_{\boldsymbol{z}=\boldsymbol{0}}\\
&= \Delta^k g(\boldsymbol{x}),
\end{aligned}$$

as $g \in C^{2m+3}$, with $2m+3 > 2(k+1)$. The evaluation of the limit $\varepsilon \to 0$ then follows as

$$\begin{aligned}\lim_{\varepsilon\to 0}&\left(\mathcal{R}^{(\ell)}_{\Lambda,\nu,\varepsilon} g(\boldsymbol{x}) + \frac{\mathcal{H}^{(2)}_{\nu,\varepsilon} g(\boldsymbol{x})}{V_\Lambda}\right)\\ &= \lim_{\varepsilon\to 0}\left(\lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d\setminus\bar{B}_\varepsilon,\Lambda} \frac{\hat{\chi}_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} h_{\boldsymbol{x}}(\boldsymbol{z}) + \frac{\mathcal{H}_{\nu,\varepsilon} h_{\boldsymbol{x}}(\boldsymbol{0})}{V_\Lambda}\right)\\ &= \lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \frac{\hat{\chi}_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} h_{\boldsymbol{x}}(\boldsymbol{z}),\end{aligned}$$

and we have recovered all terms in the HSEM expansion.

□

3. Connection to analytic number theory

In the previous section, we have established the HSEM expansion, whose main contribution is the local HSEM operator. For $\Omega = \mathbb{R}^d$, this local operator is the only contribution in the expansion. However, the coefficients of this operator are defined in terms of regularised Hadamard sum-integrals, whose numerical computation is challenging in higher dimensions. This final problem, which stands in the way of an efficient computation of singular sums by means of Hadamard integrals and local differential operators, is overcome in this section. We show that our method exhibits a deep connection to analytic number theory. It is this connection that provides us with an efficient method for the computation of the HSEM operator coefficients.

We first present an alternative representation of the HSEM operator $\mathcal{D}\!\!\!\!/\,_{\Lambda,\nu}$.

THEOREM 4.5. *For $\Lambda \in \mathfrak{L}(\mathbb{R}^d)$ and $\nu \in \mathbb{C}$, we set $\mathcal{Z}^{(0)}_{\Lambda^*,\nu} : \mathbb{R}^d \setminus \Lambda^* \to \mathbb{C}$,*

$$\mathcal{Z}^{(0)}_{\Lambda^*,\nu}(\boldsymbol{y}) = \lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{e^{-2\pi i\,\langle \boldsymbol{z},\boldsymbol{y}\rangle}}{|\boldsymbol{z}|^\nu},$$

where the function depends on the choice of the Hadamard regularisation in case that $\nu = d+2k$, $k \in \mathbb{N}_0$. For all choices, $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ can be extended to an analytic function on $\mathbb{R}^d \setminus \Lambda^* \cup \{\boldsymbol{0}\}$ and the infinite order HSEM operator admits the representation

$$\mathcal{D}\!\!\!\!/\,_{\Lambda,\nu} = \mathcal{Z}^{(0)}_{\Lambda^*,\nu}\left(-\frac{\nabla}{2\pi i}\right) = \lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{e^{\langle \boldsymbol{z},\nabla\rangle}}{|\boldsymbol{z}|^\nu},$$

in the sense of a Taylor expansion of the function $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ around zero. The finite order operators are found by truncating the Taylor expansion at the corresponding order.

Proof. We conduct the proof in close analogy to the one of Theorem 2.16. First, we show well-definedness of $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ as a distribution. The sum is investigated in the aforementioned proof, hence only a discussion of the Hadamard integral is required. Let $\beta > 0$ and define the auxiliary distribution $u_\beta \in \mathscr{D}'(\mathbb{R}^d)$ via

$$\langle u_\beta, \psi \rangle = \int_{\mathbb{R}^d} \psi(\boldsymbol{y}) \left(\fint_{\mathbb{R}^d} \hat{\chi}_\beta(\boldsymbol{z}) \frac{e^{-2\pi i \langle \boldsymbol{z}, \boldsymbol{y} \rangle}}{|\boldsymbol{z}|^\nu} \,\mathrm{d}\boldsymbol{z} \right) \mathrm{d}\boldsymbol{y}, \quad \psi \in \mathscr{D}(\mathbb{R}^d).$$

By superpolynomial decay of the smooth cutoff function $\hat{\chi}_\beta$, we can exchange the Hadamard integral with the integration over $\mathbb{R}^d$. This results in

$$\langle u_\beta, \psi \rangle = \fint_{\mathbb{R}^d} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\hat{\psi}(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} \,\mathrm{d}\boldsymbol{z}.$$

Now note that the Hadamard integral defines an extension of the function s_ν to a tempered distribution $\bar{s}_\nu \in S'(\mathbb{R}^d)$. Thus, we can write the action of u_β in the form

$$\langle u_\beta, \psi \rangle = \left\langle \hat{\chi}_\beta \bar{s}_\nu, \hat{\psi} \right\rangle.$$

Due to $\hat{\chi}_\beta \to 1$ as $\beta \to 0$ in $C^\infty(\mathbb{R}^d)$, we find by continuity of the multiplication of a distribution with a smooth function that

$$\lim_{\beta \to 0} \langle u_\beta, \psi \rangle = \left\langle \bar{s}_\nu, \hat{\psi} \right\rangle, \quad \psi \in \mathscr{D}(\mathbb{R}^d).$$

Thus $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ defines a distribution via

$$\langle \mathcal{Z}^{(0)}_{\Lambda^*,\nu}, \psi \rangle = \sum_{\boldsymbol{z} \in \Lambda}{}' \frac{\hat{\psi}(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} - \frac{1}{V_\Lambda} \left\langle \bar{s}_\nu, \hat{\psi} \right\rangle, \quad \psi \in \mathscr{D}(\mathbb{R}^d).$$

In the next step, we show that $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ can even be identified as an analytic function on $\mathbb{R}^d \setminus \Lambda^* \cup \{\boldsymbol{0}\}$. To this end, we first impose the familiar restriction $\mathrm{Re}(\nu) < -(d+1)$. Poisson summation then yields

$$\underset{\boldsymbol{z} \in \mathbb{R}^d, \Lambda}{\not\!\!\sum\!\!\!\!\!\!\int} \hat{\chi}_\beta(\boldsymbol{z}) \frac{e^{-2\pi i \langle \boldsymbol{z}, \boldsymbol{y} \rangle}}{|\boldsymbol{z}|^\nu} = V_{\Lambda^*} \sum_{\boldsymbol{z} \in \Lambda^*}{}' \chi_\beta * \hat{s}_\nu(\boldsymbol{z} + \boldsymbol{y}),$$

where the Hadamard integral coincides with the integral for this choice of ν. This type of series has been investigated by us in the proof of Theorem 2.16. Here the only important difference is that the origin is excluded in above sum. But as Lemma 2.18 also holds for all subsets of Λ^*, in particular for $\Lambda^* \setminus \{\mathbf{0}\}$, the rest of the proof follows in analogy to that of Theorem 2.16. We then recover the operator coefficients of the HSEM operator $\mathcal{D}_{\Lambda,\nu}$ by a Taylor expansion of $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ at $\mathbf{0}$.

□

In the following theorem, we show that the regularised Hadamard sum-integral generates meromorphic continuations of multidimensional lattice sums. The theorem forms the basis for the connection of our method to analytic number theory and will provide us with efficient methods for the computation of the HSEM operator coefficients. It however also represents a relevant result on its own.

THEOREM 4.6 (Meromorphic continuation of Dirichlet series). *Let $P : \mathbb{R}^d \to \mathbb{C}$ be a polynomial of order $m \in \mathbb{N}_0$. Then for $\nu \in \mathbb{C}$ such that $\operatorname{Re}(\nu) > d + m$, the regularised Hadamard sum-integral equals its associated Dirichlet series,*

$$\lim_{\beta \to 0} \sum\!\!\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d, \Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} = \sum_{\boldsymbol{z} \in \Lambda}{}' \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu},$$

where the primed sum excludes $\boldsymbol{z} = 0$. Moreover, the left hand side forms, as a function of ν, the meromorphic continuation of the Dirichlet series to $\nu \in \mathbb{C}$, whose simple poles lie at $\nu = d + 2k$, $k \in \mathbb{N}_0$, with residues

$$\frac{\omega_d}{V_\Lambda} \frac{(1/2)_k}{(2k)!(d/2)_k} \Delta^k P(\mathbf{0}).$$

The proof of this theorem requires two lemmas that investigate holomorphy of the sum-integral and of the Hadamard integral in ν.

LEMMA 4.7. *Let $P : \mathbb{R}^d \to \mathbb{C}$ be a polynomial and let $\delta > 0$ with $\delta < a_\Lambda$. Then*

$$\lim_{\beta \to 0} \sum\!\!\!\!\!\!\!\!\int_{\boldsymbol{z} \in \mathbb{R}^d \setminus B_\delta, \Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}$$

defines an entire function in ν.

PROOF. In analogy to the proof of Proposition 3.15, we use the EM expansion on unbounded domains of sufficiently high order and express the regularised sum-integral in terms of a surface integral and a volume integral that includes derivatives of $|\cdot|^{-\nu} P$. It then follows that all integrands as well as the resulting integrals are entire functions in ν.

□

LEMMA 4.8. *Let $P:\mathbb{R}^d \to \mathbb{C}$ be a polynomial of degree $m \in \mathbb{N}_0$ and let $\delta > 0$. Then for $\nu \in \mathbb{C}$, $\nu \neq d+2k$, $k \in \mathbb{N}_0$, it holds*

$$\fint_{B_\delta} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z} = -\sum_{k=0}^{\lfloor m/2\rfloor} \omega_d \frac{(1/2)_k}{(2k)!(d/2)_k} \frac{\delta^{-\nu+(2k+d)}}{\nu-(2k+d)} \Delta^k P(\boldsymbol{0}),$$

Hence the left hand side defines a meromorphic function in ν with simple poles at $\nu = d+2k$, $k \in \mathbb{N}_0$, and associated residues

$$-\omega_d \frac{(1/2)_k}{(2k)!(d/2)_k} \Delta^k P(\boldsymbol{0}).$$

PROOF. The polynomial P is equal to its Taylor series of order m around the origin,

$$P(\boldsymbol{z}) = \sum_{k=0}^{m} \frac{1}{k!} \langle \boldsymbol{z}, \nabla\rangle^k P(\boldsymbol{0}).$$

We insert this representation of the polynomial into the Hadamard integral and find that

$$\begin{aligned}
&\fint_{B_\delta} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z} \\
&= \lim_{\varepsilon\to 0}\left(\int_{B_\delta\setminus B_\varepsilon} \sum_{k=0}^{m} \frac{1}{k!} \frac{\langle \boldsymbol{z},\nabla\rangle^k}{|\boldsymbol{z}|^\nu} P(\boldsymbol{0})\,\mathrm{d}\boldsymbol{z} - \int_{\mathbb{R}^d\setminus B_\varepsilon} \sum_{k=0}^{\ell_{\nu,d}} \frac{1}{k!} \frac{\langle \boldsymbol{z},\nabla\rangle^k}{|\boldsymbol{z}|^\nu} P(\boldsymbol{0})\,\mathrm{d}\boldsymbol{z}\right) \\
&= -\sum_{k=0}^{\ell_{\nu,d}} \frac{1}{k!} \int_{\mathbb{R}^d\setminus B_\delta} \frac{\langle \boldsymbol{z},\nabla\rangle^k}{|\boldsymbol{z}|^\nu} P(\boldsymbol{0})\,\mathrm{d}\boldsymbol{z} + \sum_{k=\max\{0,\ell_{\nu,d}+1\}}^{m} \frac{1}{k!} \int_{B_\delta} \frac{\langle \boldsymbol{z},\nabla\rangle^k}{|\boldsymbol{z}|^\nu} P(\boldsymbol{0})\,\mathrm{d}\boldsymbol{z},
\end{aligned}$$

where $\ell_{\nu,d} = \lfloor \mathrm{Re}(\nu) - d\rfloor$. The integral representation of the poly-Laplace operator in Proposition 3.7 then yields

$$\begin{aligned}
\fint_{B_\delta} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z} = &-\sum_{k=0}^{\lfloor \ell_{\nu,d}/2\rfloor} \frac{1}{(2k)!} \int_{\mathbb{R}^d\setminus B_\delta} \frac{|\boldsymbol{z}|^{2k-\nu}}{p_{k,d}}\,\mathrm{d}\boldsymbol{z}\,\Delta^k P(\boldsymbol{0}) \\
&+ \sum_{k=\max\{0,\lfloor(\ell_{\nu,d}+1)/2\rfloor\}}^{\lfloor m/2\rfloor} \frac{1}{(2k)!} \int_{B_\delta} \frac{|\boldsymbol{z}|^{2k-\nu}}{p_{k,d}}\,\mathrm{d}\boldsymbol{z}\,\Delta^k P(\boldsymbol{0}),
\end{aligned}$$

where odd derivatives cancel due to the rotational symmetry of $\mathbb{R}^d \setminus B_\delta$ and B_δ. We then evaluate the integrals on the right hand side and obtain

$$\fint_{B_\delta} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z} = -\sum_{k=0}^{\lfloor m/2\rfloor} \frac{1}{(2k)!} \frac{\omega_d}{p_{k,d}} \frac{\delta^{-\nu+(2k+d)}}{\nu-(2k+d)} \Delta^k P(\boldsymbol{0}).$$

The residues follow after inserting the definition of the prefactor $p_{k,d}$ from Proposition 3.7.

□

Equipped with the previous two lemmas, we now move on to the proof of Theorem 4.6.

Proof of Theorem 4.6. In the first step, we show that the regularised Hadamard sum-integral is a meromorphic function in ν. To this end, define the auxiliary function $P_\beta = \hat{\chi}_\beta P$. For $\delta > 0$ with $\delta < a_\Lambda$, we then separate the sum-integral into two parts,

$$\begin{aligned}\lim_{\beta\to 0} \mathop{\sum\!\!\!\!\!\!\fint}_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \frac{P_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} &= \lim_{\beta\to 0} \mathop{\sum\!\!\!\!\!\!\fint}_{\boldsymbol{z}\in\mathbb{R}^d\setminus B_\delta,\Lambda} \frac{P_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} - \frac{1}{V_\Lambda}\lim_{\beta\to 0}\fint_{B_\delta} \frac{P_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z}\\ &= \lim_{\beta\to 0} \mathop{\sum\!\!\!\!\!\!\fint}_{\boldsymbol{z}\in\mathbb{R}^d\setminus B_\delta,\Lambda} \frac{P_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} - \frac{1}{V_\Lambda}\fint_{B_\delta} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z},\end{aligned}$$

where the second equality follows from the locality of the Hadamard integral together with $\hat{\chi}_\beta \to 1$ as $\beta \to 0$ in $C^\infty(\mathbb{R}^d)$. We have shown in Lemma 4.7 that the first term on the right hand side is an entire function in ν. We furthermore know from Lemma 4.8 that the second term is a meromorphic function in ν whose simple poles lie at $\nu = d + 2k$, $k \in \mathbb{N}_0$. Hence also

$$\lim_{\beta\to 0} \mathop{\sum\!\!\!\!\!\!\fint}_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \frac{P_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}$$

defines a meromorphic function in ν whose poles and associated residues readily follow from Lemma 4.8.

In the second step, we show that the regularised Hadamard sum-integral equals its associated Dirichlet series for $\mathrm{Re}(\nu) > d + m$. For these values of ν, the sum-integral converges absolutely without the β-regularisation, and we have that

$$\lim_{\beta\to 0} \mathop{\sum\!\!\!\!\!\!\fint}_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \frac{P_\beta(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} = \sideset{}{'}\sum_{\boldsymbol{z}\in\Lambda} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} - \frac{1}{V_\Lambda}\fint_{\mathbb{R}^d} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z}.$$

Due to $\ell_{\nu,d} > m$, the Hadamard integral equals zero,

$$\fint_{\mathbb{R}^d} \frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu}\,\mathrm{d}\boldsymbol{z} = \lim_{\varepsilon\to 0}\int_{\mathbb{R}^d\setminus B_\varepsilon} \left(\frac{P(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} - \sum_{k=0}^{\ell_{\nu,d}} \frac{1}{k!}\frac{\langle \boldsymbol{z},\nabla\rangle^k}{|\boldsymbol{z}|^\nu}P(\boldsymbol{0})\right)\mathrm{d}\boldsymbol{z} = 0,$$

thus showing that the sum-integral and the associated Dirichlet series coincide.

□

The HSEM operator coefficients are related to the Epstein zeta function, introduced by Epstein in [19, 20], which provides a generalisation of the Riemann zeta function to higher dimensions. This function is a well-known tool in analytic number theory [16].

DEFINITION 4.9 (Epstein zeta function). For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, $A \in \mathbb{R}^{d\times d}$ symmetric positive definite and $\nu \in \mathbb{C}$ with $\mathrm{Re}(\nu) > d$, the Epstein zeta function Z is defined by the Dirichlet series

$$Z\begin{vmatrix}\boldsymbol{x}\\ \boldsymbol{y}\end{vmatrix}(A;\nu) = {\sum_{\boldsymbol{z}\in\mathbb{Z}^d}}' \frac{e^{-2\pi i\langle \boldsymbol{z},\boldsymbol{y}\rangle}}{|\boldsymbol{z}+\boldsymbol{x}|_A^{\nu}},$$

with

$$|\boldsymbol{z}|_A = \sqrt{\boldsymbol{z}^\top A\, \boldsymbol{z}},$$

and where the primed sum excludes $\boldsymbol{z} = -\boldsymbol{x}$. The Epstein zeta function can be analytically continued to a holomorphic function in ν if not both $\boldsymbol{x} \in \mathbb{Z}^d$ and $\boldsymbol{y} \in \mathbb{Z}^d$. If on the other hand $\boldsymbol{x} \in \mathbb{Z}^d$ and $\boldsymbol{y} \in \mathbb{Z}^d$, then it can be continued to an meromorphic function in ν with a simple pole at $\nu = d$. We furthermore define the simple Epstein zeta function Z_0 such that

$$Z_0(A;\nu) = Z\begin{vmatrix}\mathbf{0}\\ \mathbf{0}\end{vmatrix}(A;\nu).$$

The Epstein zeta function has been used by Emersleben [17, 18], a PhD student of Max Born, as a tool in the precise computation of the electrostatic potential of ionic lattices. There exist series representations of the Epstein zeta function that converge exponentially fast, the most relevant example being the Chowla-Selberg formula, see [16] and references therein. With these representations, we can efficiently evaluate Epstein zeta in any number of space dimensions.

The following example uses the formula for meromorphic continuations of Dirichlet series from Theorem 4.6 and provides alternative globally convergent representations of the Epstein and Riemann zeta functions.

EXAMPLE 4.10. The Hadamard sum-integral allows us to write the simple Epstein zeta function via

$$\lim_{\beta\to 0} \sumint_{\mathbb{R}^d,\Lambda} \frac{\hat{\chi}_\beta}{|\cdot|^\nu} = Z_0\big(M_\Lambda^\top M_\Lambda;\nu\big),$$

which is holomorphic for all $\nu \in \mathbb{C}\setminus\{d\}$ with a simple pole at $\nu = d$ with residue

$$\frac{\omega_d}{V_\Lambda} = \frac{\omega_d}{\sqrt{\det(M_\Lambda^\top M_\Lambda)}}.$$

In the special case $d = 1$ and $\Lambda = \mathbb{Z}$, we recover the usual Riemann zeta function ζ,

$$\lim_{\beta\to 0} \mathop{\not{\sum}\!\!\!\!\!\!\int}_{\mathbb{R},\mathbb{Z}} \frac{\hat{\chi}_\beta}{|\cdot|^\nu} = 2\zeta(\nu).$$

Vice versa, we can represent any Epstein zeta function Z_0 by a Hadamard sum-integral. Let $A \in \mathbb{R}^{d\times d}$ symmetric and positive definite. Then the matrix A admits the unique Cholesky factorisation $A = L^\top L$ where $L \in \mathbb{R}^{d\times d}$ is a regular lower triangular matrix. After setting $\Lambda_L = L^\top \mathbb{Z}^d$, we obtain

$$Z_0(A;\nu) = Z_0(L^\top L;\nu) = \lim_{\beta\to 0} \mathop{\not{\sum}\!\!\!\!\!\!\int}_{\mathbb{R}^d,\Lambda_L} \frac{\hat{\chi}_\beta}{|\cdot|^\nu}$$

for $\nu \in \mathbb{C} \setminus \{d\}$.

If we prefer to avoid the use of Hadamard integrals in numerical applications, we can use the SEM for interior lattice points instead of the HSEM. The next corollary then shows that the required local SEM operator $\not{\mathcal{D}}_{\Lambda,\nu,\varepsilon}$ can be deduced from the HSEM operator $\not{\mathcal{D}}_{\Lambda,\nu}$.

Corollary 4.11. *Let $\ell \in \mathbb{N}_0$, $\nu \in \mathbb{C}$ such that $\nu \neq d + 2k$, $k \in \mathbb{N}_0$, and $\varepsilon > 0$ with $\varepsilon < a_\Lambda$. Then*

$$\not{\mathcal{D}}_{\Lambda,\nu,\varepsilon} = \not{\mathcal{D}}_{\Lambda,\nu} - \frac{\omega_d}{V_\Lambda} \sum_{k=0}^{\ell} \frac{(1/2)_k}{(2k)!(d/2)_k} \frac{\varepsilon^{-\nu+(2k+d)}}{\nu - (2k+d)} \Delta^k.$$

Proof. The corollary readily follows from Theorem 4.6 together with the representation of the Hadamard integral from Lemma 4.8. □

We have seen that the regularised Hadamard sum-integral generates meromorphic continuations of multidimensional lattice sums. This result provides a fruitful connection of our method to analytic number theory and gives us access to its vast range of tools, see [4] and references therein. We use these tools in the following in order to efficiently evaluate the HSEM operator coefficients. Hence, we overcome the last challenge in the theory of the HSEM expansion, making it applicable as a numerical method. In the next section, we give a short overview on how to compute the coefficients of the HSEM operator in practice and then move on to a demonstration of the numerical performance of the expansion.

4. Numerical application

4.1. Model description. In this section, we are going to implement the HSEM for a prototypical multidimensional sum that appears in a wide range of physically relevant systems and are going to show that the sum is reliably reproduces by the method. We approximate

$$\sum_{\boldsymbol{y}\in\mathbb{Z}^2}{}' f_{\boldsymbol{x}}(\boldsymbol{y})$$

with $\boldsymbol{x} \in \mathbb{Z}^2$ and

$$f_{\boldsymbol{x}}(\boldsymbol{y}) = \frac{g(\boldsymbol{y})}{|\boldsymbol{y}-\boldsymbol{x}|^\nu}.$$

where $\nu \in \mathbb{C}$. As the interpolating function g, we choose a Gaussian with width $\lambda > 0$,

$$g(\boldsymbol{y}) = e^{-|\boldsymbol{y}|^2/\lambda^2}. \tag{4.1}$$

Sums of this kind can arise in different areas of condensed matter and quantum physics. They appear in the computation of forces in crystals with long-range interactions, see [24] for a review on long-range interacting nanoscale systems. Here the interpolating function g describes the displacement of particles from their equilibrium positions. They also appear in spin lattices, where the interpolating function describes the spin orientation. The fast evaluation of lattice sums then provides the basis for a simulation of spin waves, so called magnons, which can potentially be used as information carriers in spintronics devices [26]. Finally, the above sum appears in the simulation of the discrete nonlinear Schrödinger equation with long-range interactions [35], which models, among others, charge transport in DNA strings and, in higher dimensions, light propagation in nonlinear media. Here the interpolating function can be identified as the wave function.

The choice for $\Lambda = \mathbb{Z}^2$ was made in order to allow for an implementation that can easily be verified by the reader. A reference implementation of the HSEM expansion in *Mathematica* is provided online[1], which is able to reproduce all results in this section. The method can readily be applied to higher dimensional systems after the technical task of implementing the exponentially convergent series representations for the Epstein zeta function from [16] and the resulting HSEM operator coefficients for the lattice under consideration.

4.2. Efficient computation of HSEM operator coefficients. We now discuss how the HSEM operator coefficients are computed for a particular multidimensional lattice Λ. The most general approach consists in implementing the function $\mathcal{Z}^{(0)}_{\Lambda^*,\nu}$ from Proposition 4.5. The

[1] `https://github.com/andreasbuchheit/hsem`

HSEM operator coefficients are then computed from its Taylor series at the origin,

$$\mathcal{D}_{\Lambda,\nu} = \mathcal{Z}^{(0)}_{\Lambda^*,\nu}\left(-\frac{\nabla}{2\pi i}\right) = \sum_{k=0}^{\infty} \frac{1}{(2k)!} \lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\langle \boldsymbol{z}, \nabla\rangle^k}{|\boldsymbol{z}|^\nu},$$

using the summation formulas in [16] as well as their derivatives.

The meromorphic continuation theorem 4.6 now shows that if the regularised Hadamard sum-integral converges without regularisation, it is equal to its associated lattice sum,

$$\lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^d,\Lambda} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\langle \boldsymbol{z}, \nabla\rangle^k}{|\boldsymbol{z}|^\nu} = \sum_{\boldsymbol{z}\in\Lambda}{}' \frac{\langle \boldsymbol{z}, \nabla\rangle^k}{|\boldsymbol{z}|^\nu}.$$

If, on the other hand, the regularisation is necessary, then the sum-integral generates the meromorphic continuation in ν. Of particular importance is the case $k = 0$, which yields the zero order HSEM operator. In many applications, this already forms the dominant contribution and leads to a reliable approximation to the sum. The zero order coefficient is given by a simple Epstein zeta function,

$$\lim_{\beta\to 0} \sum\!\!\!\!\!\!\int_{\mathbb{R}^d,\Lambda} \frac{\hat{\chi}_\beta}{|\cdot|^\nu} = Z_0\big(M_\Lambda^\top M_\Lambda; \nu\big),$$

where $\Lambda = M_\Lambda \mathbb{Z}^d$. This function can be efficiently computed numerically in any number of space dimensions, see [16], and there exists analytical formulas for it in some dimensions, see e.g. [51].

4.3. Results and discussion. For $\boldsymbol{x} \in \Lambda$, we approximate the sum of $f_{\boldsymbol{x}}$ over $\mathbb{Z}^2 \setminus \{\boldsymbol{x}\}$ by means of the HSEM expansion, which results in the HSEM operator of order ℓ plus the associated Hadamard integral,

$$\sum_{\boldsymbol{y}\in\mathbb{Z}^2}{}' f_{\boldsymbol{x}}(\boldsymbol{y}) \approx \mathcal{D}^{(\ell)}_{\Lambda,\nu} g(\boldsymbol{x}) + \fint_{\mathbb{R}^d} \frac{g(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^\nu}\,\mathrm{d}\boldsymbol{y}.$$

In the following, we analyse the error for different widths λ of the interpolating function and show numerically that the error scaling of the multidimensional EM expansion as found in Chapter 2 is recovered. The implementation of the HSEM operator in two dimensions is discussed in detail in Appendix 1. For details on the evaluation of the Hadamard integral, see Appendix 2.

When approximating the sum by the HSEM expansion as above, an important feature of the method becomes apparent. Whereas the approximate evaluation of the sum on the left hand side requires the computation of a sum with a large number of addends N and with a

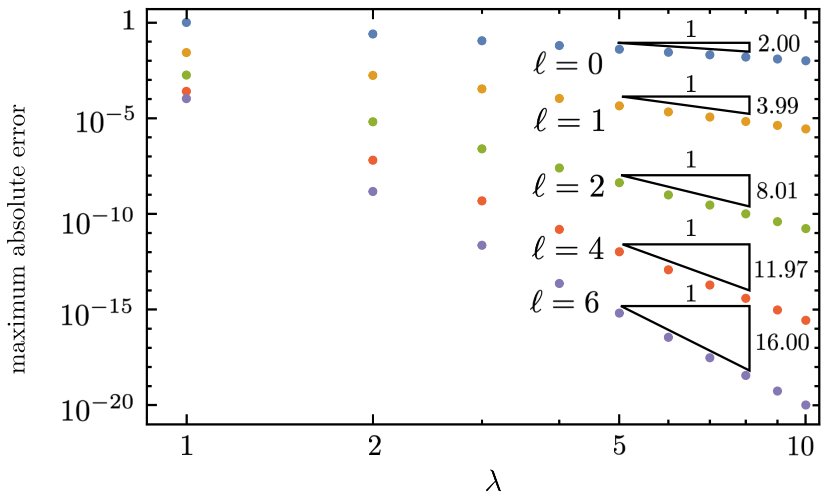

FIGURE 1. Absolute error of HSEM expansion in the maximum norm for an interaction exponent $\nu = 2.001$ and an interpolating function g as in (4.1) as a function of the scaling parameter λ for different orders ℓ of the expansion.

runtime that increases linearly with the number of terms, the evaluation of the right hand side is essentially independent of N and only depends on the complexity of the interpolating function. The HSEM operator is a local differential operator with constant coefficients that only depend on the lattice and on the interaction exponent. Hence, its action on g can be efficiently computed. The Hadamard integral over the whole space can in some cases be computed analytically. If this is not possible, we can make use of the convolution structure of the integral and of the fact that in the case of a band-limited interpolating function, quadrature rules converge exponentially fast in the number of quadrature nodes.

We choose $\nu = 2.001$ as the interaction exponent. Here $\nu = 2$ corresponds to the inverse square interaction, which appears in different models in quantum mechanics, see Ref. [29] and references therein. The case $\nu \approx d$ constitutes the most numerically challenging situation, as both short and long-range contributions remain relevant. None of the two can be neglected, hence standard continuum limits do not apply. We show the maximum absolute error at all lattices points in Fig. 1 for different expansion orders ℓ as a function of the width λ of the interpolating function. The same error scaling is observed for the interaction exponent $\nu = 1$, corresponding to the three dimensional Coulomb on a two-dimensional manifold, and the dipole interaction with $\nu = 3$. The corresponding plots are provided online[2]. The error

[2] `https://github.com/andreasbuchheit/hsem`

graphs for other exponents ν can readily be computed by adapting the parameter for ν in the code.

We observe that the maximum absolute error obeys the scaling law

$$E_\ell(\lambda) \sim \lambda^{-2(\ell+1)}.$$

The exact scaling coefficients as determined from a linear fit are shown in Fig. 1. This scaling law coincides with the one that we predict for the multidimensional EM expansion applied to a band-limited function with sufficiently small bandwidth, as well as for the SEM expansion in one dimension. Hence, the singularity of $f_{\boldsymbol{x}}$ has been well-absorbed in the HSEM operator coefficients, thus avoiding the divergence of the remainder integral. For large widths $\lambda \to \infty$, the zero order HSEM contribution already yields a reliable approximation to the sum. In contrast to that, approximations that only replace the sum by an integral yield an error that does not scale with λ and are thus are thus unreliable. For higher HSEM orders ℓ, the EM scaling law for band-limited functions is obeyed[3] and already for $\ell = 6$ and $\lambda = 10$, an absolute error smaller than 10^{-20} is obtained. We can understand these good convergence properties by the fact that the Fourier transform of $\Delta^{\ell+1} g$ has its mass concentrated inside the unit ball, and can therefore be approximated well by a band-limited function. The function essentially behaves like a band-limited function with bandwidth $\sigma < a_{\Lambda^*} = 1$. The HSEM reproduces the sum well, as long as the interpolating function does not exhibit oscillations in space with wavelengths smaller than a_{Λ^*}. Such oscillations would occur at a scale smaller than the distance between lattice points and thus can be considered unphysical. We hence observe that the HSEM converges for physically meaningful interpolation functions. It allows us to approximate singular sums in arbitrary dimensions independently of the particle number, with an error that decays exponentially in expansion order ℓ and polynomially in λ, which is proportional to the scale at which the interpolating function varies.

5. Conclusions

In this chapter, we have derived the hypersingular Euler–Maclaurin expansion. By removing the only free parameter in the expansion, a deep connection to analytic number theory is uncovered. This connection yields efficient representations for the HSEM operator coefficients, making the expansion readily applicable in practice. The numerical performance of the expansion has subsequently been analysed in a

[3] A better scaling than predicted is reached for some orders due to symmetry.

prototypical two-dimensional sum that appears in relevant systems in condensed matter and quantum physics. The same error scaling as the one predicted for the multidimensional EM expansion is observed. As a by-product of our method, new globally convergent representations for the meromorphic continuation of general multidimensional Dirichlet series are found, including the simple Epstein zeta function and the Riemann zeta function.

CHAPTER 5

Conclusions and outlook

In this work, we have derived the singular Euler–Maclaurin (SEM) expansion on multidimensional lattices, generalising the traditional Euler–Maclaurin (EM) summation formula to physically relevant singular sums. The hypersingular variant (HSEM) of the expansion is also able to describe singularities inside the integration region, which provides a reliable description of pairwise long-range interactions. If the integration region has no boundaries, then the expansion is given by the local HSEM differential operator only. Due to a fruitful connection to analytic number theory, all operator coefficients can be efficiently computed.

As an approximation to the sum is found in a runtime that is independent of the number of particles and as the approximation error decays exponentially with the order of the expansion, a powerful tool is provided that can find use in the evaluation of large sums in long-range interacting systems in condensed matter and quantum physics. Of particular interest are mesoscopic structures, where continuum limits are not applicable, yet the number of particles is too large for ad-hoc evaluations of the resulting sums. This situation arises for instance in the study of metamaterials. The numerical performance of the new method has been demonstrated by efficiently computing singular two-dimensional sums that appear, among others, in the simulation of spin lattices and in the study of the discrete nonlinear Schrödinger equation with long-range interactions.

Apart from being applicable as a numerical method, the new expansion can be used as an analytical tool in various fields of study. For the proof of the multidimensional SEM expansion, we have first derived the multidimensional EM expansion, including sharp error bounds, which is a relevant result on its own. The EM expansion has subsequently been used for proving the existence of the β-limit inside the Bernoulli-$\mathcal{A}$ functions. In similar fashion, the EM expansion can be used to prove existence and derive bounds for new mathematical objects that are based on limits of multidimensional sums. The multidimensional SEM expansion can be applied in rigorous derivations of mean field limits of long-range interacting systems, even in the case of nonlinear interactions. Higher orders of the expansion then track finite size corrections, which become relevant if the system is mesoscopic, if the interaction exponent is equal or close to the dimension of the system, or if high precision is required.

The connection of our work to analytic number theory has provided us with a fast way for evaluating the operator coefficients in the HSEM expansion. As a by-product, we have found new globally convergent series representations of the Epstein zeta function, and, in case of one-dimension, the Riemann zeta function. These elegant representations in terms of regularised Hadamard sum-integrals could potentially be of interest in number theory.

The new expansion opens up a vast range of possibilities for further developments. While we have derived the multidimensional SEM expansion for algebraic singularities, the one-dimensional treatment shows that it is possible to generalise it to a significantly larger set of interaction functions. Furthermore, our proofs for the multidimensional expansion do not rely significantly on the periodicity of the lattice. It is thus to be expected that the results can be generalised to quasi-lattices, like the Penrose lattice. In a next step, one could then try to replace lattices by random distributions of particles. Finally, in terms of long term goals, it would be interesting to consider discreteness effects in fundamental physics, e.g. in loop quantum gravity. Here the SEM expansion could be used as a tool for the precise quantification of the resulting finite size effects.

APPENDIX A

HSEM expansion in two dimensions

1. HSEM operator coefficients

We present a simple approach for computing the HSEM operator coefficient for $d=2$, which does not rely on derivatives of Epstein zeta functions and which makes use use of efficient summation formulas that have been found in the analysis of the Riemann hypothesis [39]. For a two-dimensional square lattice, it is well-known that [51, Eq. (9)]

$$\sum_{\boldsymbol{z}\in\mathbb{Z}^2}{}' \frac{1}{|\boldsymbol{z}|^\nu} = 4\zeta(\nu/2)\beta_D(\nu/2).$$

Here β_D is the Dirichlet beta function. The Dirichlet series can be analytically extended to $\nu\in\mathbb{C}\setminus\{2\}$. The meromorphic continuation of

$$C_n(\nu) = \sum_{\boldsymbol{z}\in\mathbb{Z}^2}{}' \frac{z_1^{2n}}{|\boldsymbol{z}|^{\nu+2n}}, \quad \nu\in\mathbb{C}\setminus\{2\},$$

in ν can be efficiently computed for $n\in\mathbb{N}$ by means of [39, Eq. (2.3)]

$$\begin{aligned} C_n(\nu) &= \frac{2\sqrt{\pi}\,\Gamma(\nu/2+n-1/2)\zeta(\nu-1)}{\Gamma(\nu/2+n)} \\ &\quad + \frac{8\pi^{\nu/2}}{\Gamma(\nu/2+n)} \sum_{z_1=1}^{\infty}\sum_{z_2=1}^{\infty} \left(\frac{z_2}{z_1}\right)^{(\nu-1)/2} (z_1 z_2 \pi)^n K_{(\nu-1)/2+n}(2\pi z_1 z_2), \end{aligned}$$

where $K_\nu(x)$ is the modified Bessel function of the second kind. Here, the double sum converges exponentially in both variables. With the above two lattice sums, we can now generate the whole HSEM operator in $d=2$ dimensions by using an expansion in solid harmonics.

We first note that only terms with even higher-order derivatives contribute in the HSEM operator due to symmetry. For $n\in\mathbb{N}$, we then

This chapter is based on the appendix in [7].

obtain

$$\lim_{\beta\to 0} \sum\!\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^2,\mathbb{Z}^2} \hat{\chi}_\beta(\boldsymbol{z}) \frac{\langle \boldsymbol{z}, \nabla\rangle^{2n}}{|\boldsymbol{z}|^\nu}$$

$$= \sum_{m=0}^{n} a_{2m}^{(2n)} \lim_{\beta\to 0} \sum\!\!\!\!\!\!\!\!\int_{\boldsymbol{z}\in\mathbb{R}^2,\mathbb{Z}^2} \hat{\chi}_\beta(\boldsymbol{z}) \frac{|\boldsymbol{z}|^{2(n-m)} A_{2m}(\boldsymbol{z})}{|\boldsymbol{z}|^\nu} A_{2(n-m)}(\nabla)\Delta^{n-m},$$

with the solid harmonic $A_k : \mathbb{R}^2 \to \mathbb{R}$,

$$A_k(\boldsymbol{y}) = \mathrm{Re}\Big((y_1 + iy_2)^k\Big),$$

and with the coefficients

$$a_0^{(k)} = \frac{1}{2\pi}\int_0^{2\pi} \cos^k(\phi)\,\mathrm{d}\phi, \qquad a_n^{(k)} = \frac{1}{\pi}\int_0^{2\pi} \cos(n\phi)\cos^k(\phi)\,\mathrm{d}\phi.$$

We now show that

$$\sum_{\boldsymbol{z}\in\mathbb{Z}^2}{}' \frac{A_{2m}(\boldsymbol{z})}{|\boldsymbol{z}|^{\nu+2m}} = Z_0(I_2,\nu) + \sum_{k=1}^{m} \frac{1}{(2k)!} T_{2m}^{(2k)}(0)\, C_k(\nu), \tag{A.1}$$

where $I_2 \in \mathbb{R}^{2\times 2}$ is the identity matrix and where T_{2m} are the Chebyshev polynomial of the first kind of order $2m$. We note that

$$A_{2m}(\boldsymbol{z}) = |\boldsymbol{z}|^{2m}\cos(2m\phi)$$

for the polar angle ϕ and $\boldsymbol{z} = |\boldsymbol{z}|(\cos\phi, \sin\phi)$. We then write $\cos(2m\phi)$ in terms of powers of $\cos\phi$ by means of the Chebyshev polynomial T_{2m},

$$\cos(2m\phi) = T_{2m}(\cos\phi) = \sum_{k=0}^{2m} T_{2m}^{(k)} \cos^k(\phi).$$

We insert this relation in the right hand side of (A.1) and observe that odd orders do not contribute due to the symmetry of the lattice. Then as

$$|\boldsymbol{z}|^{2k}\cos^{2k}(\phi) = z_1^{2k},$$

we recover the desired representation.

2. Evaluation of the Hadamard integral

We briefly discuss the evaluation of the Hadamard integral. For the particular choice of g as in (4.1) and for $d = 2$, it is possible to determine the Hadamard integral analytically. As g is a Schwartz function, it holds that

$$⨍_{\mathbb{R}^d} \frac{g(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^\nu}\,\mathrm{d}\boldsymbol{y} = \mathcal{F}\Big((\mathcal{F}|\cdot|^{-\nu})(\mathcal{F}g)\Big)(\boldsymbol{x}),$$

using the convolution theorem for distributions. We then obtain

$$\fint_{\mathbb{R}^d} \frac{g(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^{\nu}} \,\mathrm{d}\boldsymbol{y} = \frac{\pi\Gamma(1-\nu/2)}{\lambda^{\nu-2}} M\big(\nu/2, 1, -|\boldsymbol{x}/\lambda|^2\big),$$

where M is the Kummer confluent hypergeometric function, see e.g. [43, Eq. (13.2.2)].

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