Fast cubature of high dimensional biharmonic potential based on Approximate Approximations

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August 29, 2018

Abstract. We derive new formulas for the high dimensional biharmonic potential acting on Gaussians or Gaussians times special polynomials. These formulas can be used to construct accurate cubature formulas which are fast and effective also in very high dimensions. Numerical tests show that the formulas are accurate and provide the predicted approximation rate $O(h^8)$ up to the dimension 10^7.

AMS subject classifications. 65D32, 41A30, 41A63.

Keywords: Biharmonic potential, higher dimensions, separated representations, multidimensional convolution.

1 Introduction

The present paper is devoted to the approximation of the high dimensional biharmonic potential

$$\mathscr{B}_n f(\mathbf{x}) = \frac{\Gamma(n/2)}{4\pi^{n/2}(n-2)(n-4)} \int_{\mathbb{R}^n} \frac{f(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{n-4}} d\mathbf{y}, \qquad \mathbf{x} \in \mathbb{R}^n, \quad n \geq 3, n \neq 4, \quad (1.1)$$

(cf. [11, p.235] or [15, p.100]) for integrable f, by using approximate approximations (cf.[10] and the references therein). Approximate approximations allow to construct efficient high order cubature formulas for convolution integral operators even with singular kernel functions ([9]). Due to the operation number proportional to h^{-n}, where h denotes size of a uniform grid on the support of the density, these methods are practical only for small n. By combining approximate approximations with separated representations ([12, 13]) we derive a method for approximating volume potentials which is accurate and fast in high dimensions. First results on the fast cubature of high dimensional harmonic potential have been obtained in [3, 4]. The procedure has been applied

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in [5, 6] to advection-diffusion potentials and in [7] to parabolic problems. In [8] our approach has been extended to the computation of the Schrödinger potential, where standard cubature methods are very expansive due to the fast oscillations of the kernel. In this paper we derive new formulas for the biharmonic potential acting on Gaussians or special polynomial times Gaussians. These formulas can be used to construct fast and accurate cubature formulas.

We construct an approximation of $\mathscr{B}_n f$ if we replace f by functions with analytically known biharmonic potential. Specifically, we approximate the density $f \in C_0^N(\mathbb{R}^n)$ with the approximate quasi-interpolant

$$f_{h,\mathscr{D}}(\mathbf{x}) = \mathscr{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m})\eta\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathscr{D}}}\right), \tag{1.2}$$

where h and $\mathscr{D}$ are positive and η is a smooth and rapidly decaying function of the Schwarz space $\mathscr{S}(\mathbb{R}^n)$. The generating function is chosen so that $\mathscr{B}_n\eta$ can be computed analytically or efficiently numerically. If the generating function η satisfies the moment condition of order N

$$\int_{\mathbb{R}^n} \mathbf{x}^\alpha \eta(\mathbf{x}) d\mathbf{x} = \delta_{0,\alpha}, \qquad 0 \le |\alpha| < N, \tag{1.3}$$

then ([10, p.21])

$$|f(\mathbf{x}) - f_{h,\mathscr{D}}(\mathbf{x})| \le c(\sqrt{\mathscr{D}}h)^N \|\nabla_N f\|_{L_\infty} + \sum_{k=0}^{N-1} \varepsilon_k (h\sqrt{\mathscr{D}})^k |\nabla_k f(\mathbf{x})|$$

with

$$0 < \varepsilon_k \le \sum_{\mathbf{m}\in\mathbb{Z}^n\setminus\{0\}} |\nabla_k \mathscr{F}\eta(\sqrt{\mathscr{D}}\mathbf{m})|; \quad \lim_{\mathscr{D}\to\infty} \sum_{\mathbf{m}\in\mathbb{Z}^n\setminus\{0\}} |\nabla_k \mathscr{F}\eta(\sqrt{\mathscr{D}}\mathbf{m})| = 0$$

and

$$|\nabla_k f(\mathbf{x})| = \sum_{|\alpha|=k} \frac{|\partial^\alpha f(\mathbf{x})|}{\alpha!}.$$

Here $\mathscr{F}\eta$ denotes the Fourier transform of η

$$\mathscr{F}\eta(\mathbf{y}) = \int_{\mathbb{R}^n} \eta(\mathbf{x}) \mathrm{e}^{-2i\pi\langle\mathbf{x},\mathbf{y}\rangle} d\mathbf{x}.$$

Hence, for any *saturation error* $\varepsilon > 0$, one can fix the parameter $\mathscr{D} > 0$ so that

$$|f(\mathbf{x}) - f_{h,\mathscr{D}}(\mathbf{x})| = \mathscr{O}((\sqrt{\mathscr{D}}h)^N + \varepsilon)\|f\|_{W_\infty^N},$$

where $W_\infty^N = W_\infty^N(\mathbb{R}^n)$ denotes the Sobolev space of L_∞-functions whose generalized derivatives up to the order N also belong to L_∞. Then the linear combination

$$\mathscr{B}_n f_{h,\mathscr{D}}(\mathbf{x}) = \frac{h^4}{\mathscr{D}^{n/2-2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \mathscr{B}_n \eta\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathscr{D}}}\right) \tag{1.4}$$

gives rise to a new class of semi-analytic cubature formulas with the property that, for any prescribed accuracy $\varepsilon > 0$, one can fix the parameter $\mathscr{D}$ so that (1.4) differs in some uniform or L_p-norm from the integral (1.1) by

$$\mathscr{O}((\sqrt{\mathscr{D}}h)^N + (\sqrt{\mathscr{D}}h)^4 \varepsilon) \qquad \text{as} \qquad h \to 0\,,$$

where N is determined by (1.3). Estimates of the cubature error for general generating functions are proved in Section 2.

Therefore, to construct cubature formulas for (1.1) it remains to compute the integral $\mathscr{B}_n \eta$. This can be taken analytically or transformed to a simple one-dimensional integral. If we choose the generating functions

$$\eta(\mathbf{x}) = \pi^{-n/2} L_{M-1}^{(n/2)}(|\mathbf{x}|^2) \mathrm{e}^{-|\mathbf{x}|^2}$$

with the generalized Laguerre polynomials $L_M^{(\gamma)}$ then $\mathscr{B}_n \eta$ can be taken analytically. η satisfies the moment conditions (1.3) with $N = 2M$ and (1.4) gives rise to semi-analytic cubature formulas for $\mathscr{B}_n f$ of order h^{2M} modulo the saturation error. In Section 3 we describe these formulas when $M = 1$ that is for the exponential $\pi^{n/2}\mathrm{e}^{-|\mathbf{x}|^2}$ and, in Section 4, when $M > 1$.

If the generating function is the tensor product of one-dimensional functions of the form

$$\eta(\mathbf{x}) = \prod_{j=1}^{n} \pi^{-1/2} L_{M-1}^{(1/2)}(x_j^2) \mathrm{e}^{-x_j^2}\,,$$

each of them satisfying the moment conditions (1.3) of order $2M$, then $\mathscr{B}_n \eta$ is transformed to a one-dimensional integral with a separable integrand, i.e., a product of functions depending only on one of the variables. This is considered in Section 5 where we obtain, for example, the integral representation

$$\mathscr{B}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{1}{16} \int_0^\infty \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}}\, t\, dt, \qquad n \geq 5.$$

These one-dimensional integrals with separable integrand in combination with a quadrature rule lead to accurate separated representations of the potential acting on the generating function. In Section 6 for functions f with separated representations, i.e., within a given accuracy they can be represented as a sum of products of univariate functions, we derive formulas which reduces the n-dimensional convolution (1.1) to one-dimensional discrete convolutions. Thus for the computation of (1.1) only one-dimensional operations are used. We derive formulas of an arbitrary order fast and accurate in high dimensions. We provide results of numerical experiments which show the efficiency of the method up to approximation order $O(h^8)$ and dimensions $n = 10^7$.

2 Cubature error

The estimate of the cubature error

$$\mathscr{B}_n f_{h,\mathscr{D}}(\mathbf{x}) - \mathscr{B}_n f(\mathbf{x}) = \mathscr{B}_n (f_{h,\mathscr{D}} - f)(\mathbf{x})$$

for the biharmonic potential (1.1) is a consequence of the structure of the quasi-interpolation error, which is proved in general form in [10, Thm 2.28]. Suppose that f has generalized derivatives of order N. Using Taylor expansions of f for the nodes $h\mathbf{m}$, $\mathbf{m} \in \mathbb{Z}^n$, and Poisson's summation formula the quasi-interpolant can be written as

$$f_{h,\mathscr{D}}(\mathbf{x}) = (-h\sqrt{\mathscr{D}})^N f_N(\mathbf{x}) + \sum_{|\alpha|=0}^{N-1} \frac{(h\sqrt{\mathscr{D}})^{|\alpha|}}{\alpha!(2\pi i)^{|\alpha|}} \partial^\alpha f(\mathbf{x})\, \sigma_\alpha(\mathbf{x},\eta,\mathscr{D}) \tag{2.1}$$

with the function

$$f_N(\mathbf{x}) = \frac{1}{\mathscr{D}^{n/2}} \sum_{|\alpha|=N} \frac{N}{\alpha!} \sum_{\mathbf{m}\in\mathbb{Z}^n} \Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathscr{D}}}\Big)^\alpha \eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathscr{D}}}\Big) \int_0^1 s^{N-1} \partial^\alpha f(s\mathbf{x}+(1-s)h\mathbf{m})\, ds\,,$$

containing the remainder of the Taylor expansions, and the fast oscillating functions

$$\sigma_\alpha(\mathbf{x},\eta,\mathscr{D}) = \sum_{\nu\in\mathbb{Z}^n} \partial^\alpha \mathscr{F}\eta(\sqrt{\mathscr{D}}\nu)\, \mathrm{e}^{\frac{2\pi i}{h}\langle \mathbf{x},\nu\rangle}\,. \tag{2.2}$$

It follows from (2.2) that due to the moment condition (1.3) the second sum in (2.1) transforms to

$$f(\mathbf{x}) + \sum_{|\alpha|=0}^{N-1} \frac{(h\sqrt{\mathscr{D}})^{|\alpha|}}{\alpha!(2\pi i)^{|\alpha|}} \partial^\alpha f(\mathbf{x})\, \varepsilon_\alpha(\mathbf{x},\eta,\mathscr{D})\,,$$

where we denote

$$\varepsilon_\alpha(\mathbf{x},\eta,\mathscr{D}) = \sum_{\nu\in\mathbb{Z}^n\setminus 0} \partial^\alpha \mathscr{F}\eta(\sqrt{\mathscr{D}}\nu)\, \mathrm{e}^{\frac{2\pi i}{h}\langle \mathbf{x},\nu\rangle} = \sigma_\alpha(\mathbf{x},\eta,\mathscr{D}) - \delta_{0|\alpha|}\,.$$

We denote by $W_p^N = W_p^N(\mathbb{R}^n)$ the Sobolev space of $L_p = L_p(\mathbb{R}^n)$ functions whose generalized derivatives up to order N belong to L_p, with the norm

$$\|f\|_{W_p^N} = \sum_{l=0}^{N} |f|_{W_p^l}, \quad |f|_{W_p^l} = \sum_{|\alpha|=l} \|\partial^\alpha f\|_{L_p}\,.$$

If $f \in W_p^N$ with $N > n/p$, $1 \le p \le \infty$, then f_N can be estimated by

$$\|f_N\|_{L_p} \le C_N |f|_{W_p^N}, \qquad |f|_{W_p^N} = \sum_{|\alpha|=N} \|\partial^\alpha f\|_{L_p}\,,$$

with a constant C_N depending only on η, n, and p. Hence (2.1) leads to the representation of the quasi-interpolation error

$$f_{h,\mathscr{D}}(\mathbf{x}) - f(\mathbf{x}) = (-h\sqrt{\mathscr{D}})^N f_N(\mathbf{x}) + \sum_{|\alpha|=0}^{N-1} \frac{(h\sqrt{\mathscr{D}})^{|\alpha|}}{\alpha!(2\pi i)^{|\alpha|}} \partial^\alpha f(\mathbf{x}) \varepsilon_\alpha(\mathbf{x},\eta,\mathscr{D}), \tag{2.3}$$

which implies in particular the error estimate in L_p

$$\|f - f_{h,\mathscr{D}}\|_{L_p} \le C_N (h\sqrt{\mathscr{D}})^N |f|_{W_p^N} + \sum_{k=0}^{N-1} \frac{(h\sqrt{\mathscr{D}})^k}{(2\pi)^k} \sum_{|\alpha|=k} \frac{\|\varepsilon_\alpha(\cdot,\eta,\mathscr{D})\|_{L_\infty} \|\partial^\alpha f\|_{L_p}}{\alpha!} . \tag{2.4}$$

Thus the quasi-interpolation error consists of a term ensuring $\mathscr{O}(h^N)$-convergence and of the so-called saturation error, which, in general, does not converge to zero as $h \to 0$. However, due to the fast decay of $\partial^\alpha \mathscr{F}\eta$, one can choose $\mathscr{D}$ large enough to ensure that

$$\|\varepsilon_\alpha(\cdot,\mathscr{D},\eta)\|_{L_\infty} \le \sum_{\nu \in \mathbb{Z}^n \setminus 0} |\partial^\alpha \mathscr{F}\eta(\sqrt{\mathscr{D}}\nu)| < \varepsilon \tag{2.5}$$

for given small $\varepsilon > 0$.

From Sobolev's theorem we have that for $n \ge 5$, $1 < p < n/4$, and $q = np/(n-4p)$ the integral (1.1) converges absolutely for almost every $\mathbf{x}$ and the operator $\mathscr{B}_n$ is a bounded mapping from L_p into L_q (cf. [16, p. 119]). Hence

$$\|\mathscr{B}_n f_{h,\mathscr{D}} - \mathscr{B}_n f\|_{L_q} \le A_{p,q} \|f_{h,\mathscr{D}} - f\|_{L_p} , \tag{2.6}$$

where $A_{p,q}$ denotes the norm of $\mathscr{B}_n : L_p \to L_q$. Then, from (2.4) and (2.5),

Theorem 2.1. *Let $n \ge 5$, $1 < p < n/4$, $q = np/(n-4p)$ and $f \in W_p^N$ with $N > n/p$. Then, for any $\varepsilon > 0$ there exists $\mathscr{D} > 0$ such that*

$$\|\mathscr{B}_n f_{h,\mathscr{D}} - \mathscr{B}_n f\|_{L_q} \le A_{p,q} \Big(C_N (h\sqrt{\mathscr{D}})^N |f|_{W_p^N} + \varepsilon \sum_{k=0}^{N-1} \frac{(h\sqrt{\mathscr{D}})^k}{(2\pi)^k} \|\nabla_k f\|_{L_p} \Big) . \tag{2.7}$$

We used the notation

$$\|\nabla_k f\|_{L_p} = \sum_{|\alpha|=k} \frac{\|\partial^\alpha f\|_{L_p}}{\alpha!} .$$

It turns out, that under the conditions of Theorem 2.1 the cubature formula $\mathscr{B}_n f_{h,\mathscr{D}}$ converges to $\mathscr{B}_n f$. Since the biharmonic potential is a smoothing operator and by (2.3) the saturation error of the quasi-interpolant is a small, fast oscillating function, estimate (2.7) can be sharpened to the form that $\mathscr{B}_n f_{h,\mathscr{D}}$ approximates $\mathscr{B}_n f$ with the error $\mathscr{O}(h^N + \varepsilon h^4)$.

We denote by $H_p^s = H_p^s(\mathbb{R}^n)$ the Bessel potential space defined as the closure of compactly supported smooth functions with respect to the norm

$$\|u\|_{H_p^s} = \|\mathscr{F}^{-1}((1+4\pi^2|\cdot|^2)^{s/2}\mathscr{F}u)\|_{L_p} = \|(1-\Delta)^{s/2}u\|_{L_p} .$$

We shall use the error estimate for the quasi-interpolant (1.2) in the spaces H_p^s obtained in [10, p.83] which yields, in the case $s = -4$, the following result.

Theorem 2.2. *[10, p.83] Suppose that $\eta \in \mathscr{S}(\mathbb{R}^n)$ satisfies the moments conditions* (1.3) *of order N. Then, for any $f \in H_p^L$, $1 < p < \infty$, $L \geq N \geq 4$ with $L > n/p$, there exist constants c_η and c_p, not depending on f and h such that $f_{h,\mathscr{D}}$ defined in* (1.2) *satisfies*

$$\|f - f_{h,\mathscr{D}}\|_{H_p^{-4}} \leq c_\eta (h\sqrt{\mathscr{D}})^N \|f\|_{H_p^L} + c_p h^4 \sum_{k=0}^{N-5} \frac{(h\sqrt{\mathscr{D}})^k}{(2\pi)^{k+4}} \varepsilon_k(\mathscr{D}) \sum_{|\alpha|=k} \|\partial^\alpha f\|_{H_p^4} \quad (2.8)$$

with the numbers

$$\varepsilon_k(\mathscr{D}) = \max_{|\alpha|=k} \sum_{\nu \in \mathbb{Z}^n \setminus 0} \left| \partial^\alpha \mathscr{F}\eta(\sqrt{\mathscr{D}}\nu) \right| .$$

Theorem 2.2 leads to the following error estimate for the quasi-interpolation procedure.

Theorem 2.3. *Suppose that $\eta \in \mathscr{S}(\mathbb{R}^n)$ satisfies the moments conditions* (1.3) *of order N. Let $n \geq 5$, $1 < p < n/4$, $q = np/(n-4p)$ and $f \in W_p^L$ with $L \geq N \geq 4$ and $L > n/p$. Then there exist constants c_η , c_p and c_q, not depending on $f, h, \mathscr{D}$, such that*

$$\|\mathscr{B}_n f - \mathscr{B}_n f_{h,\mathscr{D}}\|_{L_q} \leq c_\eta (h\sqrt{\mathscr{D}})^N \|f\|_{W_p^L} + \\ h^4 \sum_{k=0}^{N-5} (h\sqrt{\mathscr{D}})^k \frac{\varepsilon_k(\mathscr{D})}{(2\pi)^{k+2}} \sum_{l=0}^{4} \left(A_{p,q} c_p |f|_{W_p^{l+k}} + c_q |f|_{W_q^{l+k}} \right) .$$

Proof. Since

$$\mathscr{B}_n f - \mathscr{B}_n f_{h,\mathscr{D}} = \mathscr{B}_n (f - f_{h,\mathscr{D}})$$

we obtain, keeping in mind (2.6),

$$\begin{aligned} \|\mathscr{B}_n(f - f_{h,\mathscr{D}})\|_{L_q} &= \|\mathscr{B}_n(I - \Delta\Delta)(I - \Delta\Delta)^{-1}(f - f_{h,\mathscr{D}})\|_{L_q} \\ &\leq \|\mathscr{B}_n(I - \Delta\Delta)^{-1}(f - f_{h,\mathscr{D}})\|_{L_q} + \|\mathscr{B}_n \Delta\Delta(I - \Delta\Delta)^{-1}(f - f_{h,\mathscr{D}})\|_{L_q} \\ &\leq A_{p,q}\|(I - \Delta\Delta)^{-1}(f - f_{h,\mathscr{D}})\|_{L_p} + \|(I - \Delta\Delta)^{-1}(f - f_{h,\mathscr{D}})\|_{L_q} . \end{aligned}$$

Since $(1 + 4\pi^2|\xi|^2)^2$ can be bounded from above and from below by $(1 + 16\pi^4|\xi|^4)$, the norm in H_p^{-4} is equivalent to

$$\|\mathscr{F}^{-1}((1 + 16\pi^4|\cdot|^4)^{-1}\mathscr{F}u)\|_{L_p} = \|(1 - \Delta\Delta)^{-1}u\|_{L_p}$$

and we deduce that

$$\|\mathscr{B}_n(f - f_{h,\mathscr{D}})\|_{L_q} \leq A_{p,q}\|f - f_{h,\mathscr{D}}\|_{H_p^{-4}} + \|f - f_{h,\mathscr{D}}\|_{H_q^{-4}} .$$

The condition $p < n/4$ ensures that W_p^L is continuously embedded in W_q^{L-4} ([16, p.124]). Hence by the estimate (2.8) the assertion follows immediately. □

3 Action on Gaussians

Consider the generating function $\eta_2(\mathbf{x}) = \pi^{-n/2} \mathrm{e}^{-|\mathbf{x}|^2}$. The moment conditions (1.3) are fulfilled with $N = 2$. If we replace f in (1.1) by

$$f_{h,\mathscr{D}}(\mathbf{x}) = (\pi\mathscr{D})^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \mathrm{e}^{-|\mathbf{x}-h\mathbf{m}|^2/(h^2\mathscr{D})},$$

then we obtain a cubature for (1.1)

$$\mathscr{B}_n f_{h,\mathscr{D}}(\mathbf{x}) = \frac{(h\sqrt{\mathscr{D}})^4}{(\pi\mathscr{D})^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \Phi_2\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathscr{D}}}\right) \tag{3.1}$$

with

$$\Phi_2(\mathbf{x}) := \mathscr{B}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}).$$

Theorem 3.1. *Let $n \geq 3, n \neq 4$. The biharmonic potential acting on the Gaussian allows the following representation*

$$\mathscr{B}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{1}{4(n-2)(n-4)} {}_1F_1\left(\frac{n-4}{2}, \frac{n}{2}, -|\mathbf{x}|^2\right), \tag{3.2}$$

where ${}_1F_1$ denotes the Kummer or confluent hypergeometric function.

Proof. The cubature of the 3-dimensional biharmonic potential $\mathscr{B}_3 f$ is considered in [10, p.119]. To determine the action of the biharmonic potential on the Gaussian the general formula

$$(Q * \mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{2\pi^{n/2} \mathrm{e}^{-|\mathbf{x}|^2}}{|\mathbf{x}|^{n/2-1}} \int_0^\infty Q(r) \mathrm{e}^{-r^2} I_{n/2-1}(2r|\mathbf{x}|)\, r^{n/2} dr \tag{3.3}$$

with the modified Bessel functions of the first kind I_n ([1, p.374]) and $Q(r) = -r/(8\pi)$ is used. Then (3.3) gives

$$\mathscr{B}_3(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = -\frac{\mathrm{e}^{-|\mathbf{x}|^2}}{8} - \frac{\sqrt{\pi}}{16} \frac{\mathrm{erf}(|\mathbf{x}|)}{|\mathbf{x}|} (2|\mathbf{x}|^2 + 1). \tag{3.4}$$

(3.4) can also be expressed by means of the confluent hypergeometric functions as

$$\mathscr{B}_3(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = -\frac{1}{4} {}_1F_1\left(-\frac{1}{2}, \frac{3}{2}, -|\mathbf{x}|^2\right).$$

Let $n \geq 5$. The convolution of two radial functions can be transformed to a one-dimensional integral by using the Fourier transforms of the radial functions. Indeed (cf. [10, (2.15) p.22])

$$\int_{\mathbb{R}^n} Q(|\mathbf{x}-\mathbf{y}|) f(|\mathbf{y}|) d\mathbf{y} = \frac{2\pi}{|\mathbf{x}|^{n/2-1}} \int_0^\infty \mathscr{F}Q(r) \mathscr{F}f(r) J_{n/2-1}(2\pi r|\mathbf{x}|) r^{n/2} dr. \tag{3.5}$$

Since $\mathscr{F}(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \pi^{n/2}\mathrm{e}^{-\pi^2|\mathbf{x}|^2}$ and $\mathscr{F}(|\cdot|^{4-n})(\mathbf{x}) = \frac{\pi^{n/2-4}}{\Gamma(\frac{n-4}{2})}|\mathbf{x}|^{-4}$ (cf. [14, p.156]) we have from (3.5) that

$$\mathscr{B}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{\pi^{n/2-3}}{8|\mathbf{x}|^{n/2-1}} \int\limits_0^\infty \mathrm{e}^{-\pi^2 r^2} J_{n/2-1}(2\pi r|\mathbf{x}|) r^{n/2-4} dr\,,$$

where we used the relation

$$\Gamma\left(\frac{n}{2}\right) = \frac{(n-2)(n-4)}{4}\Gamma\left(\frac{n-4}{2}\right).$$

This integral can be expressed by means of the Kummer or confluent hypergeometric function ${}_1F_1(a,c,z)$ (cf. [2, (8.6.14)]). (3.2) follows. □

In particular, for $n = 5$, (3.2) gives

$$\mathscr{B}_5(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{1}{16}\left(\frac{\mathrm{e}^{-|\mathbf{x}|^2}}{|\mathbf{x}|^2} + \sqrt{\pi}\frac{\mathrm{erf}(|\mathbf{x}|)}{2|\mathbf{x}|^3}(2|\mathbf{x}|^2 - 1)\right)$$

and, for $n = 6$,

$$\mathscr{B}_6(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{\mathrm{e}^{-|\mathbf{x}|^2} - 1 + |\mathbf{x}|^2}{16|\mathbf{x}|^4}$$

(cf. [1, 13.6]).
In dimension $n = 4$ the biharmonic potential has the form

$$\mathscr{B}_4 f(\mathbf{x}) = -\frac{1}{4\pi^2}\int_{\mathbb{R}^4} \ln|\mathbf{x}-\mathbf{y}| f(\mathbf{y}) d\mathbf{y}$$

and the following representation formula holds.

Theorem 3.2. *The biharmonic potential acting on the Gaussian function admits the representation*

$$\mathscr{B}_4(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{1}{16}\left(\frac{\mathrm{e}^{-|\mathbf{x}|^2} - 1}{|\mathbf{x}|^2} - 2\log|\mathbf{x}| - E_1(|\mathbf{x}|^2)\right) \tag{3.6}$$

where $E_1(r)$ is the exponential integral

$$E_1(r) = \int_r^\infty \frac{\mathrm{e}^{-t}}{t} dt\,.$$

Proof. We use that the radial function $g(r) = \Phi_2(\mathbf{x})$, $r = |\mathbf{x}|$, is solution of the differential equation

$$\frac{1}{r^3}\frac{d}{dr}\left(r^3\frac{d}{dr}\left(\frac{1}{r^3}\frac{d}{dr}\left(r^3\frac{d}{dr}\right)\right)\right) g(r) = \mathrm{e}^{-r^2}, \quad r > 0\,,$$

satisfying the conditions

$$g(r) \approx -\frac{1}{8}\log r \quad as \quad r \to \infty,$$

$$g(0) = -\frac{1}{4}\int_0^\infty r^3 \log(r) \mathrm{e}^{-r^2} dr = \frac{\gamma-1}{16}, \quad g'(0) = 0$$

with the Euler constant γ. Denote by $\mathscr{L}_n$ the inverse of the Laplace operator, the harmonic potential

$$(\mathscr{L}_n f)(\mathbf{x}) = -\frac{\Gamma(n/2-1)}{4\pi^{n/2}} \int_{\mathbb{R}^n} \frac{f(y)}{|\mathbf{x}-\mathbf{y}|^{n-2}} d\mathbf{y},$$

which provides the unique solution of the Poisson equation

$$\Delta u = f \quad \text{in} \quad \mathbb{R}^n, \qquad |u(\mathbf{x})| \le c|\mathbf{x}|^{n-2} \quad |\mathbf{x}| \to \infty.$$

Hence we have

$$\frac{1}{r^3}\frac{d}{dr}\left(r^3 \frac{d}{dr}\right) g = \mathscr{L}_4(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}).$$

From the relation (cf. [10, p.75])

$$\mathscr{L}_4(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{\mathrm{e}^{-|\mathbf{x}|^2}-1}{4|\mathbf{x}|^2}$$

we deduce that g solves

$$g''(r) + 3\frac{g'(r)}{r} = \frac{\mathrm{e}^{-r^2}-1}{4r^2}, \quad g(0) = \frac{\gamma-1}{16}, \quad g'(0) = 0.$$

We obtain

$$g'(r) = \frac{1}{8}\left(\frac{1}{r^3} - \frac{\mathrm{e}^{-r^2}}{r^3} - \frac{1}{r}\right)$$

and, finally

$$g(r) = \frac{1}{8}\int_0^r \left(\frac{1}{s^3} - \frac{\mathrm{e}^{-s^2}}{s^3} - \frac{1}{s}\right) ds + g(0) = \frac{1}{16}\int_0^{r^2} \left(\frac{1}{t} - \frac{\mathrm{e}^{-t}}{t} - 1\right)\frac{dt}{t}$$

$$+ g(0) = \frac{1}{16}\left(\frac{\mathrm{e}^{-r^2}-1}{r^2} - E_1(r^2) - 2\log r\right)$$

with the exponential integral E_1 ([1, 5.1.1]). □

(3.1), together with (3.2) and (3.6), gives rise to second order semi-analytic cubature formulas for the biharmonic operator in any dimension $n \ge 3$.

4 Action on higher-order basis functions

Now we consider the biharmonic potential

$$\Phi_{2M}(\mathbf{x}) := \mathscr{B}_n(L_{M-1}^{(n/2)}(|\cdot|^2)\mathrm{e}^{-|\cdot|^2})(\mathbf{x})$$

of the radial function $L_{M-1}^{(n/2)}(|\mathbf{x}|^2)\mathrm{e}^{-|\mathbf{x}|^2}$ with the generalized Laguerre polynomials

$$L_k^{(\gamma)}(y) = \frac{\mathrm{e}^y y^{-\gamma}}{k!}\left(\frac{d}{dy}\right)^k (\mathrm{e}^{-y}y^{k+\gamma}), \quad \gamma > -1\,.$$

The radial functions

$$\eta_{2M}(\mathbf{x}) = \pi^{-n/2} L_{M-1}^{(n/2)}(|\mathbf{x}|^2)\mathrm{e}^{-|\mathbf{x}|^2} \tag{4.1}$$

satisfy the moment conditions of order $2M$ ([10, p.56]) and give rise to approximation formulas of order $2M$ modulo the saturation error. If we give an analytic formula for Φ_{2M}, then we obtain the following semi-analytic cubature for (1.1)

$$\mathscr{B}_n f_{h,\mathscr{D}}(\mathbf{x}) = \frac{(h\sqrt{\mathscr{D}})^4}{(\pi\mathscr{D})^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m})\Phi_{2M}\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathscr{D}}}\right) \tag{4.2}$$

Theorem 4.1. *For $M > 1$ we have*

$$\Phi_{2M}(\mathbf{x}) = \mathscr{B}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) + \frac{1}{16|\mathbf{x}|^{n-2}}\gamma(\frac{n}{2}-1,|\mathbf{x}|^2) + \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{16}\sum_{j=0}^{M-3}\frac{L_j^{(n/2-1)}(|\mathbf{x}|^2)}{(j+1)(j+2)}$$

with the lower incomplete Gamma function

$$\gamma(a,x) = \int_0^x t^{a-1}\mathrm{e}^{-t}dt\,.$$

Proof. We use the relation [10, (3.18)]

$$L_{M-1}^{(n/2)}(|\mathbf{x}|^2)\mathrm{e}^{-|\mathbf{x}|^2} = \sum_{j=0}^{M-1}\frac{(-1)^j}{j!4^j}\Delta^j\mathrm{e}^{-|\mathbf{x}|^2} = \mathrm{e}^{-|\mathbf{x}|^2} - \frac{1}{4}\Delta\mathrm{e}^{-|\mathbf{x}|^2} + \sum_{j=2}^{M-1}\frac{(-1)^j}{j!4^j}\Delta^j\mathrm{e}^{-|\mathbf{x}|^2}\,.$$

Let $\mathscr{L}_n$ be the inverse of the Laplace operator, that is $\mathscr{L}_n\Delta = I$. Then $\mathscr{B}_n(\Delta\mathrm{e}^{-|\cdot|^2}) = \mathscr{L}_n(\mathrm{e}^{-|\cdot|^2})$ and we have

$$\mathscr{B}_n(\,L_{M-1}^{(n/2)}(|\cdot|^2)\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \mathscr{B}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) - \frac{1}{4}\mathscr{L}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) + \sum_{j=2}^{M-1}\frac{(-1)^j}{j!4^j}\Delta^{j-2}\mathrm{e}^{-|\mathbf{x}|^2}\,.$$

From the relations ([10, p.75])

$$\mathscr{L}_n(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = -\frac{1}{4|\mathbf{x}|^{n-2}}\gamma(\frac{n}{2}-1,|\mathbf{x}|^2), \quad n\geq 3\,,$$

with the lower incomplete Gamma function $\gamma(a,\mathbf{x})$ and ([10, (4.24)])

$$\sum_{j=2}^{M-1}\frac{(-1)^j}{j!4^j}\Delta^{j-2}\mathrm{e}^{-|\mathbf{x}|^2} = \frac{1}{16}\sum_{s=0}^{M-3}\frac{(-1)^s}{4^s(s+2)!}\Delta^s\mathrm{e}^{-|\mathbf{x}|^2} = \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{16}\sum_{j=0}^{M-3}\frac{L_j^{(n/2-1)}(|\mathbf{x}|^2)}{(j+1)(j+2)}$$

we conclude the proof. □

From the relation ([1, 6.5.16])

$$\gamma(\frac{1}{2},x^2) = \sqrt{\pi}\,\mathrm{erf}(x)$$

and the recurrence relation ([1, 6.5.22])

$$\gamma(a+1,x^2) = a\gamma(a,x) - \mathrm{e}^{-x}x^2$$

we see that in the case of odd space dimension the biharmonic potential of the Gaussian is expressed using the error function erf. In the case of even space dimension the biharmonic potential of the Gaussian is expressed by elementary functions since ([1, 6.5.13])

$$\gamma(k,x) = (k-1)!\left(1-\mathrm{e}^{-x}\sum_{j=0}^{k-1}\frac{x^j}{j!}\right), \qquad k\in\mathbf{N}.$$

In particular we have

$$\Phi_{2M}(\mathbf{x}) = -\frac{\mathrm{e}^{-|\mathbf{x}|^2}}{8} - \frac{\sqrt{\pi}|\mathbf{x}|}{8}\mathrm{erf}(|\mathbf{x}|) + \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{16}\sum_{j=0}^{M-3}\frac{L_j^{(1/2)}(|\mathbf{x}|^2)}{(j+1)(j+2)} \qquad \text{for} \quad n=3,$$

$$\Phi_{2M}(\mathbf{x}) = -\frac{\log|\mathbf{x}|}{8} - \frac{E_1(|\mathbf{x}|^2)}{16} + \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{16}\sum_{j=0}^{M-3}\frac{L_j^{(1)}(|\mathbf{x}|^2)}{(j+1)(j+2)} \qquad \text{for} \quad n=4,$$

$$\Phi_{2M}(\mathbf{x}) = \frac{\sqrt{\pi}}{16}\frac{\mathrm{erf}(|\mathbf{x}|)}{|\mathbf{x}|} + \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{16}\sum_{j=0}^{M-3}\frac{L_j^{(3/2)}(|\mathbf{x}|^2)}{(j+1)(j+2)} \qquad \text{for} \quad n=5,$$

$$\Phi_{2M}(\mathbf{x}) = \frac{1-\mathrm{e}^{-|\mathbf{x}|^2}}{16|\mathbf{x}|^2} + \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{16}\sum_{j=0}^{M-3}\frac{L_j^{(2)}(|\mathbf{x}|^2)}{(j+1)(j+2)} \qquad \text{for} \quad n=6.$$

Theorem 4.1 shows that Φ_{2M+2} can be obtained from Φ_{2M} by adding some rapidly decaying terms. We conclude that the approximation of the density f by the quasi-interpolant (1.2) with the basis functions (4.1) leads to the semi-analytic approximation of the biharmonic potential (4.2) and the corresponding analytic expression for Φ_{2M} has to be used.

5 Separated representation of the biharmonic potential acting on Gaussians

In this section we take, as in [3], the tensor product generation function

$$\eta_{2M}(\mathbf{x}) = \prod_{j=1}^{n}\widetilde{\eta}_{2M}(x_j); \quad \widetilde{\eta}_{2M}(x_j) = \frac{(-1)^{M-1}}{2^{2M-1}\sqrt{\pi}(M-1)!}\frac{H_{2M-1}(x_j)\mathrm{e}^{-x_j^2}}{x_j}, \qquad (5.1)$$

which satisfies the moment conditions of order $2M$, where H_k are the Hermite polynomials

$$H_k(x) = (-1)^k e^{x^2} \left(\frac{d}{dx}\right)^k e^{-x^2}.$$

The n-dimensional potential $\mathscr{B}_n$ applied to the basis function η_{2M} can be transformed to a one-dimensional integral with separable integrand, i.e., a product of functions depending only on one of the variables. In Section 6 we will show how these one-dimensional integrals, in combination with a quadrature rule, lead to accurate separated representations of the potential acting on the generating function. Hence, for functions f with separated representations, we derive fast formulas which reduces the n-dimensional convolution (1.1) by one-dimensional discrete convolutions.

We start with second order approximations, i.e. $M = 1$.

Theorem 5.1. *The biharmonic potential* $\mathscr{B}_n(e^{-|\cdot|^2})$ *admits the following one-dimensional integral representation*

$$\mathscr{B}_3(e^{-|\cdot|^2})(\mathbf{x}) = -\frac{1}{8}\int_0^\infty e^{-|\mathbf{x}|^2/(1+t)} \left(\frac{1}{(1+t)^{3/2}} + \frac{t|\mathbf{x}|^2}{(1+t)^{5/2}}\right) dt\,, \tag{5.2}$$

$$\mathscr{B}_n(e^{-|\cdot|^2})(\mathbf{x}) = \frac{1}{16}\int_0^\infty \frac{e^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}}\, t\, dt, \quad n \geq 5\,. \tag{5.3}$$

Proof. We use the integral formula [1, 13.2.1]

$${}_1F_1(a,c,z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\int_0^1 e^{z\tau}\tau^{a-1}(1-\tau)^{-a+c-1}d\tau, \quad \mathrm{Re}\,(c) > \mathrm{Re}\,(a) > 0\,. \tag{5.4}$$

Let $n \geq 5$. With the substitution $\tau = 1/(1+t)$ we get

$$\begin{aligned}
{}_1F_1\left(\frac{n-4}{2}, \frac{n}{2}, -|\mathbf{x}|^2\right) &= \frac{\Gamma(\frac{n}{2})}{\Gamma(\frac{n}{2}-2)}\int_0^\infty e^{-|\mathbf{x}|^2/(1+t)} \frac{1}{(1+t)^{n/2-3}} \frac{t}{1+t} \frac{dt}{(1+t)^2} \\
&= \frac{(n-2)(n-4)}{4}\int_0^\infty \frac{e^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}}\, t\, dt\,.
\end{aligned}$$

From (3.2) we get (5.3).
From the recurrence relation (cf. [1, 13.4.4]) we have

$${}_1F_1\left(-\frac{1}{2}, \frac{3}{2}, -|\mathbf{x}|^2\right) = {}_1F_1\left(\frac{1}{2}, \frac{3}{2}, -|\mathbf{x}|^2\right) + \frac{2}{3}|\mathbf{x}|^2\, {}_1F_1\left(\frac{1}{2}, \frac{5}{2}, -|\mathbf{x}|^2\right).$$

The integral formula (5.4) gives

$${}_1F_1\left(\frac{1}{2}, \frac{3}{2}, -|\mathbf{x}|^2\right) = \frac{1}{2}\int_0^1 \frac{e^{-|\mathbf{x}|^2\tau}}{\tau^{1/2}} d\tau = \frac{1}{2}\int_0^\infty \frac{e^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{3/2}} dt\,,$$

$$ {}_1F_1(\frac{1}{2},\frac{5}{2},-|\mathbf{x}|^2) = \frac{3}{4}\int_0^\infty \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{5/2}}\, t\, dt\,. $$

(5.2) follows from (3.2). □

In the next theorem we derive one-dimensional integral representations for the potential $\mathscr{B}_n$ acting on the basis functions (5.1).

Theorem 5.2. *For $M > 1$ we have*

$$ \mathscr{B}_3(\eta_{2M}(\cdot))(\mathbf{x}) = -\frac{1}{8\pi^{3/2}}\left(\int_0^\infty \prod_{j=1}^{3} \frac{\mathrm{e}^{-x_j^2/(1+t)}}{\sqrt{1+t}} Q_M(x_j,t)dt \right. $$

$$ \left. + \int_0^\infty \sum_{i=1}^{3} \frac{\mathrm{e}^{-x_i^2/(1+t)}}{\sqrt{1+t}} R_M(x_i,t) \prod_{\substack{j=1\\ j\neq i}}^{3} \frac{\mathrm{e}^{-x_j^2/(1+t)}}{\sqrt{1+t}} Q_M(x_j,t) t\, dt \right) \quad (5.5) $$

$$ \mathscr{B}_n(\eta_{2M}(\cdot))(\mathbf{x}) = \frac{1}{16\pi^{n/2}}\int_0^\infty \prod_{j=1}^{n} \frac{\mathrm{e}^{-x_j^2/(1+t)}}{\sqrt{1+t}} Q_M(x_j,t)\, t\, dt\,, \qquad n \geq 5 \quad (5.6) $$

with η_{2M} in (5.1) *and*

$$ Q_M(x,t) = \sum_{k=0}^{M-1} \frac{(-1)^k}{k!4^k} \frac{1}{(1+t)^k} H_{2k}\left(\frac{x}{\sqrt{1+t}}\right); $$

$$ R_M(x,t) = \sum_{k=0}^{M-1} \frac{(-1)^k}{k!4^k} \frac{1}{(1+t)^k} \mathscr{S}_{2k}\left(\frac{x}{\sqrt{1+t}}\right); \quad (5.7) $$

$$ \mathscr{S}_k(y) = y^2 H_k(y) - 2kyH_{k-1}(y) + k(k-1)H_{k-2}(y)\,. \quad (5.8) $$

$Q_M(x,t)$ and $R_M(x,t)$ are polynomials in x whose coefficients depend on t.

Proof. To get a one-dimensional integral representation of $\mathscr{B}_n(\prod_{j=1}^n \widetilde{\eta}_{2M})$ we use the relation ([10, p.55])

$$ \widetilde{\eta}_{2M}(y) = \frac{1}{\sqrt{\pi}} \sum_{k=0}^{M-1} \frac{(-1)^k}{k!4^k} \frac{d^{2k}}{dy^{2k}} \mathrm{e}^{-y^2}\,. $$

Let $n \geq 5$. The solution of the equation

$$ \Delta\Delta u = \prod_{j=1}^{n} \widetilde{\eta}_{2M}(x_j) $$

is given by the integral

$$
\begin{aligned}
&\frac{1}{16}\prod_{j=1}^{n}\frac{1}{\sqrt{\pi}}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx_j^{2k}}\int_0^\infty \frac{e^{-x_j^2/(1+t)}}{(1+t)^{n/2}}\,t\,dt \\
&\qquad = \frac{1}{16}\int_0^\infty \left(\prod_{j=1}^{n}\frac{1}{\sqrt{\pi}}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx_j^{2k}}e^{-x_j^2/(1+t)}\right)\frac{t\,dt}{(1+t)^{n/2}} \\
&\qquad = \frac{1}{16}\int_0^\infty \left(\prod_{j=1}^{n}\frac{1}{\sqrt{\pi}}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{e^{-x_j^2/(1+t)}}{(1+t)^{k+1/2}}H_{2k}\left(\frac{x_j}{\sqrt{1+t}}\right)\right)t\,dt\,,
\end{aligned}
$$

that is (5.6).
Let $n=3$. Keeping in mind (5.2), we get

$$
\begin{aligned}
\mathscr{B}_3(e^{-|\mathbf{x}|^2})(\mathbf{x}) = &-\frac{1}{8\pi^{3/2}}\prod_{j=1}^{3}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx_j^{2k}}\int_0^\infty \frac{e^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{3/2}}dt \\
&-\frac{1}{8\pi^{3/2}}\prod_{j=1}^{3}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx_j^{2k}}\int_0^\infty \frac{|\mathbf{x}|^2 e^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{5/2}}t\,dt.
\end{aligned}
$$

The first term in the r.h.s is similar to that considered in the case $n \geq 5$.
Concerning the second term, we have

$$
\frac{d^{2k}}{dx^{2k}}\left(\frac{x^2}{1+t}e^{-x^2/(1+t)}\right) = \frac{1}{(1+t)^k}\frac{d^{2k}}{dy^{2k}}\left(y^2 e^{-y^2}\right)_{y=x/\sqrt{1+t}} = \frac{e^{-x^2/(1+t)}}{(1+t)^k}\mathscr{S}_{2k}\left(\frac{x}{\sqrt{1+t}}\right)
$$

with $\mathscr{S}_k(y)$ in (5.8). Then

$$
\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx^{2k}}\left(\frac{x^2}{1+t}e^{-x^2/(1+t)}\right) = R_M(x,t)e^{-x^2/(1+t)}
$$

with $R_M(x,t)$ defined in (5.7). It follows that the second integral can be written as

$$
\begin{aligned}
&\prod_{j=1}^{3}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx_j^{2k}}\int_0^\infty \frac{|\mathbf{x}|^2 e^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{5/2}}t\,dt \\
&\qquad = \int_0^\infty \prod_{j=1}^{3}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!4^k}\frac{d^{2k}}{dx_j^{2k}}|\mathbf{x}|^2 e^{-|\mathbf{x}|^2/(1+t)}\frac{t\,dt}{(1+t)^{5/2}} \\
&\qquad = \int_0^\infty \sum_{i=1}^{3}R_M(x_i,t)\prod_{\substack{j=1\\ j\neq i}}^{3}Q_M(x_j,t)\frac{e^{-|\mathbf{x}|^2/(1+t)}t\,dt}{(1+t)^{3/2}}\,,
\end{aligned}
$$

which leads to (5.5). □

The polynomials $Q_M(x,t)$ and $R_M(x,t)$ for $M = 1,2,3,4$ are given by

$$Q_1(x,t) = 1\,, \qquad Q_2(x,t) = -\frac{x^2}{(1+t)^2} + \frac{1}{2(1+t)} + 1,$$

$$Q_3(x,t) = Q_2(x,t) + \frac{x^4}{2(1+t)^4} - \frac{3x^2}{2(1+t)^3} + \frac{3}{8(1+t)^2}\,,$$

$$Q_4(x,t) = Q_3(x,t) - \frac{x^6}{6(1+t)^6} + \frac{5x^4}{4(1+t)^5} - \frac{15x^2}{8(1+t)^4} + \frac{5}{16(1+t)^3}\,,$$

$$R_1(x,t) = \frac{x^2}{1+t}\,, \qquad R_2(x,t) = -\frac{x^4}{(1+t)^3} + \frac{x^2}{1+t} + \frac{5x^2}{2(1+t)^2} - \frac{1}{2(1+t)},$$

$$R_3(x,t) = R_2(x,t) + \frac{x^6}{2(1+t)^5} - \frac{7x^4}{2(1+t)^4} + \frac{39x^2}{8(1+t)^3} - \frac{3}{4(1+t)^2},$$

$$R_4(x,t) = R_3(x,t) - \frac{x^8}{6(1+t)^7} + \frac{9x^6}{4(1+t)^6} - \frac{65x^4}{8(1+t)^5} + \frac{125x^2}{16(1+t)^4} - \frac{15}{16(1+t)^3}.$$

6 Implementation and numerical results

In this section we consider the fast computation of the biharmonic potential based on (5.1). From (4.2) and (5.6) we derive the cubature formula

$$\mathscr{B}^{(n)}_{M,h} f(\mathbf{x}) = \frac{(h\sqrt{\mathscr{D}})^4}{16(\pi\mathscr{D})^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \int_0^\infty \prod_{j=1}^n Q_M\left(\frac{x_j - hm_j}{h\sqrt{\mathscr{D}}}, t\right) t\,dt\,, \quad n \geq 5\,.$$

At the grid points $h\mathbf{k} = (hk_1, ..., hk_n)$ we obtain

$$\mathscr{B}^{(n)}_{M,h} f(h\mathbf{k}) = \frac{(h\sqrt{\mathscr{D}})^4}{16} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) a^{(M)}_{\mathbf{k}-\mathbf{m}} \tag{6.1}$$

where

$$a^{(M)}_{\mathbf{k}} = \frac{1}{(\pi\mathscr{D})^{n/2}} \int_0^\infty \prod_{j=1}^n \mathrm{e}^{-k_j^2/(\mathscr{D}(1+t))} Q_M\left(\frac{k_j}{\sqrt{\mathscr{D}}}, t\right) t\,dt\,. \tag{6.2}$$

The product structure of the integrand leads to new cubature formulas if the density f admits the so-called separated representation. The idea is the following. If f is given as product of univariate functions

$$f(\mathbf{x}) = \prod_{j=1}^n f_j(x_j)$$

then the values on the grid $h\mathbf{k}$ of the cubature formula can be written as

$$\mathscr{B}^{(n)}_{M,h} f(h\mathbf{k}) = \frac{(h\sqrt{\mathscr{D}})^4}{16(\pi\mathscr{D})^{n/2}} \int_0^\infty \prod_{j=1}^n \sum_{m_j\in\mathbb{Z}} f_j(hm_j) \mathrm{e}^{-(k_j-m_j)^2/(\mathscr{D}(1+t))} Q_M\left(\frac{k_j - m_j}{\sqrt{\mathscr{D}}}, t\right) t\,dt\,.$$

A suitable quadrature of this integral with nodes τ_s and quadrature weights ω_s leads to

$$\mathscr{B}_{M,h}^{(n)} f(h\mathbf{k}) \approx \frac{(h\sqrt{\mathscr{D}})^4}{16(\pi\mathscr{D})^{n/2}} \sum_s \omega_s \prod_{j=1}^{n} \sigma_j(k_j, \tau_s)$$

with

$$\sigma_j(k,\tau) = \sum_{m\in\mathbb{Z}} f_j(hm) \mathrm{e}^{-(k-m)^2/(\mathscr{D}(1+\tau))} Q_M\left(\frac{k-m}{\sqrt{\mathscr{D}}}, \tau\right) \tau.$$

Then the value of the integral operator on the grid $h\mathbf{k}$ can be obtained by computing one-dimensional sums, and therefore the computational complexity of the algorithm scales linearly in the physical dimension.

We use an efficient quadrature based on the classical trapezoidal rule, which is exponentially converging for rapidly decaying smooth functions on the real line. We make the substitutions

$$t = \mathrm{e}^{\xi}, \quad \xi = a(\sigma + \mathrm{e}^{\sigma}), \quad \sigma = b(u - \mathrm{e}^{-u})$$

with positive constants a and b proposed in [17] (see also [3, 4]). Then the integrals (6.2) are transformed to integrals over $\mathbb{R}$ with integrands decaying doubly exponentially in u. After the substitution we have

$$a_{\mathbf{k}}^{(M)} = \frac{1}{(\pi\mathscr{D})^{n/2}} \int_{-\infty}^{\infty} \prod_{j=1}^{n} \mathrm{e}^{-k_j^2/(\mathscr{D}(1+\Phi(u)))} Q_M\left(\frac{k_j}{\sqrt{\mathscr{D}}}, \Phi(u)\right) \Phi(u)\Phi'(u) du$$

with the functions

$$\begin{aligned} \Phi(u) &= \exp(ab\,(u - \mathrm{e}^{-u}) + a\exp(b(u - \mathrm{e}^{-u}))), \\ \Phi'(u) &= \Phi(u) ab(1 + \mathrm{e}^{-u})(1 + \exp(b(u - \mathrm{e}^{-u}))). \end{aligned}$$

Thus the trapezoidal rule of step τ can provide very accurate approximations of the integral for a relatively small number of nodes τs

$$a_{\mathbf{k}}^{(M)} \approx \frac{\tau}{(\pi\mathscr{D})^{n/2}} \sum_s \prod_{j=1}^{n} \mathrm{e}^{-k_j^2/(\mathscr{D}(1+\Phi(\tau s)))} Q_M\left(\frac{k_j}{\sqrt{\mathscr{D}}}, \Phi(\tau s)\right) \Phi(\tau s)\Phi'(\tau s)$$

Assume that f, within a prescribed accuracy, can be represented as sum of products of one-dimensional functions

$$f(\mathbf{x}) = \sum_{p=1}^{P} \beta_p \prod_{j=1}^{n} f_j^{(p)}(x_j) + \mathscr{O}(\varepsilon) \tag{6.3}$$

with suitable functions $f_j^{(p)}$ chosen such that the separation rank P is small. We derive the approximation of the convolutional sum (6.1) using one-dimensional operations

$$\begin{aligned} \mathscr{B}_{M,h}^{(n)} f(h\mathbf{k}) \approx &\frac{(h\sqrt{\mathscr{D}})^4}{16(\pi\mathscr{D})^{n/2}} \tau \sum_{p=1}^{P} \beta_p \sum_s \Phi(\tau s)\Phi'(\tau s) \\ &\times \prod_{j=1}^{n} \sum_{m_j} f_j^{(p)}(hm_j) \left(\mathrm{e}^{-(k_j-m_j)^2/(\mathscr{D}(1+\Phi(\tau s)))} Q_M\left(\frac{k_j - m_j}{\sqrt{\mathscr{D}}}, \Phi(\tau s)\right)\right). \end{aligned}$$

We provide results of some experiments which show the accuracy and numerical order of the method. We compute the biharmonic potential of the density

$$f(\mathbf{x}) = 4\mathrm{e}^{-|\mathbf{x}|^2}\left(n(n+2) - 4(n+2)|\mathbf{x}|^2 + 4|\mathbf{x}|^4\right), \tag{6.4}$$

which has exact values $\mathscr{B}_n f(\mathbf{x}) = \mathrm{e}^{-|\mathbf{x}|^2}$. In Table 1 we compare the exact values of $\mathscr{B}_n f$ and the approximate values $\mathscr{B}^{(n)}_{4,0.025} f$ at some grid points $(x_1, 0, ..., 0) \in \mathbb{R}^n$ for space dimensions $n = 5, 10, 10^2, ..., 10^8$.

n		5		10		100	
x_1	exact	abs. error	rel. error	abs. error	rel. error	abs. error	rel. error
0	0.100E+01	0.129E-09	0.129E-09	0.258E-09	0.258E-09	0.258E-08	0.258E-08
1	0.368E+00	0.286E-10	0.777E-10	0.760E-10	0.207E-09	0.930E-09	0.253E-08
2	0.183E-01	0.171E-11	0.933E-10	0.404E-11	0.220E-09	0.465E-10	0.254E-08
3	0.123E-03	0.112E-12	0.910E-09	0.943E-13	0.764E-09	0.381E-12	0.309E-08
4	0.113E-06	0.435E-13	0.386E-06	0.948E-14	0.843E-07	0.973E-14	0.864E-07
n		1 000		10 000		100 000	
x_1	exact	abs. error	rel. error	abs. error	rel. error	abs. error	rel. error
0	0.100E+01	0.258E-07	0.258E-07	0.258E-06	0.258E-06	0.258E-05	0.258E-05
1	0.368E+00	0.947E-08	0.257E-07	0.948E-07	0.258E-06	0.949E-06	0.258E-05
2	0.183E-01	0.472E-09	0.257E-07	0.472E-08	0.258E-06	0.472E-07	0.258E-05
3	0.123E-03	0.324E-11	0.263E-07	0.319E-10	0.258E-06	0.318E-09	0.258E-05
4	0.113E-06	0.123E-13	0.110E-06	0.385E-13	0.342E-06	0.300E-12	0.266E-05
n		1 000 000		10 000 000		100 000 000	
x_1	exact	abs. error	rel. error	abs. error	rel. error	abs. error	rel. error
0	0.100E+01	0.258E-04	0.258E-04	0.258E-03	0.258E-03	0.258E-02	0.258E-02
1	0.368E+00	0.949E-05	0.258E-04	0.948E-04	0.258E-03	0.947E-03	0.258E-02
2	0.183E-01	0.472E-06	0.258E-04	0.472E-05	0.258E-03	0.472E-04	0.258E-02
3	0.123E-03	0.318E-08	0.258E-04	0.318E-07	0.258E-03	0.318E-06	0.258E-02
4	0.113E-06	0.291E-11	0.259E-04	0.290E-10	0.258E-03	0.290E-09	0.258E-02

Table 1: Exact value of $\mathscr{B}_n f(x_1, 0, \ldots, 0)$, absolute error and relative error using $\mathscr{B}^{(n)}_{4,0.025}$

In Table 2 we report on the absolute errors and approximation rates for the biharmonic potential $\mathscr{B}_n f(1, 0, ..., 0)$ in the space dimensions $n = 5 \times 10^k$, $k = 0, ..., 4$. The approximate values are computed by the cubature formulas $\mathscr{B}^{(n)}_{M,h}$ for $M = 1, 2, 3, 4$. We use uniform grids of size $h = 0.1 \times 2^{-k}$, $k = 1, ..., 5$. For high dimensional cases the second order formula fails whereas the eighth order formula $\mathscr{B}^{(n)}_{4,h}$ approximates with the predicted approximation rates. Table 3 shows that the cubature method is effective also for much higher space dimensions and the approximation rate is reached. For all calculations the same quadrature rule is used for computing the one-dimensional integral, the parameters are $\mathscr{D} = 5$, $a = 6$ and $b = 5$, $\tau = 0.003$ and 300 summands in the quadrature sum.

In the remainder of this section we compute the 3-dimensional biharmonic potential by means of the approximating formula (5.5). For functions of the form (6.3) we obtain that, at the points of the uniform grid $\{h\mathbf{k}\}$, the 3-dimensional integral $\mathscr{B}_3 f$ is

$M = 4$

n	5		50		500		5000		50000	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.15E-05		0.25E-04		0.26E-03		0.26E-02		0.25E-01	
20	0.70E-08	7.77	0.11E-06	7.81	0.12E-05	7.81	0.12E-04	7.81	0.12E-03	7.76
40	0.29E-10	7.94	0.46E-09	7.95	0.47E-08	7.95	0.47E-07	7.95	0.47E-06	7.95
80	0.15E-12	7.55	0.18E-11	7.99	0.19E-10	7.99	0.19E-09	7.99	0.19E-08	7.99
160	0.38E-13	2.02	0.10E-13	7.44	0.86E-13	7.75	0.84E-12	7.80	0.61E-11	8.26
					$M = 3$					
10	0.30E-04		0.60E-03		0.62E-02		0.58E-01		0.30E+00	
20	0.53E-06	5.83	0.10E-04	5.86	0.11E-03	5.85	0.11E-02	5.74	0.11E-01	4.82
40	0.86E-08	5.96	0.17E-06	5.96	0.17E-05	5.96	0.17E-04	5.96	0.17E-03	5.94
80	0.13E-09	5.99	0.26E-08	5.99	0.27E-07	5.99	0.27E-06	5.99	0.27E-05	5.99
160	0.21E-11	5.97	0.41E-10	6.00	0.43E-09	6.00	0.43E-08	6.00	0.43E-07	6.00
					$M = 2$					
10	0.74E-03		0.15E-01		0.13E+00		0.36E+00		0.37E+00	
20	0.49E-04	3.91	0.10E-02	3.89	0.10E-01	3.63	0.92E-01	1.98	0.35E+00	0.08
40	0.31E-05	3.98	0.63E-04	3.98	0.67E-03	3.96	0.66E-02	3.79	0.61E-01	2.50
80	0.20E-06	3.99	0.40E-05	3.99	0.42E-04	3.99	0.42E-03	3.98	0.42E-02	3.87
160	0.12E-07	4.00	0.25E-06	4.00	0.26E-05	4.00	0.26E-04	4.00	0.26E-03	3.99
					$M = 1$					
10	0.26E-01		0.37E+00		0.37E+00		0.37E+00		0.37E+00	
20	0.68E-02	1.95	0.35E+00	0.07	0.35E+00	0.07	0.37E+00	0.00	0.37E+00	0.00
40	0.17E-02	1.99	0.20E+00	0.82	0.20E+00	0.82	0.37E+00	0.00	0.37E+00	0.00
80	0.43E-03	2.00	0.65E-01	1.61	0.65E-01	1.61	0.32E+00	0.22	0.37E+00	0.00
160	0.11E-03	2.00	0.17E-01	1.90	0.17E-01	1.90	0.14E+00	1.15	0.37E+00	0.01

Table 2: Absolute errors and approximation rates for $\mathscr{B}_n f(1,0,\ldots,0)$ using $\mathscr{B}_{M,h}^{(n)}$.

$M = 4$

n	100000		1000000		10000000	
h^{-1}	error	rate	error	rate	error	rate
10	0.49E-01		0.28E+00		0.37E+00	
20	0.23E-03	7.71	0.23E-02	6.90	0.23E-01	4.02
40	0.95E-06	7.95	0.95E-05	7.95	0.95E-04	7.91
80	0.37E-08	7.99	0.37E-07	7.99	0.37E-06	7.99
160	0.13E-10	8.20	0.20E-09	7.58	0.11E-08	8.41
			$M = 3$			
10	0.36E+00		0.37E+00		0.37E+00	
20	0.21E-01	4.08	0.16E+00	1.16	0.37E+00	0.00
40	0.35E-03	5.92	0.35E-02	5.57	0.33E-01	3.47
80	0.55E-05	5.99	0.55E-04	5.98	0.55E-03	5.92
160	0.86E-07	6.00	0.86E-06	6.00	0.86E-05	6.00

Table 3: Absolute errors and approximation rates for $\mathscr{B}_n f(1,0,\ldots,0)$ using $\mathscr{B}_{M,h}^{(n)}$.

	$M=4$			$M=3$		
h^{-1}	absolute error	relative error	ate	absolute error	relative error	rate
10	0.236E-06	0.474E-05		0.822E-05	0.165E-03	
20	0.965E-09	0.194E-07	7.93	0.137E-06	0.275E-05	5.91
40	0.381E-11	0.765E-10	7.99	0.217E-08	0.436E-07	5.98
80	0.150E-13	0.301E-12	7.99	0.341E-10	0.685E-09	5.99
160	0.438E-14	0.879E-13	1.77	0.538E-12	0.108E-10	5.99

	$M=2$			$M=1$		
h^{-1}	absolute error	relative error	rate	absolute error	relative error	rate
10	0.217E-03	0.435E-02		0.359E-02	0.722E-01	
20	0.143E-04	0.287E-03	3.92	0.925E-03	0.186E-01	1.96
40	0.907E-06	0.182E-04	3.98	0.233E-03	0.468E-02	1.99
80	0.569E-07	0.114E-05	3.99	0.583E-04	0.117E-02	2.00
160	0.356E-08	0.715E-07	4.00	0.146E-04	0.293E-03	2.00

Table 4: Relative errors, absolute errors and approximation rates for $\mathscr{B}_3 f(1,1,1)$ using $\mathscr{B}^{(3)}_{M,h}$.

approximated by

$$\begin{aligned}\mathscr{B}_3 f(h\mathbf{k}) \approx &-\frac{h^4 \mathscr{D}^{5/2}}{8\pi^{3/2}} \tau \sum_{p=1}^{P} \beta_p \sum_s \Phi'(\tau s) \\ &\times \Bigg(\prod_{i=1}^{3} \sum_{m_i} f_j^{(p)}(hm_i) \mathrm{e}^{-(k_i-m_i)^2/(\mathscr{D}(1+\Phi(\tau s)))} Q_M\Big(\frac{k_i-m_i}{\sqrt{\mathscr{D}}}, \Phi(\tau s)\Big) \\ &\quad + \Phi(\tau s) \sum_{i=1}^{3} \sum_{m_i} \mathrm{e}^{-(k_i-m_i)^2/(\mathscr{D}(1+\Phi(\tau s)))} R_M\Big(\frac{k_i-m_i}{\sqrt{\mathscr{D}}}, \Phi(\tau s)\Big) f_i^{(p)}(hm_i) \\ &\quad \times \prod_{\substack{j=1 \\ j\neq i}}^{3} \sum_{m_j} \mathrm{e}^{-(k_j-m_j)^2/(\mathscr{D}(1+\Phi(\tau s)))} Q_M\Big(\frac{k_j-m_j}{\sqrt{\mathscr{D}}}, \Phi(\tau s)\Big) f_j^{(p)}(hm_j) \Bigg).\end{aligned}$$

In Table 4 we report on the relative and absolute errors, and the approximation rate for the 3-dimensional biharmonic potential $\mathscr{B}_3 f$ at the point $(1,1,1)$ of the density (6.4), which has exact value e^{-3}. The numerical results confirm the h^{2M} convergence of the cubature formula when $M = 1,2,3,4$.

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