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Tensor product approximations of high dimensional potentials

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Abstract

The paper is devoted to the efficient computation of high-order cubature formulas for volume potentials obtained within the framework of approximate approximations. We combine this approach with modern methods of structured tensor product approximations. Instead of performing high-dimensional discrete convolutions the cubature of the potentials can be reduced to a certain number of one-dimensional convolutions leading to a considerable reduction of computing resources. We propose one-dimensional integral representions of high-order cubature formulas for n-dimensional harmonic and Yukawa potentials, which allow low rank tensor product approximations.

1 Introduction

The construction of efficient representations of multi-variate integral operators plays a crucial role in the numerics of higher dimensional problems arising in a wide range of modern applications. Let us mention multi-dimensional integral equations and volume potentials of elliptic and parabolic partial differential operators in $\mathbb{R}^n$, $n \geq 3$.

In the present paper we study the combination of high-order semi-analytic cubature formulas for volume potentials with modern methods of structured tensor product approximations. The cubature formulas have been obtained in [5, 6] using the method of approximate approximations, see also [7] and the reference therein.

The application of tensor product approximations to the approximation of volume potentials is described for example in [3, 4, 2]. The main idea is to derive accurate tensor product approximations of the density u and the kernel g of the convolution integral of the form

$$u(\mathbf{x}) = \sum_{p=1}^{R} u_p \prod_{j=1}^{n} v_j^{(p)}(x_j)\,,$$

where $\mathbf{x} = (x_1, \dots, x_n)$ and

$$g(\mathbf{x}) = \sum_{q=1}^{R} b_q \prod_{j=1}^{n} g_j^{(q)}(x_j)\,,$$

such that the convolution integral can be approximated by one-dimensional convolutions

$$\int\limits_{\mathbb{R}^n} g(\mathbf{x}-\mathbf{y}) u(\mathbf{y})\, d\mathbf{y} \approx \sum_{p,q=1}^{R} b_q u_p \prod_{j=1}^{n} \int\limits_{\mathbb{R}} g_j^{(q)}(x_j - y) v_j^{(p)}(y)\, dy\,.$$

Then the numerical computation of the integral does not require to perform an n-dimensional discrete convolution, for example, instead one has to compute pq one-dimensional discrete convolutions, which can lead to a considerable reduction of computing time and memory requirements, and gives the possibility to treat real world problems.

In this note we present some variants for the tensor product approximation of high order cubature for harmonic, Yukawa and heat potentials as integral operators in $\mathbb{R}^n$. After a brief introduction into cubature formulas based on approximate approximations and their error behavior, we describe their representations as one-dimensional integrals suitable for tensor product approximation. For the example of the harmonic potential in $\mathbb{R}^n$, $3 \le n \le 6$, we report on numerical tests for second and fourth order formulas, which provide estimates of the tensor rank required to approximate the action of the potential on a basis function with a prescribed relative error. Further we report on numerical tests for the Yukawa potential, which can be approximated accurately with a very small number of tensors in a wide range of arguments. In the final section 5 we study the volume heat potential in $\mathbb{R}^n$, derive approximation results and describe its tensor product approximation.

2 Semi-analytic cubature formulas for potentials

Here we collect some results on high-order cubature formulas for the volume potentials of the differential operators $-\Delta$ and $-\Delta + a^2$, $\operatorname{Re} a^2 > 0$, in $\mathbb{R}^n$.

2.1 Harmonic potentials in $\mathbb{R}^n$

The harmonic potential is the inverse of the Laplace operator and given in $\mathbb{R}^n$ by the formula

$$\mathcal{L}_n u(\mathbf{x}) = \frac{\Gamma(\frac{n}{2}-1)}{4\pi^{n/2}} \int\limits_{\mathbb{R}^n} \frac{u(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{n-2}}\, d\mathbf{y}\ , \quad n \ge 3\ . \tag{2.1}$$

The volume potential provides the unique solution of the Poisson equation

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

The theory of *approximate approximations* proposes semi-analytic cubature formulas for harmonic potentials by using quasi-interpolation of the density u by functions for which the integral operator can be taken analytically. For example, approximate u by the quasi-interpolant

$$u_h(\mathbf{x}) = \mathcal{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} u(h\mathbf{m})\, \eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{\sqrt{\mathcal{D}}h}\Big)\,, \tag{2.2}$$

with a suitable generating function η. Then the sum

$$\mathcal{L}_n u_h(\mathbf{x}) = \frac{h^2}{\mathcal{D}^{n/2-1}} \sum_{\mathbf{m}\in\mathbb{Z}^n} u(h\mathbf{m}) \mathcal{L}_n \eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{\sqrt{\mathcal{D}}h}\Big) \tag{2.3}$$

is a cubature of the harmonic potential. If one wants to compute the harmonic potential of u on the given grid $\{h\mathbf{k}\}$ then one has to compute the discrete convolution

$$\mathcal{L}_n u_h(h\mathbf{k}) = \frac{h^2}{\mathcal{D}^{n/2-1}} \sum_{\mathbf{m}\in\mathbb{Z}^n} a_{\mathbf{k}-\mathbf{m}}\, u(h\mathbf{m})\,, \quad \mathbf{k}\in\mathbb{Z}^n\,, \tag{2.4}$$

with the coefficients

$$a_{\mathbf{k}} = a_{\mathbf{k}}(\mathcal{D}) = \mathcal{L}_n\eta\Big(\frac{\mathbf{k}}{\sqrt{\mathcal{D}}}\Big) = \frac{\Gamma(\frac{n}{2}-1)}{4\pi^{n/2}} \int\limits_{\mathbb{R}^n} \frac{\eta(\mathbf{y})}{|\mathbf{k}/\sqrt{\mathcal{D}}-\mathbf{y}|^{n-2}}\, d\mathbf{y}\,. \tag{2.5}$$

It has been shown that for sufficiently smooth and compactly supported functions the cubature formula (2.3) provide approximations with the error $O(h^{2M})+O(\mathrm{e}^{-\mathcal{D}\pi^2}\, h^2)$ if the function η is chosen as

$$\eta_{2M}(\mathbf{x}) = \pi^{-n/2}\, L_{M-1}^{(n/2)}(|\mathbf{x}|^2)\ \mathrm{e}^{-|\mathbf{x}|^2}\,, \tag{2.6}$$

where $L_j^{(\gamma)}$ are the generalized Laguerre polynomials

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

Additionally, there holds the analytic representation

$$\mathcal{L}_n\eta_{2M}\Big(\frac{\mathbf{k}}{\sqrt{\mathcal{D}}}\Big) = \frac{1}{\pi^{n/2}}\frac{\mathcal{D}^{n/2-1}}{4|\mathbf{k}|^{n-2}}\,\gamma\Big(\frac{n}{2}-1,\frac{|\mathbf{k}|^2}{\mathcal{D}}\Big) + \frac{\mathrm{e}^{-|\mathbf{k}|^2/\mathcal{D}}}{\pi^{n/2}} \sum_{j=0}^{M-2} \frac{L_j^{(n/2-1)}(|\mathbf{k}|^2/\mathcal{D})}{4(j+1)}\,. \tag{2.7}$$

Here γ is the lower incomplete Gamma function defined by

$$\gamma(a,x) = \int\limits_0^x \tau^{a-1}\,\mathrm{e}^{-\tau}\ d\tau\,. \tag{2.8}$$

In the case $k\in\mathbf{N}$

$$\gamma(k,x) = (k-1)!\Big(1-\mathrm{e}^{-x}\sum_{j=0}^{k-1}\frac{x^j}{j!}\Big)\,,$$

whereas for odd space dimension n one can use

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

with the error function erf and the recurrence relation

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

to derive analytic expressions for $\mathcal{L}_n\eta_{2M}$.

The asymptotic error estimate $O(h^{2M})+O(\mathrm{e}^{-\mathcal{D}\pi^2}\,h^2)$ for the cubature formula (2.3) is based on the error estimate $O(h^{2M})+\varepsilon$ for the quasi-interpolant (2.2) if the sufficiently smooth and decaying generating function η is subject to the moment condition

$$\int_{\mathbb{R}^n} \eta(\mathbf{x})\, d\mathbf{x} = 1 \ , \ \int_{\mathbb{R}^n} \mathbf{x}^{\boldsymbol{\alpha}} \eta(\mathbf{x})\, d\mathbf{x} = 0, \quad \forall\, \boldsymbol{\alpha} \ , \ 1 \le |\boldsymbol{\alpha}| < 2M \, . \tag{2.9}$$

The saturation error ε does not converge to zero for $h \to 0$, but because of

$$\varepsilon = O\Big(\max_{\mathbf{x}} \Big| \sum_{\mathbf{k} \in \mathbb{Z}^n \setminus \{\mathbf{0}\}} \mathcal{F}\eta(\sqrt{\mathcal{D}}\mathbf{k})\, \mathrm{e}^{2\pi i (\mathbf{k},\mathbf{x})/h} \Big| \Big) \tag{2.10}$$

can be made arbitrarily small if the parameter $\mathcal{D}$ is sufficiently large. Additionally, the harmonic potential maps the fast oscillating saturation term (2.10) into a function with norm of order $O(h^2 \varepsilon)$, which establishes the error estimate $O(h^{2M}) + O(\mathrm{e}^{-\mathcal{D}\pi^2} h^2)$ for the approximation of the harmonic potential by using quasi-interpolation of the density with the generating function (2.6).

So in numerical computations with $\mathcal{D} \ge 3$ the formulas (2.4-2.7) behave like high order cubature formulas for harmonic potentials in $\mathbb{R}^n$. The approximation of the potential on the grid $\{h\mathbf{k}\}$ can be done by fast convolutional methods, but one has to store the values $\{a_{\mathbf{k}}\}$ for a quite large subset of $\mathbf{k} \in \mathbb{Z}^n$.

2.2 Yukawa potentials in $\mathbb{R}^n$

The fundamental solution of the operator $-\Delta + a^2$, $\mathrm{Re}\, a^2 > 0$ in $\mathbb{R}^n$ is given as

$$\kappa_a(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \Big(\frac{|\mathbf{x}|}{a} \Big)^{1-n/2} K_{n/2-1}(a|\mathbf{x}|) \, ,$$

where K_ν is the modified Bessel function of the second kind, also known as Macdonald function, [1, 9.6]. Thus the volume potential

$$\int_{\mathbb{R}^n} \kappa_a(\mathbf{x} - \mathbf{y}) u(\mathbf{y})\, d\mathbf{y}$$

for $n = 3$ also called Yukawa potential, provides the solution of the equation

$$(-\Delta + a^2) f = u \quad \text{in } \mathbb{R}^n \, .$$

To derive a cubature formula for that potential we look for a solution of

$$-\Delta f + a^2 f = \mathrm{e}^{-|\mathbf{x}|^2}, \ \mathbf{x} \in \mathbb{R}^n \, ,$$

which is given as the one-dimensional integral

$$f(\mathbf{x}) = \frac{\mathrm{e}^{-|\mathbf{x}|^2}\ a^{n/2-1}}{|2\mathbf{x}|^{n/2-1}} \int_0^\infty K_{n/2-1}(ar)\, I_{n/2-1}(2|\mathbf{x}|r)\, r\ \mathrm{e}^{-r^2}\ dr \, , \tag{2.11}$$

where I_ν is the modified Bessel function of the first kind, see [7, Section 5.2].

Using the known analytic expressions of $I_{n+1/2}$ and $K_{n+1/2}$ (cf. [1]) it is possible to derive analytic formula of (2.11) for odd space dimension n. In particular, if $n = 3$, then

$$f(\mathbf{x}) = \frac{\sqrt{\pi}}{8} \frac{\mathrm{e}^{-|\mathbf{x}|^2}}{|\mathbf{x}|} \Big(\mathrm{w}\left(i(\frac{a}{2} - |\mathbf{x}|)\right) - \mathrm{w}\left(i(\frac{a}{2} + |\mathbf{x}|)\right) \Big), \tag{2.12}$$

where w denotes the scaled complementary error function

$$\mathrm{w}(z) = \mathrm{e}^{-z^2} \operatorname{erfc}(-iz) = \mathrm{e}^{-z^2} \Big(1 + \frac{2i}{\sqrt{\pi}} \int\limits_0^z \mathrm{e}^{t^2} \, dt \Big), \tag{2.13}$$

and

$$\operatorname{erfc}(\tau) = 1 - \operatorname{erf}(\tau) \tag{2.14}$$

is the complementary error function.

Using the representation from [7, Theorem 3.5]

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

one can derive as in the case of harmonic potentials semi-analytic cubature formulas for the Yukawa potential with the approximation rate $O(h^{2M}) + O(\mathrm{e}^{-\mathcal{D}\pi^2} \, h^2)$.

3 Tensor product expansions of potentials acting on Gaussians

To obtain a tensor product approximation of the second order cubature formula

$$\frac{\mathcal{D}h^2}{(\pi\mathcal{D})^{n/2}} \sum_{\mathbf{m} \in \mathbb{Z}^n} u(h\mathbf{m}) \, \mathcal{L}_n\big(\mathrm{e}^{-|\cdot|^2} \big)(\mathbf{r}_\mathbf{m}) \tag{3.1}$$

for the harmonic potential with

$$\mathbf{r}_\mathbf{m} = \frac{\mathbf{x} - h\mathbf{m}}{\sqrt{\mathcal{D}}h} \quad \text{and} \quad \mathcal{L}_n\big(\mathrm{e}^{-|\cdot|^2} \big)(\mathbf{x}) = \frac{1}{4|\mathbf{x}|^{n-2}} \gamma\Big(\frac{n}{2} - 1, |\mathbf{x}|^2 \Big) ,$$

we use the formula obtained in [8]

$$\mathcal{L}_n\big(\mathrm{e}^{-|\cdot|^2} \big)(\mathbf{x}) = \frac{1}{4} \int\limits_0^\infty \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}} \, dt \, ,$$

which is valid for $n \geq 3$. The simple quadrature of the integral

$$\mathcal{L}_n\big(\mathrm{e}^{-|\cdot|^2} \big)(\mathbf{x}) \approx \sum_{k=1}^R \omega_k \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+\tau_k)}}{(1+\tau_k)^{n/2}} = \sum_{k=1}^R \omega_k \prod_{j=1}^n \frac{\mathrm{e}^{-x_j^2/(1+\tau_k)}}{(1+\tau_k)^{n/2}}$$

with certain quadrature weights ω_k and nodes τ_k gives already a tensor product approximation. Hence, for $\mathbf{x} = (x_1, \dots, x_n)$ and $\mathbf{m} = (m_1, \dots, m_n)$

$$\mathcal{L}_n\big(\mathrm{e}^{-|\cdot|^2}\big)\Big(\frac{\mathbf{x}-h\mathbf{m}}{\sqrt{\mathcal{D}}h}\Big) \approx \frac{\mathcal{D}h^2}{4(\pi\mathcal{D})^{n/2}} \sum_{k=1}^{R} \omega_k \prod_{j=1}^{n} \frac{\mathrm{e}^{-(x_j-hm_j)^2/(\mathcal{D}h^2(1+\tau_k))}}{(1+\tau_k)^{n/2}}$$

which implies that one can approximate

$$\mathcal{L}_n u_h(h\mathbf{k}) \approx \frac{\mathcal{D}h^2}{4(\pi\mathcal{D})^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} u(h\mathbf{m}) \sum_{k=1}^{R} \omega_k \prod_{j=1}^{n} \frac{\mathrm{e}^{-(k_j-m_j)^2/(\mathcal{D}(1+\tau_k))}}{(1+\tau_k)^{n/2}},$$

$\mathbf{k} = (k_1, \dots, k_n)$.

To obtain a similar tensor product approximation for higher order cubature formula we note that one obtains the same convergence order $O(h^{2M}) + O(\mathrm{e}^{-\mathcal{D}\pi^2}\, h^2)$ as in the case of generating functions (2.6) if the density is approximated by the sum

$$\mathcal{M}_M u(\mathbf{x}) = (\pi\mathcal{D})^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} u(h\mathbf{m}) \prod_{j=1}^{n} \widetilde{\eta}_{2M}\Big(\frac{x_j - hm_j}{\sqrt{\mathcal{D}}h}\Big),$$

where the generating function is the tensor product of the one-dimensional generating functions

$$\widetilde{\eta}_{2M}(x) = L_{M-1}^{(1/2)}(x^2)\,\mathrm{e}^{-x^2}\,. \tag{3.2}$$

and obviously satisfies the moment condition (2.9).

To get the one-dimensional integral representation of $\mathcal{L}_n\Big(\prod_{j=1}^{n}\widetilde{\eta}_{2M}\Big)$ we use the relation

$$\widetilde{\eta}_{2M}(x) = \sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k}\,\frac{d^{2k}}{dx^{2k}}\,\mathrm{e}^{-x^2} = \mathrm{e}^{-x^2} \sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k}\, H_{2k}(x) = \mathrm{e}^{-x^2} \sum_{k=0}^{M-1} L_k^{(-1/2)}(x^2)\,,$$

where $H_k(x)$ denotes the Hermite polynomial

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

Then the solution of the Poisson equation

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

is given by the integral

$$\begin{aligned}
&\frac{1}{4}\prod_{j=1}^{n}\Big(\sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k}\,\frac{d^{2k}}{dx_j^{2k}} \int_0^\infty \frac{\mathrm{e}^{-x_j^2/(1+t)}}{(1+t)^{1/2}}\,dt\Big)\\
&= \frac{1}{4}\int_0^\infty \prod_{j=1}^{n}\Big(\sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k}\,\frac{d^{2k}}{dx_j^{2k}}\,\mathrm{e}^{-x_j^2/(1+t)}\Big)\frac{dt}{(1+t)^{n/2}}\\
&= \frac{1}{4}\int_0^\infty \prod_{j=1}^{n} \mathrm{e}^{-x_j^2/(1+t)}\Big(\sum_{k=0}^{M-1} \frac{1}{(1+t)^{k+1/2}}\, L_k^{(-1/2)}\Big(\frac{x_j^2}{1+t}\Big)\Big)\,dt\,.
\end{aligned}$$

Again, a tensor product representation of this integral and consequently of the convolution matrix for the high order cubature of the harmonic potential is given by a quadrature of the last integral.

So the problem is reduced to find efficient quadrature formulas for the parameter dependent integrals

$$
\begin{aligned}
I_1(\mathbf{x}) &= \int_0^\infty \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}}\,dt = \int_0^\infty \prod_{j=1}^n \frac{\mathrm{e}^{-x_j^2/(1+t)}}{\sqrt{1+t}}\,dt\,, \\
I_M(\mathbf{x}) &= \int_0^\infty \prod_{j=1}^n \mathrm{e}^{-x_j^2/(1+t)} \Big(\sum_{k=0}^{M-1} \frac{1}{(1+t)^{k+1/2}}\, L_k^{(-1/2)}\Big(\frac{x_j^2}{1+t}\Big)\Big)\,dt\,.
\end{aligned}
\tag{3.3}
$$

More precisely, one has to find a certain quadrature rule with minimal number of summands which approximates the integrals with prescribed error for the parameters $x_j = (k_j - m_j)/\sqrt{\mathcal{D}}$ within the range $|x_j| \le K$ and some given bound K.

3.1 Quadratures

It is well known that classical trapezoidal rule is exponentially converging for certain classes of integrands, for example periodic functions and rapidly decaying functions on the real line. For example, Poisson's summation formula yields that

$$
h \sum_{k=-\infty}^{\infty} f(kh) = \sum_{j=-\infty}^{\infty} \hat{f}\big(\frac{2\pi j}{h}\big) \tag{3.4}
$$

for any sufficiently smooth function, say of the Schwarz class $\mathcal{S}(\mathbb{R})$. Here $\hat{f}$ is the Fourier transform

$$
\hat{f}(\lambda) = \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-2\pi i x\lambda}\,dx\,.
$$

Thus,

$$
\int_{-\infty}^{\infty} f(x)\,dx - h \sum_{k=-\infty}^{\infty} f(kh) = \sum_{j\neq 0} \hat{f}\big(\frac{2\pi j}{h}\big)\,,
$$

which indicates that by choosing special substitutions such that the integrand transforms to a rapidly decaying function with rapidly decaying Fourier transform, the trapezoidal rule of step size h can provide very accurate approximations of the integral.

Here we follow a proposal made by J. Waldvogel [9] to compute accurately integrals of analytic functions. We make the substitutions

$$
t = \mathrm{e}^{\xi}\,, \quad \xi = a(\tau + \mathrm{e}^{\tau}) \quad \text{and} \quad \tau = b(u - \mathrm{e}^{-u})\,, \tag{3.5}
$$

where $a, b > 0$ are certain constants. Then the integrals (3.3) are transformed to integrals over $\mathbb{R}$ of doubly exponentially decaying integrands f, i.e. $|f(u)| \le c\exp(-\alpha\exp(|u|))$ for $|u| \to \infty$ with certain constants $c, \alpha > 0$. It is known (cf. e.g.

[4]) that by suitable truncation of the infinite sum in the trapezoidal rule of step size h provides exponentially convergent numerical quadrature algorithms with the error estimate $O(\mathrm{e}^{-c/h})$.

After the substitution we have

$$I_1(\mathbf{x}) = ab \int_{-\infty}^{\infty} \exp\Big(-\frac{|\mathbf{x}|^2}{1+\phi(u)}\Big) \frac{(1+\mathrm{e}^{-u})(1+\exp(b(u-\mathrm{e}^{-u})))\,\phi(u)}{(1+\phi(u))^{n/2}}\, du\,,$$

where we set

$$\phi(u) = \exp(ab(u-\mathrm{e}^{-u}) + a\exp(b(u-\mathrm{e}^{-u})))\,.$$

Similarly

$$I_M(\mathbf{x}) = ab \int_{-\infty}^{\infty} \prod_{j=1}^{n} g_j(u)du \quad \text{with the functions}$$

$$g_j(u) = (1+\mathrm{e}^{-u})(1+\exp(b(u-\mathrm{e}^{-u})))\,\phi(u)\exp\Big(-\frac{x_j^2}{1+\phi(u)}\Big) \sum_{k=0}^{M-1} \frac{L_k^{(-1/2)}\Big(\frac{x_j^2}{1+\phi(u)}\Big)}{(1+\phi(u))^{k+1/2}}\,.$$

The integrals are approximated by the finite sum

$$\int_{-\infty}^{\infty} f(u,\mathbf{x})\,du \approx h \sum_{k=-N_0}^{N_1} f(hk,\mathbf{x}),\ |\mathbf{x}| \le K. \tag{3.6}$$

3.2 Numerical Results

3.2.1 Approximation to the integral $I_1(\mathbf{x})$

We assume in (3.5) $a = b = 1$. Figure 1 illustrates the graph of the integrand function $f(u,\mathbf{x})$, $u \in (-4,4)$, $n = 3$, for different values of $|\mathbf{x}| \le 10^3$. A similar behavior holds for $n = 4,5,6$.

Table 1 presents the maximum step h_0 and the minimum number of quadrature points required to achieve the relative error ϵ, uniformly in $|\mathbf{x}| \in [0,10^3]$. We have considered the space dimension $n = 3\,,4\,,5\,,6$.

It is possible to play with different parameters a and b in order to diminish the number of summands in the quadrature formula. Consider e.g. the case $a = 6$ and $b = 5$. Figure 2 shows the graph of $f(u,|\mathbf{x}|)$, $u \in (0,0.85)$ for different values of $|\mathbf{x}|$. The numerical results for this quadrature are given in Table 2.

3.2.2 Approximation to the integral $I_2(\mathbf{x})$

Next, we discuss the computation of the integral

$$I_2(\mathbf{x}) = \int_0^{\infty} \prod_{j=1}^{n} \mathrm{e}^{-\frac{x_j^2}{t+1}} \left(\frac{1}{\sqrt{t+1}} + \frac{1}{(t+1)^{3/2}}(\frac{1}{2} - \frac{x_j^2}{t+1})\right) dt.$$

$n = 3$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.264	18
10^{-3}	0.137	38
10^{-5}	0.072	82
10^{-7}	0.055	116
10^{-9}	0.043	161
10^{-11}	0.036	205

$n = 4$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.198	20
10^{-3}	0.095	52
10^{-5}	0.072	77
10^{-7}	0.051	121
10^{-9}	0.040	164
10^{-11}	0.033	206

$n = 5$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.181	21
10^{-3}	0.088	59
10^{-5}	0.065	83
10^{-7}	0.060	96
10^{-9}	0.037	169
10^{-11}	0.033	200

$n = 6$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.156	26
10^{-3}	0.090	55
10^{-5}	0.059	90
10^{-7}	0.044	130
10^{-9}	0.035	178
10^{-11}	0.029	220

Table 1: The approximation of $I_1(\mathbf{x})$ for $|\mathbf{x}| \leq 10^3$, with $a = b = 1$ in (3.5).

$n = 3$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.0297	10
10^{-3}	0.0125	28
10^{-5}	0.0077	61
10^{-7}	0.0055	111
10^{-9}	0.0042	170
10^{-11}	0.0034	247

$n = 4$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.0234	10
10^{-3}	0.0107	30
10^{-5}	0.0070	58
10^{-7}	0.0049	107
10^{-9}	0.0037	169
10^{-11}	0.0033	217

$n = 5$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.0380	7
10^{-3}	0.0120	27
10^{-5}	0.0069	57
10^{-7}	0.0046	112
10^{-9}	0.0034	179
10^{-11}	0.0031	221

$n = 6$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.0185	12
10^{-3}	0.0083	36
10^{-5}	0.0058	70
10^{-7}	0.0042	117
10^{-9}	0.0037	158
10^{-11}	0.0028	242

Table 2: The approximation of $I_1(\mathbf{x})$ for $|\mathbf{x}| \leq 10^3$, with the choice $a = 6; b = 5$ in (3.5).

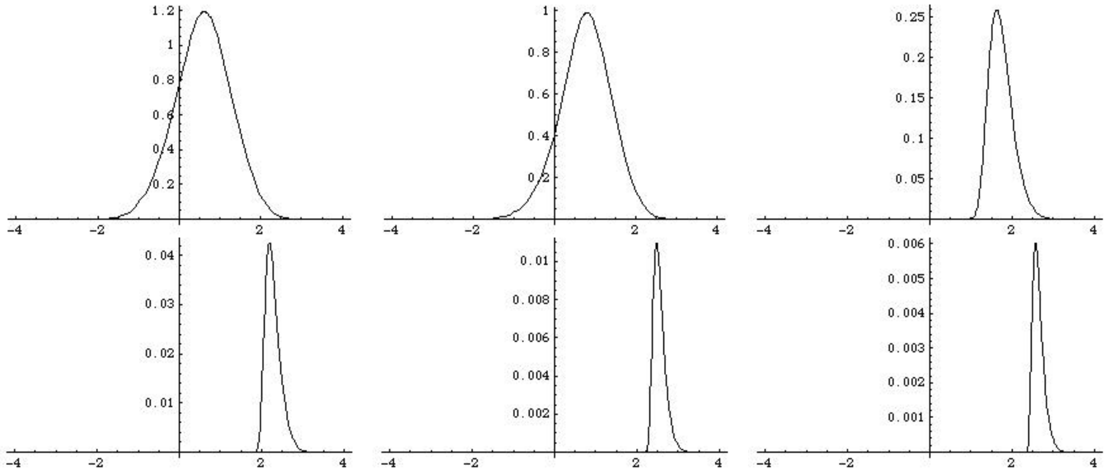

Figure 1: The plot of the integrand function $f(u, \mathbf{x})$ ($a = b = 1$) in $I_1(\mathbf{x})$ for $|\mathbf{x}| = 0, 1, 10, 100, 500, 1000$ (from the left to the right) in the interval $u \in (-4, 4)$.

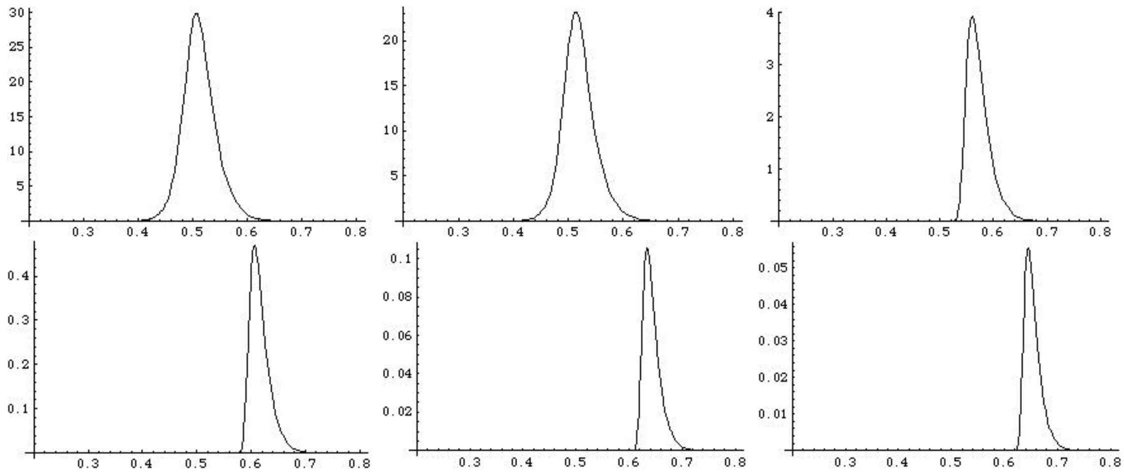

Figure 2: The plot of the integrand function $f(u, \mathbf{x})$ ($a = 6, b = 5$) in $I_1(\mathbf{x})$ for $|\mathbf{x}| = 0, 1, 10, 100, 500, 1000$ (from the left to the right) in the interval $u \in (0, 0.85)$.

using the variable transformations (3.5) and the trapezoidal rule (3.6), for $n = 3$ and $n = 4$. In the numerical results below, for the sake of simplicity, we assumed $\mathbf{x} = (x, x, x)$, with $|\mathbf{x}| \leq 10^3$.

Numerical results for this quadrature are presented in Table 3, with the parameters $a = b = 1$, and in Table 4 in the case $a = 6$, $b = 5$.

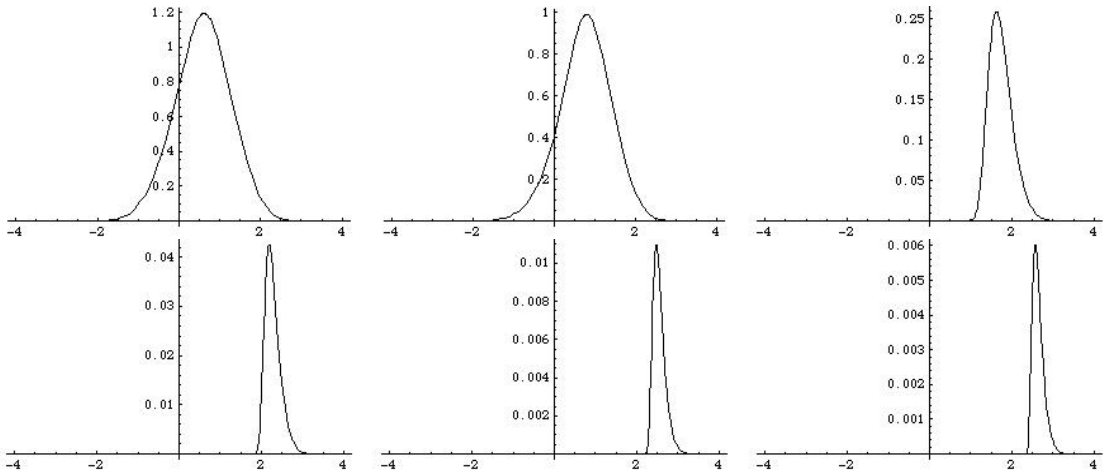

Figure 3: The plot of the integrand function $f(u, \mathbf{x})$ in $I_2(\mathbf{x})$ for $|\mathbf{x}| = 0, 1, 10, 100, 500, 1000$ (from the left to the right) in the interval $u \in (-4, 4)$, $a = 1, b = 1$.

4 Yukawa potential

To derive a tensor product approximation of the second and higher order cubature formulas for the Yukawa potential we use the relation

$$\int_{\mathbb{R}^n} \kappa_a(\mathbf{x}-\mathbf{y})\, \mathrm{e}^{-|\mathbf{y}|^2}\, d\mathbf{y} = \frac{1}{4} \int_0^\infty \frac{\mathrm{e}^{-a^2 t/4}\, \mathrm{e}^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}}\, dt\,,$$

obtained in [8] and is valid for all $n \geq 2$, see also [7, Theorem 6.4]. Hence, an approximate solution of the equation in $\mathbb{R}^n$

$$-\Delta f + a^2 f = u$$

is given by

$$f_h(\mathbf{x}) = \frac{\mathcal{D}h^2}{4(\pi\mathcal{D})^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} u(h\mathbf{m}) \int_0^\infty \frac{\mathrm{e}^{-a^2\mathcal{D}h^2 t/4}\ \mathrm{e}^{-|\mathbf{x}-h\mathbf{m}|^2/(\mathcal{D}h^2(1+t))}}{(1+t)^{n/2}}\, dt\,,$$

which converges with the order $O(h^2)$ to f.

Analogously to the case of harmonic potentials we consider the integral

$$\int_{\mathbb{R}^n} \kappa_a(\mathbf{x}-\mathbf{y}) \prod_{j=1}^n \widetilde{\eta}_{2M}(y_j)\, d\mathbf{y} = \prod_{j=1}^n \Big(\sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k} \frac{\partial^{2k}}{\partial x_j^{2k}} \Big) \int_{\mathbb{R}^n} \kappa_a(\mathbf{x}-\mathbf{y})\, \mathrm{e}^{-|\mathbf{y}|^2}\, d\mathbf{y}$$

$$= \frac{1}{4} \prod_{j=1}^n \Big(\sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k} \frac{d^{2k}}{dx_j^{2k}} \int_0^\infty \mathrm{e}^{-a^2 t/4}\, \frac{\mathrm{e}^{-x_j^2/(1+t)}}{(1+t)^{1/2}}\, dt \Big)$$

$$= \frac{1}{4} \int_0^\infty \prod_{j=1}^n \mathrm{e}^{-x_j^2/(1+t)} \Big(\sum_{k=0}^{M-1} \frac{\mathrm{e}^{-a^2 t/4}}{(1+t)^{k+1/2}}\, L_k^{(-1/2)}\Big(\frac{x_j^2}{1+t}\Big)\Big)\, dt\,.$$

$n = 3$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.295	16
10^{-3}	0.133	40
10^{-5}	0.072	82
10^{-7}	0.055	118
10^{-9}	0.043	163
10^{-11}	0.036	204

$n = 4$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.198	23
10^{-3}	0.095	52
10^{-5}	0.072	77
10^{-7}	0.051	121
10^{-9}	0.040	163
10^{-11}	0.033	206

Table 3: The approximation of $I_2(\mathbf{x})$ for $|\mathbf{x}| \le 10^3$, with $a = b = 1$.

$n = 3$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.0297	10
10^{-3}	0.0125	30
10^{-5}	0.0077	63
10^{-7}	0.0052	114
10^{-9}	0.0042	175
10^{-11}	0.0034	234

$n = 4$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.0197	11
10^{-3}	0.0107	30
10^{-5}	0.0074	57
10^{-7}	0.0046	120
10^{-9}	0.0037	175
10^{-11}	0.0033	222

Table 4: The approximation of $I_2(\mathbf{x})$ for $|\mathbf{x}| \le 10^3$, with $a = 6; b = 5$.

which is the basis of the cubature formula of the order $O(h^{2M}) + O(\mathrm{e}^{-\mathcal{D}\pi^2}\, h^2)$.

To get doubly periodic integrands for the integrals

$$K_1(\mathbf{x}) = \int\limits_0^\infty \frac{\mathrm{e}^{-a^2t/4}\,\mathrm{e}^{-|\mathbf{x}|^2/(1+t)}}{(1+t)^{n/2}}\,dt = \int\limits_0^\infty \mathrm{e}^{-a^2t/4}\prod_{j=1}^{n}\frac{\mathrm{e}^{-x_j^2/(1+t)}}{\sqrt{1+t}}\,dt$$

$$K_M(\mathbf{x}) = \int\limits_0^\infty \mathrm{e}^{-a^2t/4}\prod_{j=1}^{n}\sum_{k=0}^{M-1}\frac{\mathrm{e}^{-x_j^2/(1+t)}}{(1+t)^{k+1/2}}\,L_k^{(-1/2)}\Big(\frac{x_j^2}{1+t}\Big)\,dt\,.$$

we make the substitutions

$$t = \exp(b(u - \exp(-u))\,,\ b > 0\,,$$

and apply the trapezoidal rule to

$$K_1(\mathbf{x}) = a\int\limits_{-\infty}^{\infty}\exp\Big(-\frac{|\mathbf{x}|^2}{1+\phi(u)} - \frac{c^2\phi(u)}{4}\Big)\frac{(1+\mathrm{e}^{-u})\,\phi(u)}{(1+\phi(u))^{n/2}}\,du\,,$$

$$
\begin{aligned}
K_M(\mathbf{x}) = & a \int_{-\infty}^{\infty} \mathrm{e}^{-c^2\phi(u)/4}(1+\mathrm{e}^{-u})\,\phi(u) \prod_{j=1}^{n} \exp\Big(-\frac{x_j^2}{1+\phi(u)}\Big) \\
& \times \sum_{k=0}^{M-1} \frac{1}{(1+\phi(u))^{k+1/2}}\, L_k^{(-1/2)}\Big(\frac{x_j^2}{1+\phi(u)}\Big)\, dt\,.
\end{aligned}
$$

4.1 Approximation to the integral $K_1(\mathbf{x})$

We apply the quadrature formula (3.6) to the integral $K_1(\mathbf{x})$ for $n = 3$, in the cases $a^2 = 0.01$, $a^2 = 0.1$ (Table 5), $a^2 = 1$ and $a^2 = 4$ (Table 6). We assumed $b = 1$.

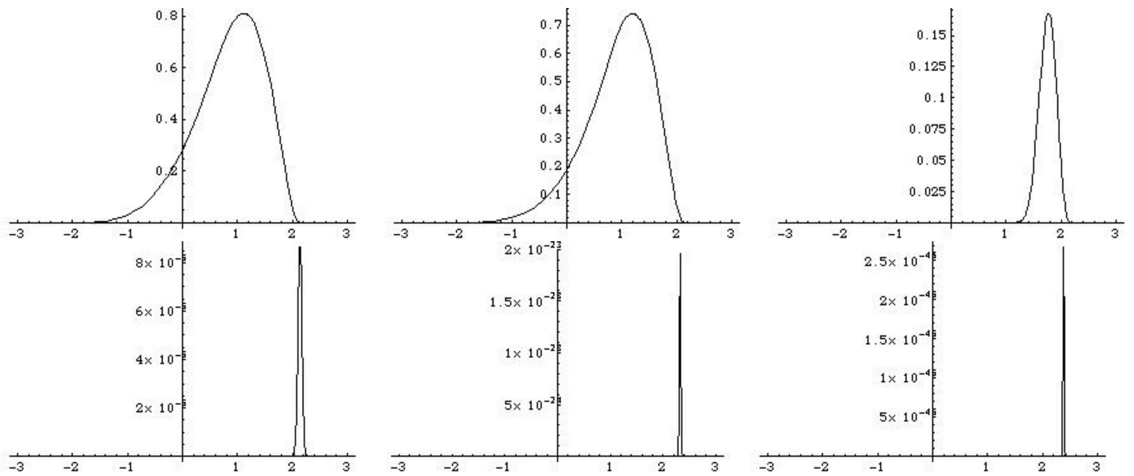

Figure 4: The plot of the integrand function $f(u, \mathbf{x})$ in $K_1(\mathbf{x})$, $a^2 = 0.01, b = 1$ for $|\mathbf{x}| = 0, 1, 10, 100, 500, 1000$ (from the left to the right) in the interval $u \in (-3, 3)$.

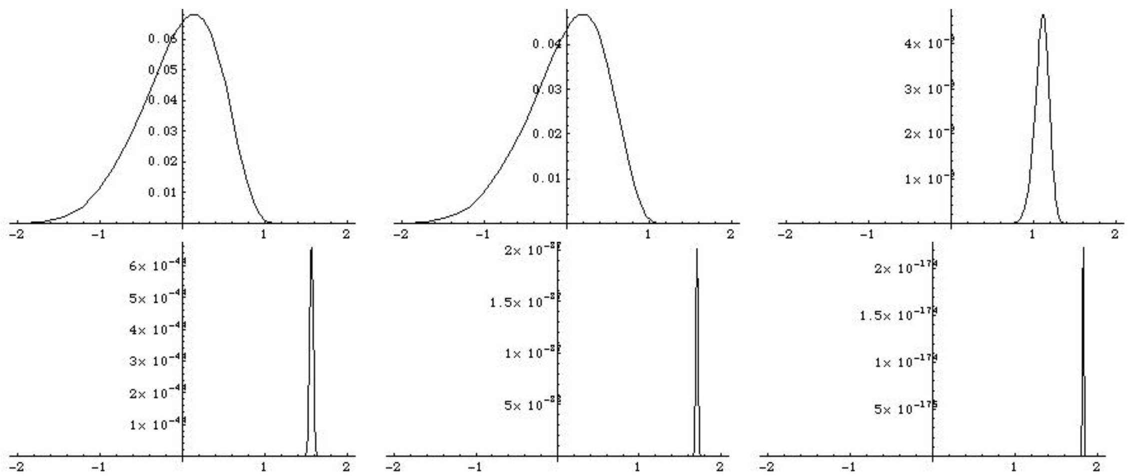

Figure 5: The plot of the integrand function $f(u, \mathbf{x})$ in $K_1(\mathbf{x})$, $a^2 = 4, b = 1$ for $|\mathbf{x}| = 0, 1, 10, 50, 100, 200$ (from the left to the right) in the interval $u \in (-2, 2)$.

$a^2 = 0.01$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.99	9
10^{-3}	0.72	15
10^{-5}	0.58	20
10^{-7}	0.47	25
10^{-9}	0.39	32
10^{-11}	0.30	43
10^{-13}	0.26	50
10^{-15}	0.25	56

$a^2 = 0.1$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.98	7
10^{-3}	0.68	12
10^{-5}	0.58	17
10^{-7}	0.42	16
10^{-9}	0.40	25
10^{-11}	0.29	36
10^{-13}	0.25	43
10^{-15}	0.23	50

Table 5: The approximation of $K_1(\mathbf{x})$ for $|\mathbf{x}| \leq 10^3$, with $a^2 = 0.01$ (on the left) and $a^2 = 0.1$ (on the right).

$a^2 = 1$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.99	6
10^{-3}	0.65	10
10^{-5}	0.48	15
10^{-7}	0.38	20
10^{-9}	0.37	22
10^{-11}	0.29	28
10^{-13}	0.25	34
10^{-15}	0.21	42

$a^2 = 4$

Relative Error	h_0	Number of quadrature points
10^{-1}	0.92	5
10^{-3}	0.58	9
10^{-5}	0.44	13
10^{-7}	0.36	17
10^{-9}	0.31	21
10^{-11}	0.27	25
10^{-13}	0.25	29
10^{-15}	0.16	46

Table 6: The approximation of $K_1(\mathbf{x})$ for $|\mathbf{x}| \leq 10^3$, with $a^2 = 1$ (on the left) and $a^2 = 4$ (on the right).

5 Heat potential

Consider the non-homogeneous (linear) heat equation

$$f_t - \nu \Delta_{\mathbf{x}} f = u(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^n,\ t \geq 0 \tag{5.1}$$

with the initial condition

$$f(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \mathbb{R}^n. \tag{5.2}$$

It well known that the solution of this Cauchy problem can be written as

$$f(\mathbf{x}, t) = \int_0^t (\mathcal{P}_{t-\lambda} u(\cdot, \lambda))(\mathbf{x})\, d\lambda\,, \tag{5.3}$$

where $\mathcal{P}_t$ is the Poisson integral

$$(\mathcal{P}_t u(\cdot,\lambda))(x) = \frac{1}{(4\pi\nu t)^{n/2}} \int\limits_{\mathbb{R}^n} \mathrm{e}^{-|\mathbf{x}-\boldsymbol{\xi}|^2/(4\nu t)} u(\boldsymbol{\xi},\lambda)\, d\boldsymbol{\xi}\,. \tag{5.4}$$

An approximation of this solution $f(\mathbf{x},t)$ can be obtained if the function f is approximated by the quasi-interpolant on the rectangular grid $(h\,\mathbf{m}, \tau\, j)$, with $h>0$ and $\tau>0$,

$$u_{h,\tau}(\mathbf{x},t) = \frac{\pi^{-(n+1)/2}}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{j\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} u(h\mathbf{m},\tau j)\, \mathrm{e}^{-(t-\tau j)^2/(\mathcal{D}_0\tau^2)}\, \mathrm{e}^{-|\mathbf{x}-h\mathbf{m}|^2/(\mathcal{D}h^2)}\,. \tag{5.5}$$

Then the sum

$$\begin{aligned}
f_{h,\tau}(\mathbf{x},t) &= \int\limits_0^t (\mathcal{P}_{t-\lambda} u_{h,\tau}(\cdot,\lambda))(\mathbf{x}) d\lambda \qquad (5.6)\\
&= \frac{(4\pi\nu)^{-n/2}}{\pi^{(n+1)/2}\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{j\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} u(h\mathbf{m},\tau j) \int\limits_0^t \frac{\mathrm{e}^{-(\lambda-\tau j)^2/(\mathcal{D}_0\tau^2)}}{(t-\lambda)^{n/2}}\, d\lambda \\
&\qquad\times \int\limits_{\mathbb{R}^n} \mathrm{e}^{-|\mathbf{x}-\boldsymbol{\xi}|^2/(4\nu(t-\lambda)) - |\boldsymbol{\xi}-h\mathbf{m}|^2/(h^2\mathcal{D})}\, d\boldsymbol{\xi} \\
&= \frac{h^n}{\pi^{(n+1)/2}\sqrt{\mathcal{D}_0}} \sum_{\substack{j\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} u(h\mathbf{m},\tau j) \int\limits_0^t \frac{\mathrm{e}^{-(\lambda-(t-\tau j))^2/(\mathcal{D}_0\tau^2)}\, \mathrm{e}^{-|\mathbf{x}-h\mathbf{m}|^2/(\mathcal{D}h^2+4\nu\lambda)}}{(\mathcal{D}h^2+4\nu\lambda)^{n/2}}\, d\lambda
\end{aligned}$$

provides an approximation of $f(\mathbf{x},t)$.

Since $u_{h,\tau}(\mathbf{x},t)$ approximates $u(\mathbf{x},t)$ with

$$|u(\mathbf{x},t) - u_{h,\tau}(\mathbf{x},t)| \le \varepsilon + c\big((\tau\sqrt{\mathcal{D}_0})^2 + (h\sqrt{\mathcal{D}})^2\big)\,, \quad \forall \mathbf{x}\in\mathbb{R}^n,\ t\in[0,T] \tag{5.7}$$

the function $f_{h,\tau}(\mathbf{x},t)$ approximates the solution $f(\mathbf{x},t)$ with the error

$$\begin{aligned}
|f(\mathbf{x},t) - f_{h,\tau}(\mathbf{x},t)| &= \frac{1}{(4\pi\nu)^{n/2}} \int\limits_0^t d\lambda \int\limits_{\mathbb{R}^n} \frac{\mathrm{e}^{-|\mathbf{x}-\boldsymbol{\xi}|^2/(4(t-\lambda))}}{(t-\lambda)^{n/2}} |u(\boldsymbol{\xi},\lambda) - u_{h,\tau}(\boldsymbol{\xi},\lambda)|\, d\boldsymbol{\xi} \\
&\le T\,||u-u_{h,\tau}||_{L^\infty(\mathbb{R}^n\times[0,T])} \le \varepsilon + c\big((\tau\sqrt{\mathcal{D}_0})^2 + (h\sqrt{\mathcal{D}})^2\big)\,, \quad \forall \mathbf{x}\in\mathbb{R}^n,\ t\in[0,T].
\end{aligned}$$

The integral

$$K_{j,\mathbf{m}}(\mathbf{x},t) = \int\limits_0^t \frac{\mathrm{e}^{-(\lambda-(t-\tau j))^2/(\mathcal{D}_0\tau^2)}\, \mathrm{e}^{-|\mathbf{x}-h\mathbf{m}|^2/(\mathcal{D}h^2+4\nu\lambda)}}{(\mathcal{D}h^2+4\nu\lambda)^{n/2}}\, d\lambda \tag{5.8}$$

cannot be taken analytically, but it allows obviously an approximate tensor product approximation. Making the substitution

$$\lambda = \frac{t}{1+\mathrm{e}^{-\xi}}$$

we derive the integral over $\mathbb{R}$

$$K_{j,\mathbf{m}}(\mathbf{x},t) = \frac{t}{4}\int\limits_{-\infty}^{\infty} \frac{\mathrm{e}^{-(\tau j - t/(1+\mathrm{e}^{\xi}))^2/(\mathcal{D}_0\tau^2)}\,\mathrm{e}^{-|\mathbf{x}-h\mathbf{m}|^2/(\mathcal{D}h^2+4\nu t/(1+\mathrm{e}^{-\xi}))}}{(\mathcal{D}h^2+4\nu t/(1+\mathrm{e}^{-\xi}))^{n/2}\cosh^2(\xi/2)}\,d\xi$$

with exponentially decaying integrand. Performing the last 2 substitutions in (3.5) we again transform the integrand to a doubly exponentially decaying function.

Approximations which converge with higher order to the solution of (5.1) can be obtained using quasi-interpolation of the right-hand side u by

$$\tilde{u}_{h,\tau}(\mathbf{x},t) = \frac{\pi^{-(n+1)/2}}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{j\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} u(h\mathbf{m},\tau j)\widetilde{\eta}_{2S}\Big(\frac{t-\tau j}{\sqrt{\mathcal{D}_0}\tau}\Big)\prod_{i=1}^{n}\widetilde{\eta}_{2M}\Big(\frac{x_i-hm_i}{\sqrt{\mathcal{D}}h}\Big) \tag{5.9}$$

where $\widetilde{\eta}_{2M}$ are defined by (3.2). Since for all $j \le 2S-1, \alpha_i \le 2M-1$ we have

$$\int\limits_{\mathbb{R}^{n+1}} t^j\,\widetilde{\eta}_{2S}(t)\prod_{i=1}^{n} x_i^{\alpha_i}\,\widetilde{\eta}_{2M}(x_i)\,dt\,d\mathbf{x} = \begin{cases} \pi^{(n+1)/2}\,, & j=\alpha_1=\ldots\alpha_n=0\,,\\ 0\,, & \text{otherwise}\,,\end{cases}$$

the following result can be derived in a standard way.

Theorem 5.1. *Given $\varepsilon > 0$ there exist $\mathcal{D} > 0$ and $\mathcal{D}_0 > 0$ such that for any $u \in W^L_\infty(\mathbb{R}^n\times\mathbb{R})$, with $L = \max(2M,2S)$, the quasi interpolant (5.9) satisfies the estimate*

$$\begin{aligned} |u\,(\mathbf{x},t) - u_{h,\tau}(\mathbf{x},t)| &\le c_1(\mathcal{D}h^2)^M + c_2(\mathcal{D}_0\tau^2)^S \\ &+\varepsilon\left(\sum_{|\alpha|=0}^{2M-1}\frac{(h\sqrt{\mathcal{D}})^{|\alpha|}}{\alpha!}||\partial_x^\alpha u||_{L^\infty(\mathbb{R}^n\times[0,T])} + \sum_{\beta=0}^{2S-1}\frac{(\tau\sqrt{\mathcal{D}_0})^{|\beta|}}{\beta!}||\partial_t^\beta u||_{L^\infty(\mathbb{R}^n\times[0,T])}\right)\end{aligned} \tag{5.10}$$

where the constants c_1 and c_2 do not depend on h, τ, $\mathcal{D}$, $\mathcal{D}_0$ and f.

To obtain the cubature we use that

$$\widetilde{\eta}_{2S}\Big(\frac{t}{\sqrt{\mathcal{D}_0}\tau}\Big) = \sum_{k=0}^{S}\frac{(-1)^k(\mathcal{D}_0\tau^2)^k}{k!\,4^k}\,\frac{\partial^{2k}}{\partial t^{2k}}\,\mathrm{e}^{-t^2/(\tau^2\mathcal{D}_0)}$$

$$\widetilde{\eta}_{2M}\Big(\frac{x_i}{\sqrt{\mathcal{D}}h}\Big) = \sum_{k=0}^{M}\frac{(-1)^k(\mathcal{D}h^2)^k}{k!\,4^k}\,\frac{\partial^{2k}}{\partial x_i^{2k}}\,\mathrm{e}^{-|\mathbf{x}|^2/(h^2\mathcal{D})}$$

Hence the heat potential of the quasi-interpolant (5.9)

$$\tilde{f}_{h,\tau}(\mathbf{x},t) = \int\limits_0^t (\mathcal{P}_{t-\lambda}\tilde{u}_{h,\tau}(\cdot,\lambda))(\mathbf{x})d\lambda$$
$$= \frac{h^n}{\pi^{(n+1)/2}\sqrt{\mathcal{D}_0}} \sum_{\substack{j\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} u(h\mathbf{m},\tau j) \sum_{k=0}^{M} \mathcal{K}_{j,\mathbf{m}}^{S,M}(\mathbf{x},t)\,, \tag{5.11}$$

where we use the notation

$$\mathcal{K}_{j,\mathbf{m}}^{S,M}(\mathbf{x},t) = \sum_{k=0}^{S} \frac{(-1)^k(\mathcal{D}_0\tau^2)^k}{k!\,4^k} \frac{\partial^{2k}}{\partial t^{2k}} \prod_{i=1}^{n}\sum_{k=0}^{M} \frac{(-1)^k(\mathcal{D}h^2)^k}{k!\,4^k} \frac{\partial^{2k}}{\partial x_i^{2k}} K_{j,\mathbf{m}}(\mathbf{x},t)$$

We have

$$\frac{\partial^{2k}}{\partial x_i^{2k}}\,\mathrm{e}^{-(x_i-hm_i)^2/(\mathcal{D}h^2+4\nu\lambda)} = (-1)^k k!\,4^k \frac{\mathrm{e}^{-(x_i-hm_i)^2/(\mathcal{D}h^2+4\nu\lambda)}}{(\mathcal{D}h^2+4\nu\lambda)^k} L_k^{(-1/2)}\Big(\frac{(x_i-m_i)^2}{\mathcal{D}h^2+4\nu\lambda}\Big)\,,$$

which by using (5.8) leads to the representation

$$\mathcal{K}_{j,\mathbf{m}}^{S,M}(\mathbf{x},t) = \sum_{k=0}^{S} \frac{(-1)^k(\mathcal{D}_0\tau^2)^k}{k!\,4^k} \frac{\partial^{2k}}{\partial t^{2k}} \int\limits_0^t \mathrm{e}^{-(\lambda-(t-\tau j))^2/(\mathcal{D}_0\tau^2)} \prod_{i=1}^{n} g_M(\lambda, x_i-m_i)d\lambda\,,$$

admitting again a tensor product approximation. Here we denote by g_M the function

$$g_M(\lambda,x) = \sum_{k=0}^{M} \frac{(\mathcal{D}h^2)^k}{(\mathcal{D}h^2+4\nu\lambda)^{k+1/2}} L_k^{(-1/2)}\Big(\frac{x^2}{\mathcal{D}h^2+4\nu\lambda}\Big)\,\mathrm{e}^{-x^2/(\mathcal{D}h^2+4\nu\lambda)}\,.$$

From Theorem 5.1 it is easy to deduce that $f_{h,\tau}$ approximates the solution f with the order $\mathcal{O}((\sqrt{\mathcal{D}_0}\tau)^{2S}+(\sqrt{\mathcal{D}}h)^{2M})$ plus the saturation error.

Theorem 5.2. *For any $\varepsilon > 0$ there exist $\mathcal{D} > 0$ and $\mathcal{D}_0 > 0$ such that, for all $u \in W_\infty^L(\mathbb{R}^n\times\mathbb{R})$, with $L = \max(2M, 2S)$, the quasi-interpolant (5.11) approximates the solution of the Cauchy problem for the heat equation (5.1)-(5.2) with the error estimate*

$$|f(\mathbf{x},t) - f_{h,\tau}(\mathbf{x},t)| \le c_{1,T}(\mathcal{D}h^2)^M + c_{2,T}(\mathcal{D}_0\tau^2)^S$$
$$+\,\varepsilon\left(\sum_{|\alpha|=0}^{2M-1} \frac{(h\sqrt{\mathcal{D}})^{|\alpha|}}{\alpha!}||\partial_x^\alpha u||_{L^\infty(\mathbb{R}^n\times[0,T])} + \sum_{\beta=0}^{2S-1}\frac{(\tau\sqrt{\mathcal{D}_0})^\beta}{\beta!}||\partial_t^\beta u||_{L^\infty(\mathbb{R}^n\times[0,T])}\right).$$

The constants $c_{i,T}$, $i = 1,2$, depend only on M and S.

Proof. Since

$$\frac{1}{(4\pi\nu(t-\lambda))^{n/2}} \int\limits_{\mathbb{R}^n} \mathrm{e}^{-|\mathbf{x}-\boldsymbol{\xi}|^2/(4\nu(t-\lambda))} d\boldsymbol{\xi} = 1$$

we obtain that

$$\begin{aligned}|f(\mathbf{x},t) &- f_{h,\tau}(\mathbf{x},t)| \\ &= \frac{1}{(4\pi\nu)^{n/2}} \int_0^t \frac{d\lambda}{(t-\lambda)^{n/2}} \int\limits_{\mathbb{R}^n} \mathrm{e}^{-|\mathbf{x}-\boldsymbol{\xi}|^2/(4\nu(t-\lambda))} |f(\boldsymbol{\xi},\lambda) - f_{h,\tau}(\boldsymbol{\xi},\lambda)|\, d\boldsymbol{\xi} \\ &\leq T\,||u - u_{h,\tau}||_{L^\infty(\mathbb{R}^n\times[0,T])}\,, \quad \forall \mathbf{x}\in\mathbb{R}^n,\ t\in[0,T].\end{aligned}$$

From (5.10) the proof is complete.

□

5.1 Numerical example

We have tested the approximation formula (5.5) for solving the Cauchy problem

$$f_t - f_{xx} = x^2 + t^2, \qquad f(x,0) = 0, \quad x \in \mathbb{R},\ t \geq 0., \tag{5.12}$$

having the solution $f(x,t) = t^2 + \dfrac{t^3}{3} + tx^2$.

In the table 7 the difference $f_{h,\tau}(x,t) - f(x,t)$ for different values of h and τ, $\mathcal{D}_0 = \mathcal{D} = 2$, at the time $t = 0.01$ and the point $x = 0.01$ is given. The numerical results in the table confirm that the error is $\mathcal{O}(h^2 + \tau^2)$.

$\tau^{-1} \setminus h^{-1}$	4	8	16	32	64	128
4	$1.25\,10^{-3}$	$7.81\,10^{-4}$	$6.64\,10^{-4}$	$6.35\,10^{-4}$	$6.27\,10^{-4}$	$6.25\,10^{-4}$
8	$7.81\,10^{-4}$	$3.12\,10^{-4}$	$1.95\,10^{-4}$	$1.66\,10^{-4}$	$1.58\,10^{-4}$	$1.56\,10^{-4}$
16	$6.64\,10^{-4}$	$1.95\,10^{-4}$	$7.81\,10^{-5}$	$4.88\,10^{-5}$	$4.15\,10^{-5}$	$3.96\,10^{-5}$
32	$6.34\,10^{-4}$	$1.66\,10^{-4}$	$4.88\,10^{-5}$	$1.95\,10^{-5}$	$1.22\,10^{-5}$	$1.03\,10^{-5}$
64	$6.27\,10^{-4}$	$1.58\,10^{-4}$	$4.15\,10^{-5}$	$1.22\,10^{-5}$	$4.88\,10^{-6}$	$3.05\,10^{-6}$
128	$6.25\,10^{-4}$	$1.56\,10^{-4}$	$3.96\,10^{-5}$	$1.03\,10^{-5}$	$3.05\,10^{-6}$	$1.22\,10^{-6}$

Table 7: Error table for solving (5.12) with (5.5)

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