CONVERGENCE OF THE HAMILTONIAN PARTICLE-MESH METHOD FOR BAROTROPIC FLUID FLOW

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Abstract. We prove convergence of the Hamiltonian Particle-Mesh (HPM) method, initially proposed by J. Frank, G. Gottwald, and S. Reich, on a periodic domain when applied to the irrotational shallow water equations as a prototypical model for barotropic compressible fluid flow. Under appropriate assumptions, most notably sufficiently fast decay in Fourier space of the global smoothing operator, and a Strang–Fix condition of order 3 for the local partition of unity kernel, the HPM method converges as the number of particles tends to infinity and the global interaction scale tends to zero in such a way that the average number of particles per computational mesh cell remains constant and the number of particles within the global interaction scale tends to infinity.

The classical SPH method emerges as a particular limiting case of the HPM algorithm and we find that the respective rates of convergence are comparable under suitable assumptions. Since the computational complexity of bare SPH is algebraically superlinear and the complexity of HPM is logarithmically superlinear in the number of particles, we can interpret the HPM method as a fast SPH algorithm.

1. Introduction

Particle methods are numerical methods for continuum dynamics in which the approximation nodes move along a finite discrete set of Lagrangian trajectories. For compressible fluid flow, particle methods became popular in the context of astro- and plasmaphysical simulations as *Smoothed Particle Hydrodynamics* (SPH) in the late 1970s [11, 16, 20]. In SPH, a finite number particles, each representing a distribution of fluid mass given by a positive, compactly supported, smooth, radial kernel function centered about the particle position, interact via Newtonian forces determined from the overall mass density field. The resulting scheme is simple, possesses a Hamiltonian structure with associated physically desirable conservation laws, and can be very efficient in many interesting physical regimes. However, there are a number of drawbacks associated with basic SPH: It is a low-order scheme and also suffers from so-called tensile instabilities and spurious zero-energy modes, so that a large number of modifications have been proposed [15, 21]. Moreover, SPH convergence requires that the average particle distance decreases faster than the interaction radius, so that simulations with higher accuracy requirements need to work around the superlinear growth of the number of interactions which must be computed.

One recent variant of the SPH scheme is the Hamiltonian Particle-Mesh (HPM) method, proposed by Frank, Gottwald, and Reich [8]. The HPM method makes use

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of an auxiliary mesh on which long-range interactions can be computed efficiently. At the same time, it carefully preserves the Hamiltonian structure of the fluid system—a property which is generally lost with a particle-in-cell (PIC) approach. In particular, HPM has a proper analog of the Kelvin circulation theorem [10].

The HPM method is characterized by two separate kernels. First, it features a local partition of unity kernel which interpolates between particle values and grid values; typically, these interactions can be computed in $O(N)$ time, where N is the total number of particles. Second, it features a global smoothing kernel which provides for interactions on scales larger than the typical inter-particle distance. It is typically characterized as a discrete inverse of an elliptic operator; its action can be computed by fast methods in $O(N)$ or $O(N \ln N)$ time.

In this paper, we prove the convergence of the HPM method on a space-periodic domain and give an explicit estimate of the rate of convergence. The assumption of space-periodicity has already been used in the exploratory work of [8] as it allows for an easy implementation of global smoothing as the action of a discrete Fourier multiplier. Analytically, the space-periodic setting allows us to use Fourier analysis as our main tool. However, the HPM method extends to domains with boundaries [6], although a full proof of convergence would be much more difficult.

Our strategy of proof generalizes work by Oelschläger [23] on the convergence of the SPH method. The resulting error bounds are, under certain assumptions, comparable to those of SPH. Due to the algebraically superlinear complexity of SPH, we conclude that HPM can be interpreted as a "fast" SPH implementation. We remark that there is also a proof of convergence of SPH in the Vasershtein metric [3, 4]; this approach appears to give results which easily apply to more general polytropic fluids, but yields results which are weaker than ours or Oelschläger's and shall not play a role here.

We study the HPM method applied to the simplest possible barotropic fluid equation

$$\partial_t u + u \cdot \nabla u + \nabla \rho = 0 \,, \tag{1a}$$

$$\partial_t \rho + \nabla \cdot (\rho u) = 0 \,, \tag{1b}$$

where $u = u(x,t)$ denotes the velocity field and $\rho = \rho(x,t)$ the density, on the d-dimensional torus $\mathbb{T}^d$. When definiteness is required, we take the fundamental domain $x \in [-\pi, \pi)^d$. For $d = 2$, this system is also known as the irrotational shallow water equations, where ρ provides an approximation to the depth of a shallow layer of incompressible fluid with a free surface under gravity; often the letter h is used. In this paper, we disregard the physical connotations and write h to denote the numerical approximation to ρ.

To define the Hamiltonian Particle-Mesh method, we introduce a regular mesh with K mesh nodes in each dimension. The mesh nodes are then given by $\{x_\alpha \equiv \lambda\alpha \colon \alpha \in \mathbb{G}^d\}$ on $\mathbb{T}^d$, where $\mathbb{G} = \mathbb{Z} \cap [-\frac{K}{2}, \frac{K}{2})$ with $\lambda = 2\pi/K$. For simplicity, we assume that K is an odd integer. All results continue to hold when K is even provided we explicitly symmetrize the discrete Fourier sums which arise later.

The local partition of unity kernel is constructed from a compactly supported shape function Ψ which is assumed to satisfy a Strang–Fix condition of sufficiently high order p. The Strang–Fix condition expresses that polynomials of degree less than p can be written as countable linear combinations of integer translates of Ψ. Our result includes, in particular, the cubic B-spline used by [8] where $p = 4$. In the proof, the Strang–Fix conditions are used to show that some discrete version of integration by parts is permissible with remainders that do not blow up as the mesh size tends to zero. Once the shape function Ψ is specified, the scaled kernel

$$\psi_\lambda(x) = \lambda^{-d}\,\Psi(x/\lambda) \tag{2}$$

and its translates form a periodic partition of unity on the mesh. Details of the construction of periodic partitions of unity and a more general statement of the sufficient assumptions on Ψ shall be described in Section 2.

The global smoothing operator S_μ is defined via discrete convolution on the mesh as follows. For a mesh function $h = (h_\alpha)_{\alpha\in\mathbb{G}^d}$, the action of the smoothing operator $S_\mu h$ at grid point $\alpha \in \mathbb{G}^d$ is computed by multiplication in discrete Fourier space with a scaled Fourier symbol σ via

$$(S_\mu h)_\alpha = (2\pi)^d \sum_{\gamma\in\mathbb{G}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot x_\alpha}\,\sigma(\mu\gamma)\,\tilde{h}(\gamma)\,, \tag{3}$$

where

$$\tilde{h}(\gamma) = \frac{1}{K^d} \sum_{\beta\in\mathbb{G}^d} \mathrm{e}^{-\mathrm{i}\gamma\cdot x_\beta}\,h_\beta \tag{4}$$

denotes the discrete Fourier transform of h. A convenient choice for σ is

$$\sigma(\xi) = \frac{1}{(2\pi)^d}\,\frac{1}{(1+|\xi|^2)^q} \tag{5}$$

for sufficiently large $q > 0$. Thus, S_μ can be regarded as a discrete inverse of the q-th power of the Helmholtz operator $1-\mu\Delta$. A more general characterization of permissible kernels will be provided in Section 3.

The HPM dynamics can then be stated as follows. We represent the fluid by N particles with respective masses m_k, positions X_k, and velocities U_k, which evolve according to the system of ordinary differential equations

$$\dot{X}_k(t) = U_k(t)\,, \tag{6a}$$

$$\dot{U}_k(t) = \lambda^d \sum_{\alpha\in\mathbb{G}^d} (S_\mu h(t))(x_\alpha)\,\nabla\psi_\lambda(x_\alpha - X_k(t))\,, \tag{6b}$$

where $k = 1,\dots,N$, and S_μ acts via (3) on the grid values $h_\alpha(t)$ obtained by evaluating the approximate continuum density

$$h(x,t) = \sum_{k=1}^{N} m_k\,\psi_\lambda(x - X_k(t)) \tag{6c}$$

on the grid nodes. In other words, we set $h_\alpha(t) = h(x_\alpha, t)$. Equations (6a–c) form a closed N-particle simple mechanical system where the interaction potential is given by the expression on the right of equation (6b).

The particle masses m_k are constants of the motion which are chosen at the initial time. The total mass is defined as

$$M \equiv \sum_{k=1}^{N} m_k \approx \int_{\mathbb{T}^d} \rho(x,0)\,\mathrm{d}x\,. \tag{7}$$

The initialization procedure and the sense in which the total (numerical) mass approximates the total physical mass is made precise in Section 5.

The accuracy of the HPM approximation shall be measured in terms of the error functional

$$\begin{aligned} Q(t) &= \frac{1}{2} \sum_{k=1}^{N} m_k \left| U_k(t) - u(X_k(t), t) \right|^2 + \frac{\lambda^d}{2} \sum_{\alpha \in \mathbb{G}^d} \left| (S_\mu^r h(t))(x_\alpha) - \rho(x_\alpha, t) \right|^2 \\ &\equiv Q_{\text{kin}}(t) + Q_{\text{pot}}(t) , \end{aligned} \tag{8}$$

where S_μ^r denotes the convolution square root of S_μ, defined via $S_\mu^r S_\mu^r = S_\mu$. This error functional can be seen as a direct generalization of the HPM Hamiltonian

$$H_{\text{HPM}} = \frac{1}{2} \sum_{k=1}^{N} m_k \, |U_k|^2 + \frac{\lambda^d}{2} \sum_{\alpha \in \mathbb{G}^d} h(x_\alpha) \, (S_\mu h)(x_\alpha) , \tag{9}$$

where h is given by (6c) and, as before, S_μ acts via (3) on the grid values of h. We observe that the convolution square root S_μ^r in the expression for Q_{pot} arises as a symmetrization of the expression for the potential energy term in the HPM Hamiltonian. The structure of the Hamiltonian and of the error functional reflects the Eulerian–Lagrangian nature of the method. Our error functional is similar to the one used by Oelschläger [23] in his work on SPH, with the space integral over the density error used there replaced by its grid-approximation here.

A simplified version of our main result in the setting described so far can be stated as follows. For every $\varepsilon > 0$, fix

$$p \geq \max\left\{3, \frac{d+3}{\varepsilon} - d - 3\right\} \quad \text{and} \quad q > \max\left\{3 + \frac{d}{2}, \frac{d+3}{\varepsilon} - \frac{d}{2} - 3\right\} . \tag{10}$$

Then, in the limit $N \to \infty$ with

$$\lambda \sim N^{-1/d} \quad \text{and} \quad \mu \sim N^{-(1-\varepsilon)/d} , \tag{11}$$

we have an error bound of the form

$$Q(t) = O(N^{-2(1-\varepsilon)/d}) \tag{12}$$

over finite intervals of time so long as the exact solution of the barotropic fluid system (1) remains smooth. This statement of our result is a reformulation of Corollary 12 in Section 6.

To prove this result, we essentially take the time derivative of Q, carefully bound suitable groups of terms by Q or other quantities known to be small, and finally apply the Gronwall lemma. Many of our computations here can be seen as gridded analogues of Oelschläger's estimates; however, working on the grid introduces a whole host of essential new error terms. It is possible to obtain a direct comparison with the classical SPH method by letting $\lambda \to 0$, so that our error functional (8) converges to Oelschläger's error functional [23] and the global smoothing operator S_μ converges to a convolution operator on $\mathbb{T}^d$ with a periodic SPH blob function. Our theorem in this limit can be stated as follows.

For every $\varepsilon > 0$, fix

$$q \geq \frac{d+2}{\varepsilon} - 2 \tag{13}$$

subject to the additional restriction $q > \max\{3 + d/2, d\}$. Then, as $N \to \infty$ with

$$\mu \sim N^{-(1-\varepsilon)/d} , \tag{14}$$

we obtain an error bound for the periodic SPH method of the form

$$Q(t) = O(N^{-2(1-\varepsilon)/d}) \tag{15}$$

over finite intervals of time so long as the exact solution of the barotropic fluid system (1) remains smooth. This statement is a reformulation of Corollary 14 in Section 7; a more general statement is given in Theorem 13.

From our results, we conclude that HPM has one main advantage over the classical SPH method: The number of operations required to advance the HPM solution one step in time is of order $N \ln N$, where the logarithmic correction comes from the fast Fourier transform required to evaluate the global smoothing operator on the grid; all other operations have complexity $O(N)$. If multigrid techniques were used to compute the global smoothing, one could even obtain $O(N)$ overall complexity. On the other hand, the number of operations to advance an SPH solution with a compactly supported SPH kernel one time step is $O(N^{1+\varepsilon})$, because the number of particles within the support of the scaled SPH kernel grows like N^ε. This shows, as claimed above, that we can think of HPM as a "fast" SPH method which, in addition, preserves the Hamiltonian structure of SPH.

The HPM method does not appear to fare better than SPH when the number of particles is the same. Rather, we see additional contributions to the error arising due to the intermediate grid, which in particular lead to stricter requirements on q relative to the corresponding SPH proof. We also note that we do not make explicit use of the Hamiltonian structure, although the form of the error functional is clearly motivated by the HPM Hamiltonian. In fact, it is trivial to add any number of structure-breaking perturbations to the HPM method which, provided they decrease sufficiently fast as a function of the parameters, will not change the asserted order of the method. However, conservation is useful for maintaining qualitative and possibly probabilistic features of the solution over times long after trajectory accuracy has been lost; in the context of ODEs, this has been discussed, e.g., in [12, 14].

The results as presented here improve on those reported earlier [18, 19] in several respects. First, in [18] it was already observed that a Strang–Fix condition of order one on the partition of unity kernel Ψ is necessary for convergence. Here, we demonstrate that Strang–Fix conditions of higher order improve the order of convergence we can assert. Note that in the statement of our main result we require a Strang–Fix condition of minimal order $p = 3$. Although this is not strictly necessary, it simplifies the proofs as only then certain error terms contribute at their natural optimal order (this applies, in particular, to the proof of Lemma 3 below). As the cubic spline used by [8] already satisfies a Strang–Fix condition of order 4, $p \geq 3$ is not a serious restriction.

Second, our results here remain valid in the limit $\lambda \to 0$ with μ fixed. While this is not a practically relevant regime, it is theoretically interesting as in this limit HPM reduces to SPH so that a direct comparison of the various contributions to the error is possible.

Third, we note here that under the assumption that the global smoothing operator is even, the global smoothing error contributes only at order $O(\mu^2)$. This gives substantially better error bounds as in [18, 19, 23]. It also shows that the rate of convergence obtained here is close to optimal, because it is not possible to reduce this component of the error to something better than $O(\mu^2)$ unless the global smoothing kernel satisfies higher moment conditions. Numerically, this would very easy to realize for the HPM method (unlike SPH where a large support of the SPH blob causes a serious hit on the computational efficiency).

We do not claim that the assumptions we require are optimal. Most of them appear fairly benign, except that we have relatively strict requirements on the decay of the global smoothing kernel in Fourier space which exclude the case when σ corresponds to the Fourier symbol of the inverse of the bi-Helmholtz operator as used in the numerical work of [8]. Note that this does not imply that errors are large in practice: ongoing numerical work shows that the pre-asymptotic behavior of HPM with bi-Helmholtz smoothing in typical parameter regimes is remarkably good. However, as λ tends to zero, the tails in the spectrum of the kernel eventually become significant: Convergence of HPM to the SPH method clearly fails, and HPM with a fixed number of particles per cell also appears to fail to converge toward the exact solution. Moreover, the numerically observed rate of convergence indeed depends strongly on q, improving with larger values. The detailed results will be reported in a forthcoming paper [1].

We note that, for the SPH method, [3, 4] have first proved convergence to a regularized continuum formulation and then taken the zero regularization limit on the continuum equations. In our context, this would correspond to letting the mesh size tend to zero and the number of particles tend to infinity with μ fixed. However, it is an open question whether our methods can be adapted to this case and, in particular, which error functional should be used. Independent of this question, the study of the regularized continuum limit can give useful information on the pre-asymptotic behavior of the numerical scheme; this point of view has, for example, been taken in [7].

Another open question is the generalization to other constitutive laws. We believe that one should start with an error functional which once again comes from the Hamiltonian. However, the associated higher powers translate poorly into the Fourier representation, so that the Fourier-based approach employed here becomes increasingly unmanageable. We expect that it would be necessary to work largely in physical space, although the general structure of the argument might persist.

The remainder of this paper is structured as follows. We begin by developing a general description of the admissible partition of unity kernels (Section 2) and global smoothing operators (Section 3). In Section 4, we prove a number of crucial technical estimates. Section 5 discusses the issue of initialization of the HPM method and provides estimates on the rate of convergence of the error functional at time $t = 0$. Section 6 finally treats the full time-dependent problem; we state our main convergence result, Theorem 11, some special cases, and provide a proof essentially via a Gronwall lemma type argument. In the final Section 7, we look at the limit when $\lambda \to 0$ with μ fixed, which is the regime where HPM reduces to the classical SPH method. In the appendix, we collect definitions and basic facts about the Fourier transform and Sobolev spaces. In particular, we define the scaling of the discrete Fourier transform used here, and how it links to the periodic Fourier transform and to the Fourier transform on $\mathbb{R}^d$.

Throughout the paper, c denotes an arbitrary numerical constant. We make no attempt to label constants uniquely, so that the actual value of c may change from one line to the next. Constants which may additionally depend on the true solution (u, ρ) of the barotropic fluid model are written C; again, we make no attempt to label such constants uniquely.

2. Periodic partitions of unity

In this section, we scale a compactly supported partition of unity kernel to the mesh and explain how higher order Strang–Fix conditions characterize its order of polynomial reproduction.

2.1. **Construction.** Let $\Psi\colon \mathbb{R}^d \to [0,\infty)$ be even and compactly supported such that it generates a translation invariant partition of unity on the integers, i.e.,

$$\sum_{\alpha\in\mathbb{Z}^d} \Psi(x-\alpha) = 1 \tag{16}$$

for all $x \in \mathbb{R}^d$. Let $K \in \mathbb{N}$ large enough such that $\operatorname{supp}\Psi \subset (-K/2, K/2)^d$. Then Ψ induces a *periodic partition of unity* on $\mathbb{T}^d$ via

$$\psi_\lambda(x) = \frac{1}{\lambda^d}\,\Psi\Big(\frac{x}{\lambda}\Big) \tag{17}$$

where, as before, $\lambda = 2\pi/K$. For convenience, we extend this definition to all $x \in \mathbb{R}^d$ periodically. We then easily verify that for every $x \in \mathbb{T}^d$,

$$\lambda^d \sum_{\alpha\in\mathbb{G}^d} \psi_\lambda(x-x_\alpha) = \sum_{\alpha\in\mathbb{G}^d} \psi_1(x/\lambda-\alpha) = \sum_{\alpha\in\mathbb{Z}^d} \Psi(x/\lambda-\alpha) = 1\,. \tag{18}$$

2.2. **Basic properties.** We first remark that the partition of unity property implies that the mass on the grid is a constant of motion for the HPM method, since

$$\lambda^d \sum_{\alpha\in\mathbb{G}^d} h_\alpha = \sum_{k=1}^N m_k\,\lambda^d \sum_{\alpha\in\mathbb{G}^d} \psi_\lambda(x_\alpha - X_k) = \sum_{k=1}^N m_k = M\,. \tag{19}$$

Next, we characterize periodic partitions of unity in Fourier space by taking the Fourier transform of (18). Applying the orthogonality relation (144) to the right hand expression, and the shift formula (151) and the discrete orthogonality relation (153) to the left hand expression, we obtain

$$\delta_\beta = \lambda^d \sum_{\alpha\in G^d} \mathrm{e}^{-\mathrm{i}\beta\cdot x_\alpha}\,\hat\psi_\lambda(\beta) = (2\pi)^d\,\delta_\beta^{\mathrm{per}}\,\hat\psi_\lambda(\beta)\,. \tag{20}$$

Therefore,

$$\hat\psi_\lambda(0) = \frac{1}{(2\pi)^d} \qquad\text{and}\qquad \hat\psi_\lambda(K\gamma) = 0 \text{ for } \gamma\in\mathbb{Z}^d\setminus\{0\}\,. \tag{21}$$

Noting that, since $\operatorname{supp}\Psi \subset (-K/2, K/2)^d$,

$$\hat\psi_\lambda(\beta) = \frac{1}{(2\pi\lambda)^d}\int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\beta\cdot x}\,\Psi\Big(\frac{x}{\lambda}\Big)\,\mathrm{d}x = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\beta\cdot\lambda y}\,\Psi(y)\,\mathrm{d}y = \mathcal{F}\Psi(\lambda\beta)\,, \tag{22}$$

where $\mathcal{F}\Psi$ denotes the Fourier transform of Ψ on $\mathbb{R}^d$, we can translate (21) back to the unscaled kernel template Ψ, so that

$$\mathcal{F}\Psi(0) = \frac{1}{(2\pi)^d} \qquad\text{and}\qquad \mathcal{F}\Psi(2\pi\gamma) = 0 \text{ for } \gamma\in\mathbb{Z}^d\setminus\{0\}\,. \tag{23}$$

Since Ψ has compact support, $\mathcal{F}\Psi$ is a smooth function on $\mathbb{R}^d$. (Note that we could have arrived at (23) directly from (16) by taking an appropriate distribution-valued Fourier transform. However, since we have to rescale to the torus in any case, this route does not offer any advantage.)

With this characterization, it is straightforward to derive the following convolution error bound. The proof is similar to that of Lemma 2 and shall be omitted.

Lemma 1. *For every $s > 2 + d/2$ there exists a constant c such that for all $f \in H^s(\mathbb{T}^d)$,*

$$\sup_{x\in\mathbb{T}^d} |(\psi_\lambda * f)(x) - f(x)| \leq c\,\lambda^2\, \|f\|_{H^s} . \tag{24}$$

2.3. **Strang–Fix conditions.** We say that a compactly supported partition of unity satisfies a Strang–Fix condition of order p if, in addition to (23),

$$\mathrm{D}^\alpha \mathcal{F}\Psi(2\pi\gamma) = 0 \text{ for } \gamma \in \mathbb{Z}^d \setminus \{0\} \text{ and } |\alpha| < p . \tag{25}$$

It is long known that this condition implies that polynomials of degree less than p can be written as countable linear combinations of integer translates of Ψ [26]; Strang and Fix [28] proved that the best approximation of an $L_2(\mathbb{R}^d)$ function provided by the span of scaled translates of Ψ is of order k in the scaling parameter; see, e.g., [2] for an overview and more general results.

It is convenient to assume that the partition of unity kernel Ψ is a tensor product of a one-dimensional partition of unity kernel Θ, i.e.

$$\Psi(x) = \prod_{i=1}^d \Theta(x_i) , \tag{26}$$

so that

$$\mathcal{F}\Psi(\xi) = \prod_{i=1}^d \mathcal{F}\Theta(\xi_i) . \tag{27}$$

We note that a radial kernel cannot satisfy the periodic partition of unity condition [29], so we are not excluding an obvious case here.

2.4. **Smoothness conditions.** To prove our main result, we must assume that the partition of unity is sufficiently smooth, namely that there exists some constant c such that

$$|\mathcal{F}\Theta(\xi)| \leq \frac{c}{1+|\xi|^\nu} , \tag{28}$$

where the exponent $\nu > 0$ is to be specified later. Then an estimate of the form (28) also holds for derivatives of $\mathcal{F}\Theta$, i.e., for every $k \in \mathbb{N}$ there is a constant c_k such that

$$|\mathrm{D}^k \mathcal{F}\Theta(\xi)| \leq \frac{c_k}{1+|\xi|^\nu} . \tag{29}$$

A proof of (29) is achieved by induction in k: noting that $\mathcal{F}f(\xi) = (\mathrm{i}\xi)^{-1}\mathcal{F}f'(\xi)$, we obtain

$$|\mathcal{F}\Theta^{(i)}(\xi)| \leq c\,\frac{|\xi|^i}{1+|\xi|^\nu} \leq 2\,c\,\frac{1}{1+|\xi|^{\nu-i}} \tag{30}$$

provided $i \leq \nu$. Moreover,

$$\begin{aligned} |\mathrm{D}^k \mathcal{F}\Theta(\xi)| &= |\mathcal{F}((-\mathrm{i}x)^k\Theta)(\xi)| = |\xi|^{-1}\,|\mathcal{F}(kx^{k-1}\Theta + x^k\Theta')(\xi)| \\ &\leq k\,|\xi|^{-1}\,|\mathcal{F}(x^{k-1}\Theta)(\xi)| + |\xi|^{-1}\,|\mathcal{F}(x^k\Theta')(\xi)| . \end{aligned} \tag{31}$$

Applying this procedure $I = \lceil \nu \rceil$ times to the final term, we obtain

$$|\mathrm{D}^k \mathcal{F}\Theta(\xi)| \leq k \sum_{i=1}^{I-1} \frac{|\mathcal{F}(x^{k-1}\Theta^{(i)})(\xi)|}{|\xi|^i} + \frac{|\mathcal{F}(x^k \Theta^{(I)})(\xi)|}{|\xi|^I} \,. \tag{32}$$

For the terms in the left hand sum, an estimate of the form (29) follows from the induction assumption and (30). The corresponding bound on the final term is a consequence of the Riemann–Lebesgue lemma.

2.5. **B-splines.** The Strang–Fix and smoothness conditions are satisfied by cardinal B-splines in the following way. Start with the zero order spline

$$\theta_0 = 1_{[-1/2,1/2)^d} \,, \tag{33}$$

the characteristic function of the box, and, for $i \in \mathbb{N}$, recursively define

$$\theta_i = \theta_0 * \theta_{i-1} \,. \tag{34}$$

Since θ_0 satisfies the smoothness condition (28) with $\nu = 1$ (as is easily verified by direct computation), due to the convolution theorem for the Fourier transform, θ_i satisfies (28) with $\nu = i + 1$.

Similarly, θ_0 satisfies (21), but none of the higher order Strang–Fix conditions. Thus, again due to the convolution theorem, θ_i satisfies the Strang–Fix condition of order $i + 1$.

3. The global smoothing operator S_μ

The smoothing operator S_μ appearing in the formulation of the HPM method has a role akin the SPH blob function in that it provides for a medium range interaction between the particles. In HPM, however, it acts exclusively on grid values which allows for efficient computation via spectral methods. It is most conveniently defined as a discrete spectral approximation to a convolution operator on $L_2(\mathbb{R}^d)$. This is detailed in the following.

3.1. **Definitions.** Let $\sigma(\xi)$ denote the real and nonnegative Fourier symbol of a convolution operator on $L_2(\mathbb{R}^d)$ and let $\sigma^r(\xi) = \sqrt{\sigma(\xi)/(2\pi)^d}$ denote the Fourier symbol of its convolution square root. On our mesh, it induces a family of scaled discrete convolution operators via

$$\tilde{S}^\mu(\gamma) = \sigma(\mu\gamma) \qquad \text{and} \qquad \tilde{S}^{\mu,r}(\gamma) = \sigma^r(\mu\gamma) \tag{35}$$

for $\gamma \in \mathbb{G}^d$ with K-periodic extension to the whole of $\mathbb{Z}^d$ and arbitrary scaling parameter $\mu > 0$. Then, for any grid function f,

$$(S_\mu f)_\alpha \equiv (S^\mu \circledast f)_\alpha = \lambda^d \sum_{\beta \in \mathbb{G}^d} S^\mu_{\alpha-\beta} f_\beta = (2\pi)^d \sum_{\gamma \in \mathbb{G}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot x_\alpha} \sigma(\mu\gamma)\, \tilde{f}(\gamma) \,, \tag{36}$$

where we write S_μ to denote the operator, and S^μ to denote the corresponding discrete convolution kernel. With a corresponding definition for S^r_μ, it is easy to check that

$$S_\mu = S^r_\mu \, S^r_\mu \,. \tag{37}$$

Note that we may extend $(S_\mu f)_\alpha$ to a function on $\mathbb{T}^d$ via

$$(S_\mu f)(x) = (2\pi)^d \sum_{\gamma \in \mathbb{G}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot x} \sigma(\mu\gamma)\, \tilde{f}(\gamma) \,. \tag{38}$$

The operator S_μ is self-adjoint on the grid, and almost self-adjoint as an operator into $L_2(\mathbb{T}^d)$ in the sense that, setting

$$(S_\mu^* g)_\alpha = (2\pi)^d \sum_{\gamma \in \mathbb{G}^d} \mathrm{e}^{\mathrm{i}\gamma \cdot x_\alpha} \, \sigma(\mu\gamma) \, \hat{g}(\gamma) \tag{39}$$

for any $g \in L_2(\mathbb{T}^d)$, we have

$$\int_{\mathbb{T}^d} (S_\mu f)(x) \, \overline{g(x)} \, \mathrm{d}x = \lambda^d \sum_{\alpha \in \mathbb{G}^d} f_\alpha \, \overline{(S_\mu^* g)_\alpha} \, . \tag{40}$$

Since S_μ is a band-limited operator, the convolution square root decomposition (37) can be written

$$S_\mu = S_\mu^{r*} \, S_\mu^r \, , \tag{41}$$

where the right hand operator is interpreted as mapping into $L_2(\mathbb{T}^d)$.

3.2. **Assumptions.** We assume that σ is even, normalized such that

$$\sigma(0) = \frac{1}{(2\pi)^d} \, , \tag{42a}$$

and decays sufficiently fast, i.e., that there exists a constant c such that

$$\sigma(\xi) \leq \frac{c}{1 + |\xi|^\zeta} \, , \tag{42b}$$

where the exponent ζ is to be specified later. Further, we require that $\sigma \in C^{\ell+1}(\mathbb{R}^d)$ where, in the proof of the main Theorem 11, we will take $\ell = 2 + \lceil d/2 \rceil$. Finally, we need to assume that convolution kernel decays sufficiently fast in physical space. For our purposes, this decay condition is most conveniently formulated in terms of the Fourier symbol σ^r; we require that there exists a constant c such that, for multi-indices k with $1 \leq |k| \leq \ell$,

$$|\mathrm{D}_\xi^k [\xi \sigma^r(\xi)]| \leq c \, \sigma^r(\xi) \, , \tag{43a}$$

and for $|k| = \ell + 1$,

$$\sup_{\tau \in [0,1]} \sum_{\gamma \in \mathbb{Z}^d} \left| \mathrm{D}_\xi^k [\xi \sigma^r(\xi)] \Big|_{\xi = \gamma + \tau} \right|^2 \leq c \, . \tag{43b}$$

Condition (43b) expresses, in other words, that arbitrary translates of $\mathrm{D}_\xi^k[\xi\sigma^r(\xi)]$ are uniformly bounded in $\ell_2(\mathbb{Z}^d)$. We remark that (43a) implies that derivatives of σ up to order ℓ possess a decay estimate of the form (42b) as well. In particular, as we will require in several places in this paper, second derivatives of σ and of σ^r are uniformly bounded.

3.3. **Inverse powers of the Helmholtz operator.** All numerical studies of the HPM method so far used inverse powers of the Helmholtz operator as a simple and natural choice for the global smoothing operator. When the underlying convolution operator on $L_2(\mathbb{R}^d)$ is given by $(1 - \Delta)^{-q}$, then, in the notation of Section 3.1,

$$\sigma(\xi) = \frac{1}{(2\pi)^d} \frac{1}{(1 + |\xi|^2)^q} \qquad \text{and} \qquad \sigma^r(\xi) = \frac{1}{(2\pi)^d} \frac{1}{(1 + |\xi|^2)^{q/2}} \, . \tag{44}$$

Clearly, σ is smooth, even, properly normalized, and satisfies the decay condition (42b) provided $2q \geq \zeta$. To prove (43a), we notice that, when $k = e_i$,

$$\mathrm{D}^k \frac{\xi_j}{(1+|\xi|^2)^{q/2}} = \delta_{i-j} \frac{1}{(1+|\xi|^2)^{q/2}} + q \frac{\xi_i \, \xi_j}{(1+|\xi|^2)^{q/2+1}} \tag{45}$$

so (43a) is true for $|k| = 1$. Taking further derivatives leads to decay with a larger exponent, so that (43a) holds true for $|k| \geq 2$ as well. Finally, to prove (43b), it suffices to test for convergence of the sum, which holds whenever $d < 2q + \ell$.

3.4. **Modified smoothing operator.** For internal use in the proof of our main theorem, it is useful to define a modified smoothing operator which acts on functions $f \in L_2(\mathbb{T}^d)$,

$$\mathcal{S}_\mu f(x) = (2\pi)^d \sum_{\gamma \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot x} \, \sigma(\mu\gamma) \, \hat{f}(\gamma) \,, \tag{46}$$

with an analogous definition for $\mathcal{S}_\mu^r$. Then the following holds.

Lemma 2. *For every $s > 2 + d/2$ there exists a constant c such that for all $f \in H^s(\mathbb{T}^d)$,*

$$\sup_{x \in \mathbb{T}^d} |\mathcal{S}_\mu f(x) - f(x)| \leq c \, \mu^2 \, \|f\|_{H^s} \,. \tag{47}$$

Proof. Recall that σ is even with $\sigma(0) = (2\pi)^{-d}$ and uniformly bounded second derivative. Hence, we can estimate

$$\begin{aligned} |\mathcal{S}_\mu f(x) - f(x)| &\leq \sum_{\gamma \in \mathbb{Z}^d} |(2\pi)^d \, \sigma(\mu\gamma) - 1| \, |\hat{f}(\gamma)| \\ &\leq c \, \mu^2 \sum_{\gamma \in \mathbb{Z}^d} |\gamma|^2 \, |\hat{f}(\gamma)| \leq c \, \mu^2 \left(\sum_{\gamma \in \mathbb{Z}^d} |\gamma|^{-2s+4} \right)^{\frac{1}{2}} \|f\|_{H^s} \end{aligned} \tag{48}$$

The remaining sum on the right converges provided $s > 2 + d/2$, proving (47). □

Due to the Poisson summation formula, the difference of $S_\mu - \mathcal{S}_\mu$ depends only on the high wavenumber Fourier coefficients of f, so an estimate similar to the proof of Lemma 2 shows that, for sufficiently smooth f, $(S_\mu - \mathcal{S}_\mu) f$ is small when λ is small. However, when acting on the partition of unity kernel ψ_λ whose derivatives are not bounded uniformly in λ, it is much harder to find strong estimates on $S_\mu - \mathcal{S}_\mu$. Such bounds will be provided as Lemma 4 and Lemma 5 further below.

4. Auxiliary estimates

We begin by proving four auxiliary estimates. The first pair can be seen as discrete versions of integration by parts, the second pair concerns the difference between full and truncated Fourier series in certain integral expressions.

Lemma 3. *Suppose that the one-dimensional partition of unity kernel Θ satisfies a Strang–Fix condition of order 3 and that its Fourier coefficients have decay exponent $\nu > 2$. Then for every $s > 3 + d/2$ there exists a constant c such that for all $\rho \in H^s(\mathbb{T}^d)$,*

$$\sup_{x \in \mathbb{T}^d} \left| \nabla\rho(x) - \lambda^{2d} \sum_{\alpha,\beta \in \mathbb{G}^d} \rho(x_\alpha) \, S^{\mu,r}_{\alpha-\beta} \, \nabla\psi_\lambda(x - x_\beta) \right| \leq c \, (\lambda^2 + \mu^2) \, \|\rho\|_{H^s} \,. \tag{49}$$

Proof. We denote the second term on the left of (49) by $g(x)$ and compute

$$\begin{aligned}
\hat{g}(\gamma) &= \lambda^{2d} \sum_{\alpha,\beta\in\mathbb{G}^d} \rho(x_\alpha)\, S^{\mu,r}_{\alpha-\beta}\, \mathrm{i}\gamma\, \mathrm{e}^{-\mathrm{i}\gamma\cdot x_\beta}\, \hat{\psi}_\lambda(\gamma) \\
&= (2\pi)^{2d}\, \mathrm{i}\gamma\, \hat{\psi}_\lambda(\gamma)\, \frac{1}{K^d} \sum_{\alpha\in\mathbb{G}^d} \rho(x_\alpha)\, \mathrm{e}^{-\mathrm{i}\gamma\cdot x_\alpha}\, \sigma^r(\mu\gamma) \\
&= (2\pi)^{2d}\, \mathrm{i}\gamma\, \hat{\psi}_\lambda(\gamma)\, \sigma^r(\mu\gamma)\, \tilde{\rho}(\gamma)\,, \qquad (50)
\end{aligned}$$

where we have used the differentiation rule (150) and shift formula (151) for the Fourier transform in the first equality, the definition (152) and shift formula (158) for the discrete Fourier transform as well as the symmetry of σ^r in the second and third equalities.

We now write $\gamma = \alpha + \kappa K$ with $\alpha \in \mathbb{G}^d$ and $\kappa \in \mathbb{Z}^d$. Then

$$\begin{aligned}
|\nabla\rho(x) - g(x)| &\le \sum_{\gamma\in\mathbb{Z}^d} |\mathrm{i}\gamma\, \hat{\rho}(\gamma) - \hat{g}(\gamma)| \\
&\le \sum_{\alpha\in\mathbb{G}^d} |\mathrm{i}\alpha\, \hat{\rho}(\alpha) - \hat{g}(\alpha)| + \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|\, |\hat{\rho}(\gamma)| + \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\hat{g}(\gamma)| \\
&\equiv G_1 + G_2 + G_3\,. \qquad (51)
\end{aligned}$$

To find an estimate for G_1, we write

$$\begin{aligned}
|\mathrm{i}\alpha\, \hat{\rho}(\alpha) - \hat{g}(\alpha)| &= |\alpha|\, |\hat{\rho}(\alpha) - (2\pi)^{2d}\, \mathcal{F}\Psi(\lambda\alpha)\, \sigma^r(\mu\alpha)\, \tilde{\rho}(\alpha)| \\
&= |\alpha|\, |\hat{\rho}(\alpha) - \tilde{\rho}(\alpha)| + |\alpha|\, |1 - (2\pi)^{2d}\, \mathcal{F}\Psi(\lambda\alpha)\, \sigma^r(\mu\alpha)|\, |\tilde{\rho}(\alpha)|\,. \qquad (52)
\end{aligned}$$

We know that $\mathcal{F}\Psi(0) = \sigma^r(0) = (2\pi)^{-d}$, that $\mathcal{F}\Psi$ and σ^r are even so that their first order derivatives vanish at the origin, and that their second order derivatives are uniformly bounded, so that

$$\begin{aligned}
G_1 &\le \sum_{\alpha\in\mathbb{G}^d} |\alpha|\, |\hat{\rho}(\alpha) - \tilde{\rho}(\alpha)| + c\,(\lambda^2 + \mu^2) \sum_{\alpha\in\mathbb{G}^d} |\alpha|^3\, |\tilde{\rho}(\alpha)| \\
&\le G_2 + c\,(\lambda^2 + \mu^2) \sum_{\gamma\in\mathbb{Z}^d} |\gamma|^3\, |\hat{\rho}(\gamma)| \\
&\le G_2 + c\,(\lambda^2 + \mu^2) \Biggl(\sum_{\gamma\in\mathbb{Z}^d\setminus\{0\}} |\gamma|^{-2s+6} \Biggr)^{\frac{1}{2}} \|\rho\|_{H^s}\,, \qquad (53)
\end{aligned}$$

where, in the second inequality, we have used the Poisson summation formula (159) on both of the terms. The sum in the final expression is convergent provided $s > 3 + d/2$.

A matching upper bound for G_2 is easily found, namely

$$\begin{aligned}
G_2 &= \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^{-2-d/2}\, |\gamma|^{3+d/2}\, |\hat{\rho}(\gamma)| \\
&\le \Biggl(\sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^{-4-d} \Biggr)^{\frac{1}{2}} \|\rho\|_{H^{3+d/2}} \\
&\le c\,\lambda^2\, \|\rho\|_{H^{3+d/2}}\,. \qquad (54)
\end{aligned}$$

Finally,

$$G_3 = (2\pi)^{2d} \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} \sum_{\alpha\in\mathbb{G}^d} |\alpha+\kappa K|\, |\mathcal{F}\Psi(2\pi\kappa+\lambda\alpha)|\, \sigma^r(\mu\alpha)\, |\tilde\rho(\alpha)|\,. \tag{55}$$

Due to the Strang–Fix condition of order 3 and the smoothness condition (29),

$$\begin{aligned}
|\alpha+\kappa K|\, |\mathcal{F}\Psi(2\pi\kappa+\lambda\alpha)| &\le c\, |\lambda\alpha|^3\, |\alpha+\kappa K| \sup_{\xi\in[-\pi,\pi]^d} |\mathrm{D}^3\mathcal{F}\Psi(2\pi\kappa+\xi)| \\
&\le c\,\lambda^2\, |\alpha|^3\, |2\pi\kappa+\lambda\alpha| \sup_{\xi\in[-\pi,\pi]^d} \prod_{i=1}^d |\mathrm{D}^3\mathcal{F}\Theta(2\pi\kappa_i+\xi_i)| \\
&\le c\,\lambda^2\, |\alpha|^3 \sup_{1\le j\le d} |\kappa_j| \prod_{i=1}^d \frac{1}{1+|\kappa_i|^\nu} \\
&\le c\,\lambda^2\, |\alpha|^3 \prod_{i=1}^d \frac{1}{1+|\kappa_i|^{\nu-1}}\,.
\end{aligned} \tag{56}$$

Noting the uniform boundedness of $\sigma^r(\mu\alpha)$, we obtain

$$G_3 \le c\,\lambda^2 \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} \prod_{i=1}^d \frac{1}{1+|\kappa_i|^{\nu-1}} \sum_{\alpha\in\mathbb{G}^d} |\alpha|^3\, |\tilde\rho(\alpha)|\,. \tag{57}$$

We note that the first sum on the right converges whenever $\nu > 2$, the second sum can be estimated as in (53). □

Lemma 4. *Suppose that the one-dimensional partition of unity kernel Θ satisfies a Strang–Fix condition of order p and that its Fourier coefficients have decay exponent $\nu > 2$. Further, suppose that the smoothing kernel σ has decay exponent $\zeta > d+p$. Then there exists a constant c such that, for $\lambda \le \mu$,*

$$\sup_{x\in\mathbb{T}^d} \left| \lambda^d \sum_{\alpha\in\mathbb{G}^d} (S_\mu h)_\alpha\, \nabla\psi_\lambda(x_\alpha - x) - \int_{\mathbb{T}^d} \mathcal{S}_\mu h(y)\, \nabla\psi_\lambda(y-x)\,\mathrm{d}y \right| \le c\, M\, \frac{\lambda^{p-1}}{\mu^{p+d}}\,. \tag{58}$$

Proof. Let J denote the argument of the supremum in (58). Applying the discrete and the continuous Parseval identity, respectively, we find

$$\begin{aligned}
J &= (2\pi)^d \sum_{\gamma\in\mathbb{Z}^d} \sigma(\mu\gamma)\, \big[1_{\mathbb{G}^d}(\gamma)\, \tilde h(\gamma)\, \overline{(\nabla\psi_\lambda(\cdot-x))\tilde{}\,(\gamma)} - \hat h(\gamma)\, \overline{(\nabla\psi_\lambda(\cdot-x))\hat{}\,(\gamma)} \big] \\
&= (2\pi)^d \sum_{\gamma\in\mathbb{G}^d} \sigma(\mu\gamma)\, (\tilde h - \hat h)(\gamma)\, \overline{(\nabla\psi_\lambda(\cdot-x))\tilde{}\,(\gamma)} \\
&\quad + (2\pi)^d \sum_{\gamma\in\mathbb{G}^d} \sigma(\mu\gamma)\, \hat h(\gamma)\, \overline{[(\nabla\psi_\lambda(\cdot-x))\tilde{}\,(\gamma) - (\nabla\psi_\lambda(\cdot-x))\hat{}\,(\gamma)]} \\
&\quad - (2\pi)^d \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} \sigma(\mu\gamma)\, \hat h(\gamma)\, \overline{(\nabla\psi_\lambda(\cdot-x))\hat{}\,(\gamma)} \\
&\equiv J_1 + J_2 + J_3\,.
\end{aligned} \tag{59}$$

By the Poisson summation formula (159) and shift formula (151), we compute

$$(\tilde h - \hat h)(\gamma) = \sum_{k=1}^N m_k \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} \mathrm{e}^{-\mathrm{i}(\gamma+\kappa K)\cdot X_k}\, \hat\psi_\lambda(\gamma+\kappa K)\,. \tag{60}$$

Bounding $\hat{\psi}_\lambda(\gamma+\kappa K)$ as in (56), we obtain

$$|(\tilde{h}-\hat{h})(\gamma)| \leq c\, M \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} |\lambda\gamma|^p \prod_{i=1}^d \frac{1}{1+|\kappa_i|^\nu} \leq c\, M\, \lambda^p\, |\gamma|^p \tag{61}$$

where the sum converges whenever $\nu>1$. Moreover, noting (22) and applying the decay condition (28), we find

$$\begin{aligned} |(\nabla\psi_\lambda(\cdot - x))\tilde{}(\gamma)| &= \left| \sum_{\kappa\in\mathbb{Z}^d} \mathrm{i}(\gamma+\kappa K)\, \mathrm{e}^{-\mathrm{i}(\gamma+\kappa K)\cdot x}\, \hat{\psi}_\lambda(\gamma+\kappa K) \right| \\ &\leq c \sum_{\kappa\in\mathbb{Z}^d} |\gamma+\kappa K| \prod_{i=1}^d \frac{1}{1+|\kappa_i|^\nu} \leq \frac{c}{\lambda}\,, \end{aligned} \tag{62}$$

where, as in (56), the sum converges so long as $\nu>2$. Altogether,

$$|J_1| \leq c\, M\, \lambda^{p-1} \sum_{\gamma\in\mathbb{G}^d} \sigma(\mu\gamma)\, |\gamma|^p\,. \tag{63}$$

An integral estimate on the right hand sum yields a bound of the form (58). Similarly,

$$|J_2| \leq c\, M \sum_{\gamma\in\mathbb{G}^d} \sigma(\mu\gamma) \prod_{i=1}^d \frac{1}{1+|\lambda\gamma_i|^\nu} \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} |\lambda\gamma|^p\, |\gamma+\kappa K| \prod_{i=1}^d \frac{1}{1+|\kappa_i|^\nu}\,. \tag{64}$$

As before, this yields a bound of the form (58). Finally,

$$|J_3| \leq c\, M \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} \sigma(\mu\gamma)\, |\gamma| \leq c\, M\, \frac{\lambda^{\zeta-d-1}}{\mu^\zeta}\,. \tag{65}$$

When $\lambda\leq\mu$ and $\zeta>d+p$, this term contributes to lower order than J_1 and J_2. □

Remark 1. In estimate (58) and also in Lemma 5 below, we obtain a negative power of μ on the right. On the other hand, in the next Section 5 we will see that a very similar expression yields an estimate of $O(\mu^2)$. The difference is due to the following. We can reorder the sums in (60), writing

$$(\tilde{h}-\hat{h})(\gamma) = \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} \left(\sum_{k=1}^N m_k\, \mathrm{e}^{-\mathrm{i}(\gamma+\kappa K)\cdot X_k} \right) \hat{\psi}_\lambda(\gamma+\kappa K)\,. \tag{66}$$

Here, we have no reason to assume any structure on the distribution of the X_k, so the best we can assert is that the inner sum is bounded by M. On the other hand, when the X_k are on a regular grid, for example, as in the proof of Lemma 7 below, then the inner sum can be interpreted as a discrete Fourier transform with correspondingly much tighter bounds. It is an open question whether, as the HPM particles evolve, the particle locations retain sufficient uniformity for as long as the potential energy error remains small to assert a bound which is substantially better than the brute-force estimate used in the proof of Lemma 4.

Lemma 5. *Suppose that the one-dimensional partition of unity kernel Θ satisfies a Strang–Fix condition of order p and that its Fourier coefficients have decay exponent*

$\nu > 1$. *Further, suppose that the smoothing kernel* σ *has decay exponent* $\zeta > 2p+d$. *Then there exists a constant* c *such that, for* $\lambda \le \mu$,

$$\|\mathcal{S}_\mu^r h - S_\mu^r h\|_{L_2(\mathbb{T}^d)} \le c\, M\, \frac{\lambda^p}{\mu^{p+d/2}} \,. \tag{67}$$

Proof. As in the proof of Lemma 4, we apply the Parseval identity, so that, using (61), we obtain

$$\begin{aligned}\int_{\mathbb{T}^d} |(\mathcal{S}_\mu^r - S_\mu^r)h|^2 \,\mathrm{d}x &= \sum_{\gamma\in\mathbb{G}^d} \sigma(\mu\gamma)\, |\tilde{h}(\gamma) - \hat{h}(\gamma)|^2 + \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} \sigma(\mu\gamma)\, |\hat{h}(\gamma)|^2 \\ &\le c \sum_{\gamma\in\mathbb{Z}^d} \sigma(\mu\gamma)\, M^2\, \lambda^{2p}\, |\gamma|^{2p} + c\, M^2 \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} \sigma(\mu\gamma) \\ &\le c\, M^2\, \frac{\lambda^{2p}}{\mu^{2p+d}} + c\, M^2\, \frac{\lambda^{\zeta-d}}{\mu^\zeta} \end{aligned} \tag{68}$$

where convergence of the first sum on the second line is contingent upon $\zeta > 2p+d$. The contribution from the second sum is of lower order relative to the first under this same condition provided $\lambda \le \mu$. This completes the proof. □

Lemma 6. *Suppose that the one-dimensional partition of unity kernel* Θ *satisfies a Strang–Fix condition of order* p *and that its Fourier coefficients have decay exponent* $\nu > 1$. *Then for every* $s > p + d/2$ *there exists a constant* c *such that for all* $g \in H^s(\mathbb{T}^d)$,

$$\left| \lambda^d \sum_{\alpha\in\mathbb{G}^d} h_\alpha\, g_\alpha - \int_{\mathbb{T}^d} h(x)\, g(x) \,\mathrm{d}x \right| \le c\, M\, \lambda^p\, \|g\|_{H^s} \,. \tag{69}$$

Proof. By the continuous and discrete Parseval identities,

$$\begin{aligned} &\lambda^d \sum_{\alpha\in\mathbb{G}^d} h_\alpha\, g_\alpha - \int_{\mathbb{T}^d} h(x)\, g(x) \,\mathrm{d}x \\ &\quad = (2\pi)^d \sum_{\gamma\in\mathbb{G}^d} (\tilde{h}(\gamma) - \hat{h}(\gamma))\, \tilde{g}(\gamma) + (2\pi)^d \sum_{\gamma\in\mathbb{G}^d} \hat{h}(\gamma)\, (\tilde{g}(\gamma) - \hat{g}(\gamma)) \\ &\qquad + (2\pi)^d \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} \hat{h}(\gamma)\, \hat{g}(\gamma) \\ &\quad \equiv J_1 + J_2 + J_3 \,. \end{aligned} \tag{70}$$

Using (61) to bound $\tilde{h} - \hat{h}$ and the Poisson summation formula for $\tilde{g}$, we estimate

$$\begin{aligned} |J_1| &\le c\, M\, \lambda^p \sum_{\gamma\in\mathbb{G}^d} |\gamma|^p \left(\sum_{\kappa\in\mathbb{Z}^d} |\hat{g}(\gamma + \kappa K)| \right) \\ &\le c\, M\, \lambda^p \sum_{\gamma\in\mathbb{Z}^d} |\gamma|^p\, |\hat{g}(\gamma)| \le c\, M\, \lambda^p \left(\sum_{\gamma\in\mathbb{Z}^d\setminus\{0\}} |\gamma|^{2(p-s)} \right)^{\frac{1}{2}} \|g\|_{H^s} \,, \end{aligned} \tag{71}$$

where the sums in the above expression converge due to $s > p + d/2$. Similarly, using the uniform boundedness of the Fourier coefficients of ψ and the Poisson summation formula, we estimate

$$|J_2| \le c\,M \sum_{\gamma\in\mathbb{G}^d} \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} |\hat{g}(\gamma+\kappa K)| \le c\,M \Biggl(\sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^{-2p-d} \Biggr)^{\frac{1}{2}} \|g\|_{H^{p+d/2}} \,. \tag{72}$$

An integral estimate on the remaining sum on the right yields once again a bound of the form (69). Finally, J_3 can be bounded as in (72). □

5. Initialization

The HPM method can be initialized in many different ways. In this paper, we only consider initial particle placements on a uniform grid with mesh spacing Λ, so that the initial particle positions X_k can be identified, by enumeration, with the initialization mesh points $\{X_\beta \equiv \Lambda\beta \colon \beta \in \mathbb{H}^d\}$ where $\mathbb{H} = \mathbb{Z} \cap [-\frac{L}{2}, \frac{L}{2})$ with $\Lambda = 2\pi/L$. For simplicity, we assume that L is an integer multiple of K or vice versa, as this simplifies the argument. Similar results can be proved for more general ratios of K and L.

Then, with the same identification between enumeration index k and multi-index β, we set, at time $t=0$,

$$m_\beta = \Lambda^d\,\rho(X_\beta) \qquad \text{and} \qquad U_\beta = u(X_\beta)\,. \tag{73}$$

Lemma 7. *Suppose that the one-dimensional partition of unity kernel Θ satisfies a Strang–Fix condition of order 2, and that its Fourier coefficients have decay exponent $\nu > 1$. Fix $n \in \mathbb{N}$. For every $K \in \mathbb{N}$, let $L = nK$. Then for every $s > 2 + d/2$ there exists a constant c such that for all $\rho \in H^s(\mathbb{T}^d)$, for all $\mu \le 1$ and for all K sufficiently large, with h initialized as above,*

$$\sup_{x\in\mathbb{T}^d} |(S_\mu^r h)(x) - \rho(x)| \le c\,(\lambda^2 + \mu^2)\,\|\rho\|_{H^s}\,. \tag{74}$$

Proof. Set $g(x) = (S_\mu^r h)(x) - \rho(x)$. Then, for every $\gamma \in \mathbb{Z}^d$,

$$\hat{g}(\gamma) = (2\pi)^d\,\sigma^r(\mu\gamma)\,\tilde{h}(\gamma)\,1_{\mathbb{G}^d}(\gamma) - \hat{\rho}(\gamma)\,. \tag{75}$$

By the Poisson summation formula (159) and shift formula (151), we compute

$$\begin{aligned}
\tilde{h}(\gamma) &= \sum_{k=1}^N m_k \sum_{\kappa\in\mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}(\gamma+\kappa K)\cdot X_k}\,\hat{\psi}_\lambda(\gamma+\kappa K) \\
&= (2\pi)^d \sum_{\kappa\in\mathbb{Z}^d} \frac{1}{L^d} \sum_{\beta\in\mathbb{H}^d} \mathrm{e}^{-\mathrm{i}(\gamma+\kappa K)\cdot X_\beta}\,\rho(X_\beta)\,\mathcal{F}\Psi(2\pi\kappa+\lambda\gamma) \\
&= (2\pi)^d \sum_{\kappa\in\mathbb{Z}^d} \sum_{\iota\in\mathbb{Z}^d} \hat{\rho}(\gamma+\kappa K+\iota L)\,\mathcal{F}\Psi(2\pi\kappa+\lambda\gamma)
\end{aligned} \tag{76}$$

where, in the last step, we have identified the β-sum as a discrete Fourier transform on the Λ-grid and expressed it via the corresponding Poisson summation identity.

Now suppose that $L = nK$ for some $n \in \mathbb{N}$ and write

$$\begin{aligned}
\tilde{h}(\gamma) = (2\pi)^d\,\hat{\rho}(\gamma)\,\mathcal{F}\Psi(\lambda\gamma) &+ (2\pi)^d \sum_{\iota\in\mathbb{Z}^d\setminus\{0\}} \hat{\rho}(\gamma+\iota nK)\,\mathcal{F}\Psi(\lambda\gamma) \\
&+ (2\pi)^d \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} \sum_{\iota\in\mathbb{Z}^d} \hat{\rho}(\gamma+(\kappa+\iota n)K)\,\mathcal{F}\Psi(2\pi\kappa+\lambda\gamma)\,.
\end{aligned} \tag{77}$$

Then

$$
\begin{aligned}
\sup_{x\in\mathbb{T}^d} |g(x)| &\leq \sum_{\gamma\in\mathbb{Z}^d} |\hat{g}(\gamma)| \\
&\leq \sum_{\gamma\in\mathbb{G}^d} |1-(2\pi)^{2d}\sigma^r(\mu\gamma)\,\mathcal{F}\Psi(\lambda\gamma)|\,|\hat{\rho}(\gamma)| + \sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\hat{\rho}(\gamma)| \\
&\quad + (2\pi)^{2d}\sum_{\gamma\in\mathbb{G}^d}\sigma^r(\mu\gamma)\sum_{\iota\in\mathbb{Z}^d\setminus\{0\}} |\hat{\rho}(\gamma+\iota nK)|\,|\mathcal{F}\Psi(\lambda\gamma)| \\
&\quad + (2\pi)^{2d}\sum_{\gamma\in\mathbb{G}^d}\sigma^r(\mu\gamma)\sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}}\sum_{\iota\in\mathbb{Z}^d} |\hat{\rho}(\gamma+(\kappa+\iota n)K)|\,|\mathcal{F}\Psi(2\pi\kappa+\lambda\gamma)| \\
&\equiv G_1+G_2+G_3+G_4\,.
\end{aligned}
\tag{78}
$$

To estimate G_1, we proceed as in the proof of Lemma 3, noting that $\mathcal{F}\Psi(0) = \sigma^r(0) = (2\pi)^{-d}$ and that $\mathcal{F}\Psi$ and σ^r are even, so that their first order derivatives vanish at the origin. As the second order derivatives are uniformly bounded, we obtain

$$
\begin{aligned}
G_1 &\leq c\,(\lambda^2+\mu^2)\sum_{\gamma\in\mathbb{G}^d} |\gamma|^2\,|\hat{\rho}(\gamma)| \\
&\leq c\,(\lambda^2+\mu^2)\Bigg(\sum_{\gamma\in\mathbb{Z}^d\setminus\{0\}} |\gamma|^{-2s+4}\Bigg)^{\frac{1}{2}} \|\rho\|_{H^s}
\end{aligned}
\tag{79}
$$

where the sum converges provided $s > 2 + d/2$. Next,

$$
G_2 \leq \Bigg(\sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^{-4-d}\Bigg)^{\frac{1}{2}} \|\rho\|_{H^{2+d/2}} \leq c\,\lambda^2\,\|\rho\|_{H^{2+d/2}}\,. \tag{80}
$$

For G_3, we note that σ^r and $\mathcal{F}\Psi$ are uniformly bounded, so that G_3 has a bound of the form (80) as well. Finally, we estimate

$$
\begin{aligned}
G_4 &\leq c\sum_{\gamma\in\mathbb{G}^d}\sum_{\iota\in\mathbb{Z}^d} |\hat{\rho}(\gamma+\iota K)| \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}} |\mathcal{F}\Psi(2\pi\kappa+\lambda\gamma)| \\
&\leq c\sum_{\gamma\in\mathbb{G}^d}\sum_{\iota\in\mathbb{Z}^d} |\hat{\rho}(\gamma+\iota K)|\,|\lambda\gamma|^2 \sum_{\kappa\in\mathbb{Z}^d\setminus\{0\}}\prod_{i=1}^d \frac{1}{1+|\kappa_i|^\nu} \\
&\leq c\,\lambda^2\,\|\rho\|_{H^s}
\end{aligned}
\tag{81}
$$

where we use an estimate of the form (56) in the second step. In the last step, we note that the κ-sum converges whenever $\nu > 1$, and that the remaining double-sum can be estimated as in (79). □

Corollary 8. *Under the assumptions of Lemma 7,*

$$
Q(0) \leq c\,M\,(\lambda^2+\mu^2)\,\|\rho\|_{H^s}\,. \tag{82}
$$

Proof. The initial kinetic energy error is zero by construction. For the potential energy error, we pull out one factor of $S^r_\mu h - \rho$ in the L_∞ norm and apply Lemma 7. The remaining sums are, under the given assumptions, consistent approximations of the total mass M. □

The following lemma states the corresponding estimate for the case when the initialization grid is coarser than the computational grid. This is a computationally inefficient regime, but the result is interesting for looking at the SPH limit of HPM.

Lemma 9. *Suppose that the global smoothing operator σ has decay exponent $\zeta > 2d$. Then for every $s > 2 + d/2$ there exists a constant c such that for every $L \in \mathbb{N}$ and $K = nL$ for sufficiently large $n \in \mathbb{N}$, and for all $\rho \in H^s(\mathbb{T}^d)$ and h initialized as above,*

$$\sup_{x \in \mathbb{T}^d} |(S^r_\mu h)(x) - \rho(x)| \leq c \left(\lambda^2 + \mu^2 + \Lambda^{s-d/2} + \frac{\Lambda^{\zeta/2-d}}{\mu^{\zeta/2}} \right) \|\rho\|_{H^s} \,. \tag{83}$$

Proof. We follow the proof of Lemma 7. In place of (77) we split differently, writing

$$\begin{aligned} \tilde{h}(\gamma) &= (2\pi)^d \, \hat{\rho}(\gamma) \, \mathcal{F}\Psi(\lambda\gamma) + (2\pi)^d \sum_{\kappa \in \mathbb{Z}^d \setminus \{0\}} \hat{\rho}(\gamma + \kappa n L) \, \mathcal{F}\Psi(2\pi\kappa + \lambda\gamma) \\ &\quad + (2\pi)^d \sum_{\kappa \in \mathbb{Z}^d} \sum_{\iota \in \mathbb{Z}^d \setminus \{0\}} \hat{\rho}(\gamma + (\kappa n + \iota)L) \, \mathcal{F}\Psi(2\pi\kappa + \lambda\gamma) \,. \end{aligned} \tag{84}$$

Then G_1 and G_2 remain as before. The new G_3 reads

$$G_3 = (2\pi)^{2d} \sum_{\gamma \in \mathbb{G}^d} \sigma^r(\mu\gamma) \sum_{\kappa \in \mathbb{Z}^d \setminus \{0\}} |\hat{\rho}(\gamma + \kappa n L)| \, |\mathcal{F}\Psi(2\pi\kappa + \lambda\gamma)| \,, \tag{85}$$

which can be estimated as G_4 in the previous case. The new G_4 reads

$$\begin{aligned} G_4 &= (2\pi)^{2d} \sum_{\gamma \in \mathbb{G}^d} \sigma^r(\mu\gamma) \sum_{\kappa \in \mathbb{Z}^d} \sum_{\iota \in \mathbb{Z}^d \setminus \{0\}} |\hat{\rho}(\gamma + (\kappa n + \iota)L)| \, |\mathcal{F}\Psi(2\pi\kappa + \lambda\gamma)| \\ &= (2\pi)^{2d} \sum_{\gamma \in \mathbb{G}^d} \sigma^r(\mu\gamma) \sum_{\iota \in \mathbb{Z}^d \setminus \{0\}} |\hat{\rho}(\gamma + \iota L)| \sum_{\kappa \in \mathbb{Z}^d} |\mathcal{F}\Psi(2\pi\kappa + \lambda\gamma)| \end{aligned} \tag{86}$$

where now we can only assert convergence of the κ sum uniformly in γ due to the decay condition on $\mathcal{F}\Psi$. Hence,

$$\begin{aligned} G_4 &\leq c \sum_{\gamma \in \mathbb{H}^d} \sum_{\iota \in \mathbb{Z}^d \setminus \{0\}} |\hat{\rho}(\gamma + \iota L)| + c \sum_{\gamma \in \mathbb{G}^d \setminus \mathbb{H}^d} \sigma^r(\mu\gamma) \sum_{\iota \in \mathbb{Z}^d \setminus \{0\}} |\hat{\rho}(\gamma + \iota L)| \\ &\leq c \sum_{\gamma \in \mathbb{G}^d \setminus \mathbb{H}^d} |\hat{\rho}(\gamma)| + c \sum_{\gamma \in \mathbb{Z}^d \setminus \mathbb{H}^d} \sigma^r(\mu\gamma) \sum_{\beta \in \mathbb{Z}^d} |\hat{\rho}(\beta)| \\ &\leq c \, \Lambda^q \, \|\rho\|_{H^{q+d/2}} + c \, \frac{\Lambda^{\zeta/2-d}}{\mu^{\zeta/2}} \, \|\rho\|_{H^{1+d/2}} \end{aligned} \tag{87}$$

where we have estimated the left hand sum as in (80) and note that the first sum in the right hand term converges provided $d < \zeta/2$; an integral estimate then yields the final upper bound. Collecting terms and setting $q = s - d/2$, we obtain (83). □

With the same argument as in the proof of Corollary 8, we can state the following.

Corollary 10. *Under the assumptions of Lemma 9,*

$$Q(0) \leq c \, M \left(\lambda^2 + \mu^2 + \Lambda^{s-d/2} + \frac{\Lambda^{\zeta/2-d}}{\mu^{\zeta/2}} \right) \|\rho\|_{H^s} \,. \tag{88}$$

6. Time dependent estimates

We have now assembled all necessary tools to state and prove our main result on the convergence of the HPM method.

Theorem 11. *Assume that the barotropic fluid equations* (1) *possess a classical solution of class*

$$u, \rho \in C^1([0,T]; H^{4+d}(\mathbb{T}^d)) \tag{89}$$

for some $T > 0$. Suppose that the one-dimensional partition of unity kernel Θ is even and compactly supported as in Section 2, satisfies a Strang–Fix condition of order $p \geq 3$, has Fourier coefficients decaying with exponent $\nu > 2$ in (28)*, and satisfies*

$$|\mathcal{F}\Theta(\xi)| \geq c \qquad \text{for} \qquad \xi \in [-\pi, \pi] \tag{90}$$

with some constant c. Suppose further that the symbol σ of the global smoothing operator satisfies the conditions of Section 3.2 with $\ell = 2 + \lceil d/2 \rceil$ and decay exponent $\zeta > 2p + d$.

Now fix $n \in \mathbb{N}$. For every $K \in \mathbb{N}$, set $N = (nK)^d$ and let $X_1(t), \dots, X_N(t)$ denote the solution to the HPM system (6)*, initialized on a regular grid as described in Section 5, Lemma 7. Then there exist constants C_1 and C_2 such that for all $\mu \leq 1$ and K so large that* $\operatorname{supp}\Theta \subset (-K/2, K/2)$ *and $\lambda \leq \mu$,*

$$Q(t) \leq C_1 \, \mathrm{e}^{C_2 t} \left(\mu^2 + \frac{\lambda^{p-1}}{\mu^{p+d}} \right) \tag{91}$$

for all $t \in [0,T]$.

Remark 2. Except in $d = 1$, the L^2-sense of convergence asserted by Theorem 11 is too weak to say anything about convergence of individual trajectories. In particular, the weights m_k in the expression for the error of the particle velocities in Q_{kin} decay like N^{-1}, hence faster than the right hand side of the error estimate (91).

Let us consider a few special cases. First, under the assumption that $\mu = \lambda^a$, the two terms in the error estimate (91) scale identically when

$$a = \frac{p-1}{p+d+2} \,. \tag{92}$$

Then the following error estimates result.

Corollary 12. *Under the assumptions of Theorem 11, take $\mu = \lambda^a$, where a is given by* (92)*. Then there exist constants C_1 and C_2 such that*

$$Q(t) \leq C_1 \, \mathrm{e}^{C_2 t} \, \lambda^{\frac{2(p-1)}{p+d+2}} \tag{93}$$

for all $t \in [0,T]$.

Remark 3. The exponent in estimate (93) tends to 2 as $p \to \infty$.

If the one-dimensional partition of unity kernel is a cubic spline, then $\nu = 4$ and $p = 4$ as stated in Section 2.5. Hence, with

$$\mu = \lambda^{\frac{3}{6+d}} \tag{94}$$

and provided that $\zeta > 8 + d$, we have the error estimate

$$Q(t) \leq C_1 \, \mathrm{e}^{C_2 t} \, \lambda^{\frac{6}{6+d}} \tag{95}$$

for all $t \in [0,T]$. If we use an inverse power of the Helmholtz operator for global smoothing, we must require that $q > 4 + d/2$. Thus, our proof excludes the case studied in [8] where $q = 2$. In this case, we would not even be able to apply Theorem 11 with $p = 1$, so our approach does not even yield a proof of convergence.

Proof of Theorem 11. The time evolution of the error functional is given by

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \sum_{k=1}^{N} m_k \bigl(U_k - u(X_k)\bigr) \cdot \bigl(\dot{U}_k - \frac{\mathrm{d}}{\mathrm{d}t} u(X_k)\bigr) + \lambda^d \sum_{\alpha \in \mathbb{G}^d} \bigl((S_\mu^r h)_\alpha - \rho(x_\alpha)\bigr)\bigl((S_\mu^r \dot{h})_\alpha - \dot{\rho}(x_\alpha)\bigr) . \tag{96}$$

Inserting the particle momentum equation (6b) for $\dot{U}_k$, noting that, due to (6a) and the shallow water momentum equation (1a),

$$\frac{\mathrm{d}}{\mathrm{d}t} u(X_k) = \dot{u}(X_k) + U_k \cdot \nabla u(X_k) = -u(X_k) \cdot \nabla u(X_k) - \nabla\rho(X_k) + U_k \cdot \nabla u(X_k) \,, \tag{97}$$

noting that, due to the definition of the HPM height field (6c),

$$\dot{h}_\alpha = -\sum_{k=1}^{N} m_k \, U_k \cdot \nabla\psi_\lambda(x_\alpha - X_k) \,, \tag{98}$$

inserting the shallow water continuity equation (1b) for $\dot{h}$, and regrouping terms, we obtain

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = A_0 + A_1 + A_2 + A_3 \tag{99}$$

where

$$\begin{aligned} A_0 &= \sum_{k=1}^{N} m_k \, U_k \cdot \dot{U}_k + \lambda^{3d} \sum_{\alpha,\beta,\gamma \in \mathbb{G}^d} S^{\mu,r}_{\alpha-\beta} \, h_\beta \, S^{\mu,r}_{\alpha-\gamma} \, \dot{h}_\gamma \\ &= \sum_{k=1}^{N} m_k \, U_k \cdot \dot{U}_k + \lambda^{2d} \sum_{\alpha,\beta \in \mathbb{G}^d} S^{\mu}_{\alpha-\beta} \, h_\beta \, \dot{h}_\alpha = 0 \,, \end{aligned} \tag{100a}$$

$$A_1 = \sum_{k=1}^{N} m_k \bigl(U_k - u(X_k)\bigr) \cdot \bigl((u(X_k) - U_k) \cdot \nabla u(X_k)\bigr) \,, \tag{100b}$$

$$A_2 = \sum_{k=1}^{N} m_k \, U_k \cdot \nabla\rho(X_k) - \lambda^{2d} \sum_{\alpha,\beta \in \mathbb{G}^d} \rho(x_\alpha) \, S^{\mu,r}_{\alpha-\beta} \sum_{k=1}^{N} m_k \, U_k \cdot \nabla\psi_\lambda(x_\beta - X_k) \,, \tag{100c}$$

and

$$\begin{aligned} A_3 = &-\sum_{k=1}^{N} m_k \, u(X_k) \cdot (\dot{U}_k + \nabla\rho(X_k)) \\ &+ \lambda^{2d} \sum_{\alpha,\beta \in \mathbb{G}^d} S^{\mu,r}_{\alpha-\beta} \, h_\beta \, \nabla \cdot (\rho u)(x_\alpha) - \lambda^d \sum_{\alpha \in \mathbb{G}^d} \rho(x_\alpha) \, \nabla \cdot (\rho u)(x_\alpha) \,. \end{aligned} \tag{100d}$$

We now seek estimates for the nonzero terms A_1, A_2, and A_3. For A_1, we can proceed directly as in [23], estimating

$$|A_1| \leq \sum_{k=1}^{N} m_k \, |U_k - u(X_k)|^2 \, |\nabla u(X_k)| \leq c \, \|\nabla u\|_{L_\infty} \, Q_{\mathrm{kin}} \,. \tag{101}$$

For A_2, we estimate

$$\begin{aligned} |A_2| &= \left| \sum_{k=1}^{N} m_k \, U_k \cdot \left(\nabla \rho(X_k) - \lambda^{2d} \sum_{\alpha,\beta \in \mathbb{G}^d} \rho(x_\alpha) \, S^{\mu,r}_{\alpha-\beta} \, \nabla \psi_\lambda(x_\beta - X_k) \right) \right| \\ &\leq \sum_{k=1}^{N} m_k \, |U_k| \, \sup_{x \in \mathbb{T}^d} \left| \nabla \rho(x) - \lambda^{2d} \sum_{\alpha,\beta \in \mathbb{G}^d} \rho(x_\alpha) \, S^{\mu,r}_{\alpha-\beta} \, \nabla \psi_\lambda(x - x_\beta) \right| . \end{aligned} \tag{102}$$

Recalling (7) and using the Cauchy–Schwarz inequality, we find

$$\begin{aligned} \sum_{k=1}^{N} m_k \, |U_k| &\leq \sum_{k=1}^{N} m_k \, |u(X_k)| + \sum_{k=1}^{N} m_k \, |U_k - u(X_k)| \\ &\leq M \, \|u\|_{L_\infty} + \sqrt{M} \left(\sum_{k=1}^{N} m_k \, |U_k - u(X_k)|^2 \right)^{\frac{1}{2}} , \\ &\leq M \, \|u\|_{L_\infty} + \sqrt{M} \, \sqrt{Q} \end{aligned} \tag{103}$$

Inserting this estimate back into (102) and applying Lemma 3 to the second term on the right of (102), we find

$$|A_2| \leq (M \, \|u\|_{L_\infty} + \sqrt{M} \, \sqrt{Q}) \, c \, (\lambda^2 + \mu^2) \, \|\rho\|_{H^s} \leq C \, (\lambda^2 + \mu^2) \, (M + Q) \,. \tag{104}$$

To estimate the final group of terms, we note that

$$- \sum_{k=1}^{N} m_k \, u(X_k) \cdot \dot{U}_k \; = \; \sum_{k=1}^{N} m_k \, u(X_k) \, \cdot \, \lambda^d \sum_{\alpha \in \mathbb{G}^d} (S_\mu h)_\alpha \, \nabla \psi_\lambda (X_k \, - \, x_\alpha) \tag{105}$$

and define, as in [23],

$$Y(x) = \sum_{k=1}^{N} m_k \, \delta(x - X_k) - \rho(x) \,. \tag{106}$$

We can then write $A_3 = A_{31} + \cdots + A_{35}$ with

$$A_{31} = \sum_{k=1}^N m_k\, u(X_k) \cdot \biggl(\lambda^d \sum_{\alpha \in \mathbb{G}^d} (S_\mu h)_\alpha \, \nabla\psi_\lambda(X_k - x_\alpha) - \int_{\mathbb{T}^d} \mathcal{S}_\mu h(y)\, \nabla \psi_\lambda(X_k - y)\,\mathrm{d}y \biggr) \,, \tag{107a}$$

$$A_{32} = \int_{\mathbb{T}^d} u(x) \cdot \int_{\mathbb{T}^d} \mathcal{S}_\mu(\psi_\lambda * Y)(y)\, Y(x)\, \nabla\psi_\lambda(x-y)\,\mathrm{d}y\,\mathrm{d}x \,, \tag{107b}$$

$$A_{33} = -\sum_{k=1}^N m_k\, u(X_k) \cdot \bigl(\nabla(\psi_\lambda * \mathcal{S}_\mu(\psi_\lambda * \rho))(X_k) - \nabla\rho(X_k) \bigr) \,, \tag{107c}$$

$$A_{34} = \int_{\mathbb{T}^d} (\psi_\lambda * \mathcal{S}_\mu(\psi_\lambda * \rho))(x)\, \nabla \cdot (\rho u)(x)\,\mathrm{d}x - \lambda^d \sum_{\alpha \in \mathbb{G}^d} \rho_\alpha\, \nabla \cdot (\rho u)_\alpha \,, \tag{107d}$$

and

$$A_{35} = \lambda^d \sum_{\alpha \in \mathbb{G}^d} (S_\mu^r h)_\alpha\, \nabla \cdot (\rho u)_\alpha - \int_{\mathbb{T}^d} (\psi_\lambda * \mathcal{S}_\mu h)(x)\, \nabla \cdot (\rho u)(x)\,\mathrm{d}x \,. \tag{107e}$$

A direct application of Lemma 4 shows that

$$|A_{31}| \le c\, \|u\|_{L_\infty}\, M^2\, \frac{\lambda^{p-1}}{\mu^{p+d}} \,. \tag{108}$$

To estimate A_{32}, we adopt the strategy of [23], writing

$$\begin{aligned} A_{32} &= \int_{\mathbb{T}^d} u(x) \cdot \int_{\mathbb{T}^d} \mathcal{S}_\mu^r(\psi_\lambda * Y)(y)\, Y(x)\, \nabla \mathcal{S}_\mu^r(\psi_\lambda(x - \cdot))(y)\,\mathrm{d}y\,\mathrm{d}x \\ &= \int_{\mathbb{T}^d} \mathcal{S}_\mu^r(\psi_\lambda * Y)(y) \int_{y+\mathbb{T}^d} Y(x)\, u(x) \cdot \nabla \mathcal{S}_\mu^r(\psi_\lambda(x-\cdot))(y)\,\mathrm{d}x\,\mathrm{d}y \,, \end{aligned} \tag{109}$$

where we notice that the inner integrand is, by definition, periodic in x so that the inner integral is invariant under translations of its domain of integration. We denote this inner integral by $Z(y)$ and write

$$\begin{aligned} Z(y) &= \int_{y+\mathbb{T}^d} Y(x)\, u(x) \cdot \nabla \mathcal{S}_\mu^r(\psi_\lambda(x-\cdot))(y)\,\mathrm{d}x \\ &= \int_{y+\mathbb{T}^d} Y(x)\, u(x) \cdot \sum_{\gamma \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot(y-x)}\, \sigma^r(\mu\gamma)\, \mathrm{i}\gamma\, \mathcal{F}\Psi(\lambda\gamma) \\ &= \int_{y+\mathbb{T}^d} Y(x)\, u(x) \cdot g^{\mathrm{per}}(y-x)\,\mathrm{d}x \\ &= \int_{\mathbb{T}^d} Y(y-z)\, u(y-z) \cdot g^{\mathrm{per}}(z)\,\mathrm{d}z \\ &= \int_{\mathbb{R}^d} Y(y-z)\, u(y-z) \cdot g(z)\,\mathrm{d}z \end{aligned} \tag{110}$$

where the final equality is based on identity (142) with

$$g(z) = \int_{\mathbb{R}^d} \mathrm{e}^{i\xi\cdot z}\, \sigma^r(\mu\xi)\, \mathrm{i}\xi\, \mathcal{F}\Psi(\lambda\xi)\,\mathrm{d}\xi \,. \tag{111}$$

We now Taylor expand $u(y-z)$ about y,

$$u(y-z) = \sum_{|k|\le\ell} \frac{\mathrm{D}^k u(y)}{k!}\,(-z)^k + \sum_{|k|=\ell+1} \frac{\ell+1}{k!}\,(-z)^k \int_0^1 (1-s)^\ell\,\mathrm{D}^k u(y-sz)\,\mathrm{d}s\,, \tag{112}$$

and substitute into (109). Here k is a multi-index; we denote the part of $Z(y)$ associated with each k by Z_k, and the corresponding part of A_{32} by T_k. At lowest order,

$$\begin{aligned} Z_0(y) &= \int_{\mathbb{R}^d} Y(y-z)\,u(y)\cdot g(z)\,\mathrm{d}z \\ &= u(y)\cdot\int_{\mathbb{T}^d} Y(y-z)\,g^{\mathrm{per}}(z)\,\mathrm{d}z \end{aligned} \tag{113}$$

so that, reversing the steps taken in (110),

$$\begin{aligned} |T_0| &= \left|\int_{\mathbb{T}^d} \mathcal{S}^r_\mu(\psi_\lambda * Y)(y)\,u(y)\cdot\nabla\mathcal{S}^r_\mu(\psi_\lambda * Y)(y)\,\mathrm{d}y\right| \\ &= \frac{1}{2}\left|\int_{\mathbb{T}^d} \nabla\cdot u\,\big(\mathcal{S}^r_\mu(\psi_\lambda * Y)\big)^2\,\mathrm{d}y\right| \\ &\le \tfrac{1}{2}\,\|\mathrm{D}u\|_{L_\infty(\mathbb{T}^d)}\,\|\mathcal{S}^r_\mu(\psi_\lambda * Y)\|^2_{L_2(\mathbb{T}^d)}\,. \end{aligned} \tag{114}$$

For $1\le|k|\le\ell$,

$$T_k = \int_{\mathbb{T}^d} \mathcal{S}^r_\mu(\psi_\lambda * Y)(y)\,Z_k(y)\,\mathrm{d}y \tag{115}$$

where

$$\begin{aligned} Z_k(y) &= \frac{(-1)^{|k|}}{k!}\,\mathrm{D}^k u(y)\cdot\int_{\mathbb{R}^d} Y(y-z)\,z^k\,g(z)\,\mathrm{d}z \\ &= \frac{(-1)^{|k|}}{k!}\,\mathrm{D}^k u(y)\cdot\int_{\mathbb{T}^d} Y(y-z)\,g_k^{\mathrm{per}}(z)\,\mathrm{d}z\,, \end{aligned} \tag{116}$$

with $g_k(z) = z^k\,g(z)$. Then

$$|T_k| = c\,\|\mathrm{D}^k u\|_{L_\infty(\mathbb{T}^d)}\,\|\mathcal{S}^r_\mu(\psi_\lambda * Y)\|_{L_2(\mathbb{T}^d)}\left(\sum_{\gamma\in\mathbb{Z}^d} |\hat{Y}(\gamma)|^2\,|\mathcal{F}g_k(\gamma)|^2\right)^{\frac{1}{2}} \tag{117}$$

with

$$\begin{aligned} |\mathcal{F}g_k(\gamma)| &= \frac{1}{(2\pi)^d}\left|\int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}z\cdot\gamma}\,z^k \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}z\cdot\xi}\,\sigma^r(\mu\xi)\,\mathrm{i}\xi\,\mathcal{F}\Psi(\lambda\xi)\,\mathrm{d}\xi\,\mathrm{d}z\right| \\ &= \left|\mathrm{D}^k_\gamma\big[\gamma\,\sigma^r(\mu\gamma)\,\mathcal{F}\Psi(\lambda\gamma)\big]\right| \\ &= \left|\sum_{j\le k}\binom{k}{j}\,\mathrm{D}^j_\gamma\big[\gamma\,\sigma^r(\mu\gamma)\big]\,\mathrm{D}^{k-j}_\gamma\mathcal{F}\Psi(\lambda\gamma)\right| \\ &\le |\gamma|\,\sigma^r(\mu\gamma)\,\lambda^{|k|}\,(\mathrm{D}^k\mathcal{F}\Psi)(\lambda\gamma) + c\sum_{0<j\le k}\mu^{|j|-1}\left|\mathrm{D}^j_\beta\big[\beta\,\sigma^r(\beta)\big]\right| \\ &\le c\,(\lambda\,|\gamma|+1)\,\sigma^r(\mu\gamma)\,, \end{aligned} \tag{118}$$

where $\beta=\mu\gamma$, we employed the uniform bounds on derivatives of $\mathcal{F}\Psi$, and we used assumption (43a) on the global smoothing kernel. We must now distinguish two cases. When $\gamma \in \mathbb{G}^d$, $\lambda\,|\gamma| \leq \pi$ and, by assumption (90), $\mathcal{F}\Psi(\lambda\gamma)$ is bounded from below. When $\gamma \in \mathbb{Z}^d \setminus \mathbb{G}^d$, $\lambda\,|\gamma| > \pi$ and no such lower bound exists due to the Strang–Fix condition on Ψ. Hence,

$$|\mathcal{F}g_k(\gamma)| \leq \begin{cases} c\,\sigma^r(\mu\gamma)\,|\mathcal{F}\Psi(\lambda\gamma)| & \text{for } \gamma \in \mathbb{G}^d \\ c\,\lambda\,|\gamma|\,\sigma^r(\mu\gamma) & \text{for } \gamma \in \mathbb{Z}^d \setminus \mathbb{G}^d\,. \end{cases} \tag{119}$$

Plugging (119) into (117), further noting that $|\hat{Y}(\gamma)| \leq \|Y\|_{L_1} \leq c\,M$, we obtain

$$\begin{aligned} |T_k| &\leq C\,\|\mathcal{S}^r_\mu(\psi_\lambda * Y)\|_{L_2(\mathbb{T}^d)} \biggl(\|\mathcal{S}^r_\mu(\psi_\lambda * Y)\|_{L_2(\mathbb{T}^d)} + \lambda\,M \biggl(\sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^2\,\sigma(\mu\gamma) \biggr)^{\frac{1}{2}} \biggr) \\ &\leq C\,\|\mathcal{S}^r_\mu(\psi_\lambda * Y)\|^2_{L_2(\mathbb{T}^d)} + M^2\,\frac{\lambda^{\zeta-d}}{\mu^\zeta} \end{aligned} \tag{120}$$

provided the decay exponent of the global smoothing kernel satisfies $\zeta > d+2$. The second term in this estimate is of lower order relative to (108) when, for example, $p > 2$, as is assumed throughout.

When $|k| = \ell + 1$, we have

$$T_k = (\ell+1) \int_{\mathbb{T}^d} \mathcal{S}^r_\mu(\psi_\lambda * Y)(y) \int_0^1 (1-s)^\ell\,Z_k(y;s)\,\mathrm{d}s\,\mathrm{d}y \tag{121}$$

where

$$\begin{aligned} Z_k(y;s) &= \frac{(-1)^{|k|}}{k!} \int_{\mathbb{R}^d} Y(y-z)\,\mathrm{D}^k u(y-sz)\cdot g_k(z)\,\mathrm{d}z \\ &= (2\pi)^d\,\frac{(-1)^{|k|}}{k!} \sum_{\alpha,\gamma\in\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot y}\,\hat{Y}(\alpha)\,(\mathrm{D}^k u)\hat{}(\gamma-\alpha)\,\mathcal{F}g_k(\alpha+s(\gamma-\alpha))\,. \end{aligned} \tag{122}$$

Hence,

$$\begin{aligned} \|Z_k(y;s)\|^2_{L_2(\mathbb{T}^d)} &\leq c\,\|Y\|^2_{L_1(\mathbb{T}^d)} \sum_{\gamma\in\mathbb{Z}^d} \biggl(\sum_{\alpha\in\mathbb{Z}^d} |(\mathrm{D}^k u)\hat{}(\gamma-\alpha)|\,|\mathcal{F}g_k(\alpha+s(\gamma-\alpha))| \biggr)^2 \\ &= c\,M^2 \sum_{\beta,\beta',\gamma\in\mathbb{Z}^d} |(\mathrm{D}^k u)\hat{}(\beta)|\,|(\mathrm{D}^k u)\hat{}(\beta')|\,|\mathcal{F}g_k(\gamma+(s-1)\beta)|\,|\mathcal{F}g_k(\gamma+(s-1)\beta')| \\ &\leq c\,M^2 \biggl(\sum_{\beta\in\mathbb{Z}^d} |(\mathrm{D}^k u)\hat{}(\beta)| \biggr)^2 \sup_{\tau\in[0,1]} \sum_{\gamma\in\mathbb{Z}^d} |\mathcal{F}g_k(\gamma+\tau)|^2\,. \end{aligned} \tag{123}$$

To proceed, we estimate, similarly as in (118),

$$\begin{aligned} |\mathcal{F}g_k(\gamma)| &\leq |\gamma|\,\sigma^r(\mu\gamma)\,\lambda^{\ell+1}\,(\mathrm{D}^k\mathcal{F}\Psi)(\lambda\gamma) + \mu^\ell\,\bigl|\mathrm{D}^k_\beta\bigl[\beta\,\sigma^r(\beta)\bigr]\bigr|\,|\mathcal{F}\Psi(\lambda\gamma)| \\ &\quad + c \sum_{0<j<k} \mu^{|j|-1}\,\bigl|\mathrm{D}^j_\beta\bigl[\beta\,\sigma^r(\beta)\bigr]\bigr|\,\lambda^{|k-j|}\,|(\mathrm{D}^k\mathcal{F}\Psi)(\lambda\gamma)| \\ &\leq c\,(\mu^{\ell+1}\,|\gamma| + \mu^\ell)\,\sigma^r(\mu\gamma) + c\,\mu^\ell\,\bigl|\mathrm{D}^k_\beta\bigl[\beta\,\sigma^r(\beta)\bigr]\bigr|\,, \end{aligned} \tag{124}$$

where, as before, $\beta = \mu\gamma$. Further, we have assumed $\lambda \leq \mu$, employed the uniform bounds on derivatives of $\mathcal{F}\Psi$, and used assumption (43a) on the global smoothing kernel. Inserting (124) into (123) and using assumption (43b), each of the terms contributes the same bound, namely

$$\|Z_k(\,\cdot\,;s)\|_{L_2} \leq c\,M\,\|u\|_{H^s}\,\mu^{\ell-d/2} \tag{125}$$

for $s > \ell + 1 + d/2$ where, to obtain a finite bound from the contribution of the first term on the right of (124), the decay exponent of the global smoothing kernel σ must satisfy $\nu > d$. So, altogether,

$$|T_k| \leq C\,\|\mathcal{S}_\mu^r(\psi_\lambda * Y)\|_{L_2(\mathbb{T}^d)}^2 + M^2\,\mu^{2\ell-d}\,. \tag{126}$$

To complete the estimation of A_{32}, we define

$$\rho^{\mathrm{samp}}(x) = \sum_{\gamma\in\mathbb{G}^d} \mathrm{e}^{\mathrm{i}\gamma\cdot x}\,\tilde\rho(\gamma)\,, \tag{127}$$

and note that $Q_{\mathrm{pot}} = \frac12\,\|S_\mu^r h - \rho^{\mathrm{samp}}\|_{L_2}^2$. Hence,

$$\begin{aligned}
\|\mathcal{S}_\mu^r(\psi_\lambda * Y)\|_{L_2} &= \|\mathcal{S}_\mu^r h - \mathcal{S}_\mu^r(\psi_\lambda * \rho)\|_{L_2} \\
&\leq \|\mathcal{S}_\mu^r h - S_\mu^r h\|_{L_2} + \|S_\mu^r h - \rho^{\mathrm{samp}}\|_{L_2} + \|\rho^{\mathrm{samp}} - \mathcal{S}_\mu^r(\psi_\lambda * \rho)\|_{L_2} \\
&\leq c\,M\,\frac{\lambda^p}{\mu^{p+d/2}} + \sqrt{2\,Q_{\mathrm{pot}}} + c\,(\lambda^2+\mu^2)\,\|\rho\|_{H^s}
\end{aligned} \tag{128}$$

where, in the last inequality, the first term was estimated using Lemma 5, and the last term was estimated using Lemma 16, Lemma 2, and Lemma 1, where we require that $s > 2 + d/2$. Altogether, with $\ell = 2 + \lceil d/2 \rceil$ and $\zeta > 2p + d$, we obtain

$$|A_{32}| \leq C\,Q + C\,(\lambda^2+\mu^2) + M^2\,\frac{\lambda^{2p}}{\mu^{2p+d}}\,. \tag{129}$$

To estimate A_{33}, we proceed as in (108), here referring to Lemma 2 and Lemma 1 with $s > 3 + d/2$, thereby obtaining

$$|A_{33}| \leq c\,\|u\|_{L_\infty}\,M\,(\lambda^2+\mu^2)\,\|\rho\|_{H^{s+1}}\,. \tag{130}$$

The smoothness assumptions on ρ and u imply that the second term in (107d) is a (better than) $O(\lambda^2)$ approximation to the corresponding integral, see Lemma 15. Using Lemma 2 and Lemma 1 once again, we find that A_{34} possesses the upper bound

$$|A_{34}| \leq c\,(\lambda^2+\mu^2)\,\|\rho\|_{H^s}\,\|\rho\|_{H^{s-1}}\,\|u\|_{H^{s-1}} \tag{131}$$

so long as $s > 2 + d/2$.

Finally, to estimate A_{35}, we note the self-adjointness of the various smoothing and convolution operators and write

$$\begin{aligned}
A_{35} &= \lambda^d \sum_{\alpha\in\mathbb{G}^d} h_\alpha\,(S_\mu^r \nabla\cdot(\rho u))_\alpha - \int_{\mathbb{T}^d} h(x)\,\mathcal{S}_\mu(\psi_\lambda * \nabla\cdot(\rho u))(x)\,\mathrm{d}x \\
&= \lambda^d \sum_{\alpha\in\mathbb{G}^d} h_\alpha\,\bigl[(S_\mu^r\nabla\cdot(\rho u))_\alpha - \mathcal{S}_\mu(\psi_\lambda * \nabla\cdot(\rho u))_\alpha\bigr] \\
&\quad + \lambda^d \sum_{\alpha\in\mathbb{G}^d} h_\alpha\,g_\alpha - \int_{\mathbb{T}^d} h(x)\,g(x)\,\mathrm{d}x\,,
\end{aligned} \tag{132}$$

where $g(x) = \mathcal{S}_\mu(\psi_\lambda * \nabla \cdot (\rho u))(x)$. Applying Lemma 16, Lemma 2, and Lemma 1 to the first term on the right, and Lemma 6 to the second term on the right, we obtain

$$|A_{35}| \leq c\, M\, (\lambda^2 + \mu^2)\, \|\rho u\|_{H^s} \tag{133}$$

provided the Strang–Fix condition of the one-dimensional partition of unity kernel Θ is of order $p \geq 2$, and that $s > 3 + d/2$.

Collecting all the contributions to the differential inequality for $Q(t)$ and dropping lower order contributions, we obtain

$$\frac{\mathrm{d}Q}{\mathrm{d}t} \leq C \left(Q + \mu^2 + \frac{\lambda^{p-1}}{\mu^{p+d}} \right) \tag{134}$$

Due to the initial error bound provided by Corollary 8, the error bound (91) follows from a direct application of the Gronwall inequality. □

7. The SPH limit

All estimates in the proof of Theorem 11 are uniformly valid for λ small. We can therefore take the limit $\lambda \to 0$ and obtain the following convergence result for the SPH method on a periodic domain.

Theorem 13. *Assume that the barotropic fluid equations* (1) *possess a classical solution of class* (89) *for some* $T > 0$. *Suppose further that the symbol* σ *of the global smoothing operator satisfies the conditions of Section 3.2 with* $\ell = 2 + \lceil d/2 \rceil$ *and decay exponent* $\zeta > \max\{6 + d, 2d\}$.

Take $L \in \mathbb{N}$, *set* $N = L^d$, *and let* $X_1(t), \dots, X_N(t)$ *denote the solution to the HPM system* (6), *initialized on a regular grid as described in Section 5, Lemma 9. Then there exist constants* C_1 *and* C_2 *such that for all* $\mu \leq 1$,

$$Q(t) \leq C_1\, \mathrm{e}^{C_2 t} \left(\mu^2 + \frac{\Lambda^{\zeta/2-d}}{\mu^{\zeta/2}} \right) \tag{135}$$

for all $t \in [0, T]$.

In (135), the potential energy term in the error functional is understood in the sense that the Riemann sum has converged to the corresponding integral as $\lambda \to 0$.

Proof of Theorem 13. Take any partition of unity kernel Ψ which satisfies the assumptions of Theorem 11 with $p = 3$. Now follow the proof of Theorem 11 up to (134) and let $\lambda \to 0$. Due to the initial error bound provided by Corollary 10, also applied in the limit $\lambda \to 0$, (135) follows via the Gronwall inequality. □

Under the assumption that $\mu = \Lambda^a$, the two terms in the error estimate (135) scale identically when

$$a = \frac{\zeta - 2d}{\zeta + 4}\,. \tag{136}$$

Then the following error estimate results.

Corollary 14. *Under the assumptions of Theorem 13, take* $\mu = \lambda^a$, *where* a *is given by* (136). *Then there exist constants* C_1 *and* C_2 *such that*

$$Q(t) \leq C_1\, \mathrm{e}^{C_2 t}\, \Lambda^{\frac{2\zeta - 4d}{\zeta + 4}} \tag{137}$$

for all $t \in [0, T]$.

Remark 4. The exponent in estimate (137) tends to 2 as $\zeta \to \infty$.

Remark 5. In the case of periodic SPH, we could easily reduce our proof to a minor modification of Oelschläger's proof [23]. Comparing term by term, we note two main differences between our result and his: First, Oelschläger did not assume that the SPH kernel is even. Without this assumption, the smoothing error estimate Lemma 2 and related arguments only yield a bound of $O(\mu)$. This carries through the argument, so that the second term in (134) is also only linear in μ. An $O(\mu^2)$ estimate for SPH using symmetry of the kernel was already given by Price [24].

Second, Oelschläger takes a probabilistic view on the initialization procedure, assuming that the particles are initially random variables, independently and identically distributed with density ρ. The corresponding bound on the expected error is weaker than our deterministic initialization error bound Corollary 10, and the resulting time dependent error bound must also be read as an expected value.

Appendix A. Fourier Transforms

In two appendices we recall basic facts of Fourier analysis. Although this is entirely textbook material [13, 27], it is necessary to be very clear about conventions because our proofs interlink the Fourier transform on $\mathbb{R}^d$, the periodic Fourier transform, and the discrete Fourier transform in the limit of vanishing mesh size.

A.1. **Fourier transform on $\mathbb{R}^d$.** We denote the Fourier transform of a function $f \in L_2(\mathbb{R}^d)$ by

$$\mathcal{F}f(\xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\xi\cdot x} \, f(x) \, \mathrm{d}x \,. \tag{138}$$

The Dirac delta distribution has the representation

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\xi\cdot x} \, \mathrm{d}x = \delta(\xi) \,, \tag{139}$$

which implies the Fourier inversion formula

$$f(x) = \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\xi\cdot x} \, \mathcal{F}f(\xi) \, \mathrm{d}\xi \,. \tag{140}$$

A function $g \in L_2(\mathbb{R}^d)$ which is decaying sufficiently fast such that its Fourier transform $\mathcal{F}g$ is continuous can be periodized by setting

$$g^{\mathrm{per}}(x) = \sum_{\beta\in\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\beta\cdot x} \, \mathcal{F}g(\beta) \,. \tag{141}$$

Then, if $f \in L_2(\mathbb{T}^d)$, periodically extended to $\mathbb{R}^d$,

$$\int_{\mathbb{R}^d} f(x) \, g(x) \, \mathrm{d}x = \int_{\mathbb{T}^d} f(x) \, g^{\mathrm{per}}(x) \, \mathrm{d}x \,. \tag{142}$$

A.2. **Fourier transform on $\mathbb{T}^d$.** For $f \in L_1(\mathbb{T}^d)$, we define the Fourier transform

$$\hat{f}(\beta) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \mathrm{e}^{-\mathrm{i}\beta\cdot x} \, f(x) \, \mathrm{d}x \,, \tag{143}$$

where $\beta \in \mathbb{Z}^d$. For future reference, we note the orthogonality relation

$$\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \mathrm{e}^{\mathrm{i}\beta\cdot x} \, \mathrm{d}x = \delta_\beta \equiv \begin{cases} 1 & \text{for } \beta = 0 \\ 0 & \text{otherwise} \,, \end{cases} \tag{144}$$

which implies the Fourier inversion formula

$$f(x) = \sum_{\beta \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\beta \cdot x} \, \hat{f}(\beta) \tag{145}$$

and Parseval identity

$$\int_{\mathbb{T}^d} f(x) \, \overline{g(x)} \, \mathrm{d}x = (2\pi)^d \sum_{\gamma \in \mathbb{Z}^d} \hat{f}(\gamma) \, \overline{\hat{g}(\gamma)} \tag{146}$$

for $f, g \in L_2(\mathbb{T}^d)$, where the over-bar denotes the complex conjugate. Further, we write

$$(f * g)(x) = \int_{\mathbb{T}^d} f(y) \, g(x-y) \, \mathrm{d}y \tag{147}$$

to denote the convolution of two periodic functions (where, as before, the arguments are understood as referring to the periodic extension when not in the fundamental domain), so that

$$(f * g)\hat{\ }(\beta) = (2\pi)^d \, \hat{f}(\beta) \, \hat{g}(\beta) \tag{148}$$

and

$$(fg)\hat{\ }(\beta) = \sum_{\gamma \in \mathbb{Z}^d} \hat{f}(\gamma) \, \hat{g}(\beta - \gamma) \, . \tag{149}$$

We recall that differentiation of f transforms into multiplication of its Fourier transform by $\mathrm{i}\beta$, namely

$$\nabla f(x) = \sum_{\beta \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\beta \cdot x} \, \mathrm{i}\beta \, \hat{f}(\beta) \, ; \tag{150}$$

finally, we recall the shift formula

$$f(\cdot - y)\hat{\ }(\beta) = \mathrm{e}^{-\mathrm{i}\beta \cdot y} \, \hat{f}(\beta) \, . \tag{151}$$

A.3. **Discrete Fourier transform.** For the finite set of point values $(f_\alpha)_{\alpha \in \mathbb{G}^d}$, we define their *discrete Fourier transform*

$$\tilde{f}(\beta) = \frac{1}{K^d} \sum_{\alpha \in \mathbb{G}^d} \mathrm{e}^{-\mathrm{i}\beta \cdot x_\alpha} \, f_\alpha \, , \tag{152}$$

where $\beta \in \mathbb{G}^d$. The corresponding orthogonality relation is

$$\frac{1}{K^d} \sum_{\alpha \in \mathbb{G}^d} \mathrm{e}^{\mathrm{i}\beta \cdot x_\alpha} = \delta_\beta^{\mathrm{per}} \equiv \begin{cases} 1 & \text{for } \beta = 0 \mod K \\ 0 & \text{otherwise} \end{cases} \, , \tag{153}$$

which implies the inversion formula

$$f_\alpha = \sum_{\beta \in \mathbb{G}^d} \mathrm{e}^{\mathrm{i}\beta \cdot x_\alpha} \, \tilde{f}(\beta) \tag{154}$$

and the discrete Parseval identity

$$\lambda^d \sum_{\alpha \in \mathbb{G}^d} f_\alpha \, \overline{g_\alpha} = (2\pi)^d \sum_{\beta \in \mathbb{G}^d} \tilde{f}(\beta) \, \overline{\tilde{g}(\beta)} \, . \tag{155}$$

The above relations extend periodically to all $\alpha, \beta \in \mathbb{Z}$. We denote the discrete convolution of such periodically extended f_α and g_α by

$$(f \circledast g)_\alpha = \lambda^d \sum_{\beta \in \mathbb{G}^d} f_\beta \, g_{\alpha - \beta} \, , \tag{156}$$

so that

$$(f \circledast g)\tilde{}(\beta) = (2\pi)^d \, \tilde{f}(\beta) \, \tilde{g}(\beta) \,. \tag{157}$$

Finally, we quote the shift formula for the discrete Fourier transform,

$$(f_{\cdot - \gamma})\tilde{}(\beta) = \mathrm{e}^{-\mathrm{i}\beta\cdot x_\gamma} \, \tilde{f}(\beta) \,. \tag{158}$$

For a function $f \in C(\mathbb{T}^d)$, we can set $f_\alpha \equiv f(x_\alpha)$. If, moreover, $\hat{f} \in \ell_1(\mathbb{Z}^d)$, the Fourier transform and the discrete Fourier transform of f are related via the *Poisson summation formula*

$$\hat{f}(\beta) - \tilde{f}(\beta) = - \sum_{\kappa \in \mathbb{Z}^d \setminus \{0\}} \hat{f}(\beta + \kappa K) \tag{159}$$

for every $\beta \in \mathbb{G}^d$.

Appendix B. Sobolev spaces

We write $H^s(\mathbb{T}^d)$ to denote the Sobolev space of Lebesgue measurable functions whose weak derivatives up to order s belong to $L_2(\mathbb{T}^d)$ endowed with norm

$$\|f\|_{H^s}^2 = (2\pi)^d \sum_{\beta \in \mathbb{Z}^d} (1 + |\beta|^2)^s \, |\hat{f}(\beta)|^2 \,. \tag{160}$$

For our purposes, all functions are real-valued, although we state fundamental properties like the Parseval identity for the complex-valued case for clarity.

For later reference, we state a simple fact on the accuracy of equidistant quadrature for functions in H^s.

Lemma 15. *For every $s > d/2$ there exists a constant c such that for every $f \in H^s(\mathbb{T}^d)$,*

$$\left| \int_{\mathbb{T}^d} f(x) \, \mathrm{d}x - \lambda^d \sum_{\alpha \in \mathbb{G}^d} f(x_\alpha) \right| \leq c \, \lambda^s \, \|f\|_{H^s(\mathbb{T}^d)} \,. \tag{161}$$

Proof. By definition, the left side of (161) equals $|\hat{f}(0) - \tilde{f}(0)|$. Using the Poisson summation formula and the Cauchy–Schwarz inequality, we estimate

$$\begin{aligned} |\hat{f}(0) - \tilde{f}(0)| &\leq \sum_{\gamma \in \mathbb{Z}^d \setminus \{0\}} |\hat{f}(K\gamma)| \\ &\leq \Bigg(\sum_{\gamma \in \mathbb{Z}^d \setminus \{0\}} (K|\gamma|)^{-2s} \Bigg)^{\frac{1}{2}} \Bigg(\sum_{\gamma \in \mathbb{Z}^d \setminus \{0\}} (K|\gamma|)^{2s} \, |\hat{f}(K\gamma)|^2 \Bigg)^{\frac{1}{2}} \\ &\leq K^{-s} \Bigg(\sum_{\gamma \in \mathbb{Z}^d \setminus \{0\}} |\gamma|^{-2s} \Bigg)^{\frac{1}{2}} \|f\|_{H^s(\mathbb{T}^d)} \,, \end{aligned} \tag{162}$$

where the right hand sum converges whenever $s > d/2$. □

A direct consequence of the Poisson summation formula is the following sampling error estimate.

Lemma 16. *For every $s > d/2$ there exists a constant c such that for every $f \in H^s(\mathbb{T}^d)$,*

$$\sup_{x \in \mathbb{T}^d} \left| f(x) - \sum_{\beta \in \mathbb{G}^d} \mathrm{e}^{\mathrm{i}\beta\cdot x} \, \tilde{f}(\beta) \right| \leq c \, \lambda^{s-d/2} \, \|f\|_{H^s(\mathbb{T}^d)} \,. \tag{163}$$

Proof. Due to the Fourier inversion formula (145) in the first step and the Poisson summation formula (159) in the second step,

$$\begin{aligned}\Big| f(x) - \sum_{\beta\in\mathbb{G}^d} \mathrm{e}^{\mathrm{i}\beta\cdot x}\, \tilde f(\beta) \Big| &\le \sum_{\beta\in\mathbb{G}^d} |\hat f(\beta) - \tilde f(\beta)| + \sum_{\beta\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\hat f(\beta)| \\ &\le 2 \sum_{\beta\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\hat f(\beta)| \\ &\le 2 \Big(\sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^{-2s} \Big)^{\frac12} \Big(\sum_{\gamma\in\mathbb{Z}^d\setminus\mathbb{G}^d} |\gamma|^{2s}\, |\hat f(\gamma)|^2 \Big)^{\frac12} . \qquad (164)\end{aligned}$$

The claim follows by an integral estimate on the first sum on the last line. □

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