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Asymptotic and Numerical Analyses for Mechanical Models of Heat Baths

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A mechanical model of a particle immersed in a heat bath is studied, in which a distinguished particle interacts via linear springs with a collection of n particles with variable masses and random initial conditions; the jth particle oscillates with frequency j^p, where p is a parameter. For $p > 1/2$ the sequence of random processes that describe the trajectory of the distinguished particle tends almost surely, as $n \to \infty$, to the solution of an integro-differential equation with a random driving term; the mean convergence rate is $1/n^{p-1/2}$. We further investigate whether the motion of the distinguished particle can be well approximated by an integration scheme—the symplectic Euler scheme—when the product of time step h and highest frequency n^p is of order 1, that is, when high frequencies are underresolved. For $1/2 < p < 1$ the numerical solution is found to converge to the exact solution at a reduced rate of $|\log h|\, h^{2-1/p}$. These results shed light on existing numerical data.

KEY WORDS: Heat bath; generalized Langevin equation; Volterra equation; stiff oscillatory systems; symplectic Euler scheme; order reduction.

1. INTRODUCTION

We study a simple model of a particle in a heat bath. The heat bath consists of a collection of particles that interact with the distinguished particle through springs. Such models were introduced back in the 1960's by Ford *et al.*[1] in order to study the mechanical foundations of Brownian motion and stochastic dynamics. There exists a significant amount of related literature both for classical and quantum systems (see, e.g., refs. 2–5). In

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recent years, there has been a renewed interest in systems of this type in the context of the numerical analysis of large oscillatory systems with broad frequency spectra,[6–8] and the approximation of stochastic differential equations.[9] Kast[10] considered systems of coupled oscillators in the context of optimal prediction theory.[11, 12]

We examine a one-parameter family of models that are a variant of the Ford–Kac–Mazur model. A collection of n particles of different masses interacts with a distinguished particle through linear springs of unit strength. A parameter, p, determines the mass distribution: the jth particle has mass $m_j = j^{-2p}$. Thus, if the distinguished particle was held fixed, it would be the anchor point of n independent oscillators with frequencies $\omega_j = j^p$. The model studied by Stuart and Warren[6] is a particular instance with $p = 1$. It is a very special case as all frequencies are rationally related, resulting in periodic solutions. The generalization to $p \neq 1$ is interesting since the motion of the distinguished particle is governed by nonlocal memory effects (see later).

Following the standard approach in statistical mechanics it is assumed that all the degrees of freedom, except for the ones under explicit consideration, have random initial data. The system is assumed to be in thermodynamical equilibrium, i.e., the random initial data are distributed according to the Gibbs measure associated with the Hamiltonian of the system. In the present case, the variables of interest are the position, $Q_n(t)$, and the momentum, $P_n(t)$, of the distinguished particle; the subscript n refers to the number of particles in the heat bath. Under these assumptions, $Q_n(t)$ and $P_n(t)$ are governed by a generalized Langevin equation, which is an integro-differential equation with random forcing; the randomness stems from the postulated random initial data.

We study the "thermodynamics limit," $n \to \infty$, and find that for $p > 1/2$ the sequence of random trajectories, $Q_n(t)$, converges almost surely to a limiting processes, $Q(t)$; the convergence is uniform on any bounded time interval $[0, T]$. We estimate the discrepancy between Q_n and Q in $L^2(\Omega; L^2[0, T])$ and $L^1(\Omega; C[0, T])$, where Ω is the probability sample space; in both cases the mean convergence rate is $1/n^{p-1/2}$. Our results generalize those of Stuart and Warren,[6] who obtain mean square convergence with rate $1/n^{1/2}$ for $p = 1$.

We further investigate the numerical approximation of this model in an underresolved setting, when the product of the time step, h, and the highest frequency, n^p, is of order 1. The question is whether the trajectory of the distinguished particle can be accurately predicted without properly resolving a fraction of the spectrum. We analyze the symplectic Euler scheme, which has also been considered in refs. 6 and 8. In the limit $h \to 0$, $n \to \infty$, $n^p h \leqslant 1$, the numerical solution converges to Q_n. For $1/2 < p < 1$

the convergence rate is $|\log h|\, h^{2-1/p}$, which is less than the convergence rate of the symplectic Euler scheme for non-stiff problems. These results are in agreement with numerical data in ref. 7.

To facilitate the reading of this long and technical paper, we have organized it in the following manner: We start with a presentation of the model and the computational scheme (Sections 2–6). Both continuous and discrete systems are brought into an integral form, which is the starting point for our asymptotic analysis. Our main results are summarized in Section 7; proofs follow in Sections 8–16. Numerical results are presented in Section 17, followed by a discussion in Section 18.

2. THE MODEL

We consider a family of mechanical models that describe the motion of a particle immersed in a heat bath. The heat bath is modeled by a large collection of particles that interact with the distinguished particle via linear springs. Let Q_n, P_n denote the position and momentum of the distinguished particle, and $q=(q_1, q_2,..., q_n)$, $p=(p_1, p_2,..., p_n)$ denote the vectors of positions and momenta of a collection of n particles that constitute the heat bath. All motions are assumed to take place in one space dimension. The Hamiltonian of the system is

$$H(Q_n, P_n, q, p)=\frac{1}{2}(P_n^2+Q_n^2)+\frac{1}{2}\sum_{j=1}^{n}\left[\frac{p_j^2}{m_j}+k_j(q_j-Q_n)^2\right] \tag{1}$$

where m_j is the mass of the jth particle, and k_j is the stiffness of the spring that connects the jth particle to the distinguished particle. In this paper we consider a continuous family of models where the mass distribution is $m_j=1/j^{2p}$, $j=1, 2,..., n$, and where all the springs are of equal strength, $k_j=1$; the parameter p plays an important role in the limiting behavior of this system as $n\to\infty$. This family of models is a variant of the model introduced by Ford *et al.*,[1, 13] and is closely related to the models recently studied by Stuart and Warren[6] and Cano and Stuart.[8]

The Hamilton equations of motion are

$$\begin{cases}\dot{Q}_n=P_n\\ \dot{P}_n=-Q_n+\sum_{j=1}^{n}(q_j-Q_n)\end{cases}\qquad \begin{cases}\dot{q}_j=j^{2p}p_j\\ \dot{p}_j=-(q_j-Q_n)\end{cases} \tag{2}$$

complemented by initial conditions, $Q_n(0)=Q_0$, $P_n(0)=P_0$, $q_j(0)$, and $p_j(0)$. The assumption is that the initial conditions of the heat bath variables are random, with a joint probability measure, μ_n, given by the equilibrium Gibbs distribution,

$$\mu_n(dq \times dp) = Z^{-1} e^{-\beta H(Q_0, P_0, q, p)}\, dq\, dp$$

where Z is a normalization constant and β is the inverse temperature, which without loss of generality will be taken to be 1. For H given by (1) the measure μ_n is Gaussian and satisfies

$$\begin{aligned} E[q_j - Q_0] &= E[p_j] = 0 \\ E[(q_j - Q_0)^2] &= E[j^{2p} p_j^2] = 1 \end{aligned} \tag{3}$$

where $E[\cdot]$ denotes expectation with respect to μ_n. Thus, $q_j(0) = Q_0 + \xi_j$ and $p_j(0) = j^{-p} \eta_j$, where ξ_j and η_j are independent identically-distributed random variables drawn from a normal distribution $\mathcal{N}(0, 1)$. Our statistical setting for the initial conditions differs slightly from the one used in ref. 6, where $q_j(0)$, $p_j(0)$ are assumed to be distributed independently of Q_0, P_0.

Equation (3) suggests the following change of variables:

$$a_j = (q_j - Q_n), \qquad b_j = j^p p_j$$

leading to rescaled equations of motion:

$$\begin{cases} \dot{Q}_n = P_n \\ \dot{P}_n = -Q_n + \sum_{j=1}^n a_j \end{cases} \qquad \begin{cases} \dot{a}_j = j^p b_j - P_n \\ \dot{b}_j = -j^p a_j \end{cases} \tag{4}$$

with initial conditions $a_j(0) = \xi_j$ and $b_j(0) = \eta_j$.

3. GENERALIZED LANGEVIN EQUATION

The model equations (4) are sufficiently simple for the a_j, b_j equations to be integrated explicitly by standard methods:

$$\begin{aligned} a_j(t) &= \xi_j \cos(j^p t) + \eta_j \sin(j^p t) - \int_0^t \cos[j^p(t-s)]\, P_n(s)\, ds \\ b_j(t) &= -\xi_j \sin(j^p t) + \eta_j \cos(j^p t) + \int_0^t \sin[j^p(t-s)]\, P_n(s)\, ds \end{aligned} \tag{5}$$

Substituting $a_j(t)$ back into the $\dot{P}_n$ equation in (4) we obtain a closed set of equations for the motion of the distinguished particle:

$$
\begin{aligned}
\dot{Q}_n &= P_n \\
\dot{P}_n &= -Q_n - \int_0^t \kappa_n(t-s)\, P_n(s)\, ds + g_n(t)
\end{aligned}
\tag{6}
$$

where

$$\kappa_n(t) = \sum_{j=1}^{n} \cos(j^p t)$$

and

$$g_n(t) = \sum_{j=1}^{n} [\xi_j \cos(j^p t) + \eta_j \sin(j^p t)]$$

Equation (6) is a projection of the $(2n+2)$-dimensional system (4) onto the two-dimensional subspace (Q_n, P_n); it is an inhomogeneous integro-differential system of equations that describes the rate of change of (Q_n, P_n) as function of their past and present values. The history dependence is encapsulated by the memory kernel, $\kappa_n(t)$. The function $g_n(t)$ is a forcing that depends on the initial values, ξ_j and η_j, of the integrated variables. In the current setting, $g_n(t)$ is a random function whose expectation value is identically zero, and whose autocorrelation function is given by

$$E[g_n(t)\, g_n(0)] = \sum_{j=1}^{n} \cos(j^p t) = \kappa_n(t)$$

which is known as a fluctuation-dissipation relation. Equation (6) is an instance of the Mori–Zwanzig projection formalism,[12, 14, 15] and is also known as a generalized Langevin equation.

For $p = 1$ the memory kernel tends, as $n \to \infty$, to the Fourier series of a 2π-periodic delta function, whereas $g_n(t)$ tends, for $0 \leqslant t < \pi$, to the Fourier representation of white noise. Stuart and Warren[6] showed that $Q_n(t)$ converges in the mean square on $[0, \pi]$ to the solution of the stochastic differential equation,

$$
\begin{aligned}
\dot{Q} &= P \\
\dot{P} &= -Q - \frac{\pi}{2} P + \dot{W}
\end{aligned}
$$

where $\dot{W}(t)$ is white noise.

4. VOLTERRA EQUATION

Equation (6) can be transformed into an integral equation of Volterra type, which is a more convenient starting point for asymptotic analysis. We first write (6) as a second-order equation for $Q_n(t)$,

$$\ddot{Q}_n(t) = -Q_n(t) - \int_0^t \kappa_n(t-s)\, \dot{Q}_n(s)\, ds + g_n(t)$$

and then integrate it from 0 to t, integrating by parts the memory term,

$$\dot{Q}_n(t) = P_0 - Q_0 t - Q_0 K_n(t) \\ - \int_0^t [1+\kappa_n(t-s)]\, Q_n(s)\, ds + \int_0^t g_n(s)\, ds$$

where

$$K_n(t) = -\int_0^t [1+\kappa_n(s)]\, ds = -t - \sum_{j=1}^n \frac{\sin(j^p t)}{j^p} \tag{7}$$

A second integration from 0 to t yields a Volterra convolution equation,

$$Q_n(t) = F_n(t) + \int_0^t K_n(t-s)\, Q_n(s)\, ds \tag{8}$$

with kernel K_n and forcing

$$F_n(t) = Q_0 + P_0 t + Q_0 \sum_{j=1}^n \frac{1-\cos(j^p t)}{j^{2p}} \\ + \sum_{j=1}^n \xi_j \frac{1-\cos(j^p t)}{j^{2p}} + \sum_{j=1}^n \eta_j \left[\frac{t}{j^p} - \frac{\sin(j^p t)}{j^{2p}}\right] \tag{9}$$

An equation for $P_n(t)$ is obtained by differentiating (8):

$$P_n(t) = f_n(t) + \int_0^t K_n(t-s)\, P_n(s)\, ds \tag{10}$$

where

$$f_n(t) = \dot{F}_n(t) + Q_0 K_n(t)$$
$$= P_0 - tQ_0 + \sum_{j=1}^{n} \xi_j \frac{\sin(j^p t)}{j^p} + \sum_{j=1}^{n} \eta_j \frac{1-\cos(j^p t)}{j^p} \tag{11}$$

Note that the equation that governs $Q_n(t)$ differs from the equation that governs $P_n(t)$ only in the forcing.

5. SYMPLECTIC EULER SCHEME

From a computational point of view the equations of motion (2) form a stiff oscillatory system due to the large ratio between the highest frequency, which is of order n^p, and the lowest frequency, which is of order 1. The question addressed in refs. 6–8 is whether the motion of the distinguished particle can be accurately computed when the high frequencies are underresolved, i.e., when the time step h is small relative to the characteristic time scale of the distinguished particle, but the product $n^p h$ is not small. Cano and Stuart[8] conducted numerical experiments for a variety of systems using several numerical methods; their results indicate that convergence to the right solution is sensitive both to the system and to the numerical method. In several cases, the numerical solution was found to converge to the wrong limit. Their observation is that it is harder to approximate systems with local damping, i.e., when the memory kernel has a delta-singularity.

In this paper we analyze underresolved computations for the symplectic Euler scheme (ref. 16, p. 312). The equations are solved on a finite time interval $[0, T]$. Let h be a fixed step size, such that $Nh = T$, with N the total number of steps; $t_k = kh$ denotes the time at the kth step. The discrete variables are denoted by $\mathbb{Q}_n^k \approx Q_n(t_k)$, $\mathbb{P}_n^k \approx P_n(t_k)$, $q_j^k \approx q_j(t_k)$ and $p_j^k \approx p_j(t_k)$. The size of the heat bath, n, is chosen such to keep the product $n^p h$ approximately fixed: $n = \lfloor (\xi/h)^{1/p} \rfloor$, with $\xi \leqslant 1$.

The symplectic Euler scheme for (2) is

$$\begin{aligned}
\mathbb{Q}_n^{k+1} &= \mathbb{Q}_n^k + h\mathbb{P}_n^{k+1} \\
\mathbb{P}_n^{k+1} &= \mathbb{P}_n^k - h\mathbb{Q}_n^k + h\sum_{j=1}^{n} (q_j^k - \mathbb{Q}_n^k) \\
q_j^{k+1} &= q_j^k + hj^{2p} p_j^{k+1} \\
p_j^{k+1} &= p_j^k - h(q_j^k - \mathbb{Q}_n^k)
\end{aligned} \tag{12}$$

Changing variables into $a_j^k = q_j^k - \mathbb{Q}_n^k$ and $b_j^k = j^p p_j^k$, the discrete analog of (4) is

$$\begin{aligned}
\mathbb{Q}_n^{k+1} &= \mathbb{Q}_n^k + h\mathbb{P}_n^{k+1} \\
\mathbb{P}_n^{k+1} &= \mathbb{P}_n^k - h\mathbb{Q}_n^k + h\sum_{j=1}^{n} a_j^k \\
a_j^{k+1} &= a_j^k + hj^p b_j^{k+1} - (\mathbb{Q}_n^{k+1} - \mathbb{Q}_n^k) \\
b_j^{k+1} &= b_j^k - hj^p a_j^k
\end{aligned} \tag{13}$$

where $\mathbb{Q}_n^0 = Q_0$, $\mathbb{P}_n^0 = P_0$, $a_j^0 = \xi_j$, and $b_j^0 = \eta_j$, with $\xi_j, \eta_j \sim \mathcal{N}(0, 1)$.

Like in the continuous case, the equations for a_j^k, b_j^k can be solved explicitly; the derivation is presented in Appendix A. The solution, which is the discrete analog of (5), is

$$\begin{aligned}
\begin{pmatrix} a_j^k \\ b_j^k \end{pmatrix} &= \frac{1}{\cos(\frac{1}{2}\phi_j)} \begin{pmatrix} \cos[(k+\frac{1}{2})\,\phi_j] & \sin k\phi_j \\ -\sin k\phi_j & \cos[(k-\frac{1}{2})\,\phi_j] \end{pmatrix} \begin{pmatrix} \xi_j \\ \eta_j \end{pmatrix} \\
&\quad - \sum_{m=1}^{k} \frac{1}{\cos(\frac{1}{2}\phi_j)} \begin{pmatrix} \cos[(k-m+\frac{1}{2})\,\phi_j] & \sin[(k-m)\,\phi_j] \\ -\sin[(k-m)\,\phi_j] & \cos[(k-m-\frac{1}{2})\,\phi_j] \end{pmatrix} \\
&\quad \times \begin{pmatrix} \mathbb{Q}_n^m - \mathbb{Q}_n^{m-1} \\ 0 \end{pmatrix}
\end{aligned} \tag{14}$$

where

$$\phi_j = \cos^{-1}(1 - \tfrac{1}{2} j^{2p} h^2)$$

Our formulas can be simplified by using the following identities:

$$\begin{aligned}
\frac{\sin(k\phi_j)}{\cos(\frac{1}{2}\phi_j)} &= j^p h\, U_{k-1}(x_j) \\
\frac{\cos[(k+\frac{1}{2})\,\phi_j]}{\cos(\frac{1}{2}\phi_j)} &= U_k(x_j) - U_{k-1}(x_j)
\end{aligned} \tag{15}$$

where the U_k are the Chebyshev polynomials of the second kind (see Appendices A and B) and

$$x_j = \cos\phi_j = 1 - \tfrac{1}{2} j^{2p} h^2$$

Substituting the a_j^k component of (14) along with the identities (15) into the $\mathbb{P}_n$-equation in (13), we obtain a closed, second-order difference equation for $\mathbb{Q}_n^k$:

$$\frac{\mathbb{Q}_n^{k+1} - 2\mathbb{Q}_n^k + \mathbb{Q}_n^{k-1}}{h^2} = -\mathbb{Q}_n^k + \sum_{j=1}^{n} \xi_j [U_k(x_j) - U_{k-1}(x_j)] + h \sum_{j=1}^{n} \eta_j j^p U_{k-1}(x_j)$$
$$- \sum_{j=1}^{n} \sum_{m=1}^{k} [U_{k-m}(x_j) - U_{k-m-1}(x_j)](\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1}) \tag{16}$$

where we adopt the convention $U_{-1}(x) = 0$. Equation (16) is the discrete analog of (6); it is a two-step (leap-frog) method. The two initial conditions are deduced from (13):

$$\begin{aligned} \mathbb{Q}_n^0 &= Q_0 \\ \mathbb{Q}_n^1 &= Q_0 + hP_0 - h^2 Q_0 + h^2 \sum_{j=1}^{n} \xi_j \end{aligned} \tag{17}$$

6. DISCRETE VOLTERRA EQUATION

In analogy with the continuous case, we convert the (discrete) integro-differential equation (16) into a (discrete) integral equation. The procedure is straightforward and parallel to its continuous counterpart: it involves two summations over the discrete time index and summation by parts; the derivation is presented in Appendix C.

The resulting equation is

$$\mathbb{Q}_n^k = \mathbb{F}_n^k + h \sum_{\ell=0}^{k-1} \mathbb{K}_n^{k-\ell} \mathbb{Q}_n^\ell \tag{18}$$

$k = 0, 1, \ldots, N$, where the discrete kernel is

$$\mathbb{K}_n^k = -t_k - h \sum_{j=1}^{n} U_{k-1}(x_j) \tag{19}$$

where $t_k = kh$, $x_j = 1 - \frac{1}{2} j^{2p} h^2$, and we recall our convention that $U_{-1}(x) = 0$, thus $\mathbb{K}_n^0 = 0$. The discrete forcing is

$$\mathbb{F}_n^k = Q_0 + P_0 t_k + Q_0 \sum_{j=1}^{n} \frac{1 - [U_k(x_j) - U_{k-1}(x_j)]}{j^{2p}}$$
$$+ \sum_{j=1}^{n} \xi_j \frac{1 - [U_k(x_j) - U_{k-1}(x_j)]}{j^{2p}} + \sum_{j=1}^{n} \eta_j \left[\frac{t_k}{j^p} - h \frac{U_{k-1}(x_j)}{j^p} \right] \tag{20}$$

Equations (18), (19), and (20) are the discrete analogs of (8), (7), and (9), respectively.

7. SUMMARY OF MAIN RESULTS

The solutions Q_n, P_n of Eq. (8) are random functions, whereas the solutions $\mathbb{Q}_n$, $\mathbb{P}_n$ of Eq. (18) are N-dimensional random vectors. In both cases, the randomness stems from the random initial data ξ_j, η_j, $j=1, 2,\ldots, n$, which are independent Gaussian variables. Recall that N and n are related as $n=\lfloor(\xi/h)^{1/p}\rfloor$, $\xi \leqslant 1$, and $N=T/h$.

To analyze the limit $n, N \to \infty$, $h \to 0$ we have to construct a probability space with respect to which all random functions are defined. Consider two infinite sequences of independent Gaussian variables ξ_j, η_j, $j=1, 2,\ldots$ defined on some probability space $(\Omega, \mathscr{F}, \mathscr{P})$. For all n, Q_n and P_n are measurable mappings from Ω to some space of functions defined on $[0, T]$; similarly, $\mathbb{Q}_n$, $\mathbb{P}_n$ are measurable mappings from Ω to $\Re^N$.

To formulate our error bounds we introduce the following spaces of functions:

1. Spaces of functions defined on $[0, T]$, $C[0, T]$ and $L^p[0, T]$, with the standard corresponding norms. We will use the abbreviate notations C and L^p, respectively, but one should always keep in mind that the time interval is finite.

2. Spaces of random functions, $L^1(\Omega; C[0, T])$ and $L^2(\Omega; L^2[0, T])$, with norms

$$\|Q\|_{L^1(\Omega;\, C[0,T])} = E[\sup_{0 \leqslant t \leqslant T} |Q(t)|]$$

and

$$\|Q\|_{L^2(\Omega;\, L^2[0,T])} = \left(E\left[\int_0^T Q^2(t)\, dt\right]\right)^{1/2} \tag{21}$$

Here, we shall use the abbreviate notations, $L^1(\Omega; C)$ and $L^2(\Omega; L^2)$, respectively.

3. The space of N-dimensional (non-random) vectors, L_h^1, $N=T/h$, with norm

$$\|\mathbb{K}\|_{L_h^1} = h \sum_{k=0}^{N-1} |\mathbb{K}^k|$$

4. The space of N-dimensional random vectors, $L^2(\Omega; L_h^2)$, $N = T/h$, with norm

$$\|\mathbb{Q}\|_{L^2(\Omega;\, L_h^2)} = \left(E\left[h \sum_{k=0}^{N-1} (\mathbb{Q}^k)^2 \right] \right)^{1/2} \tag{22}$$

To relate the finite dimensional space $L^2(\Omega; L_h^2)$ to the infinite dimensional space $L^2(\Omega; L^2)$ we introduce two mapping operators: a restriction operator $r_h\colon L^2(\Omega; L^2) \mapsto L^2(\Omega; L_h^2)$ and a prolongation operator $p_h\colon L^2(\Omega; L_h^2) \mapsto L^2(\Omega; L^2)$. Specifically, r_h maps random functions $Q \in L^2(\Omega; L^2)$ into random vectors by averaging over intervals of size h,

$$(r_h Q)^k = \frac{1}{h} \int_{t_k}^{t_{k+1}} Q(s)\, ds$$

whereas p_h maps random vectors $\mathbb{Q} \in L^2(\Omega; L_h^2)$ into piecewise-constant random functions,

$$(p_h \mathbb{Q})(t) = \sum_{k=0}^{N-1} \mathbb{Q}^k \chi_k(t)$$

where $\chi_k(t)$ is the indicator function of the interval $[t_k, t_{k+1})$. These approximations are first-order accurate, which is the order of the symplectic Euler scheme.

A sequence $\mathbb{Q}_n \in L^2(\Omega; L_h^2)$ is said to converge discretely to $Q \in L^2(\Omega; L^2)$ if

$$\lim_{h \to 0} \|\mathbb{Q}_n - r_h Q\|_{L^2(\Omega;\, L_h^2)} = 0$$

and it is said to converge globally if

$$\lim_{h \to 0} \|p_h \mathbb{Q}_n - Q\|_{L^2(\Omega;\, L^2)} = 0$$

One can show that discrete and global convergence are equivalent in the current setting.

We can now formulate our main results:

Theorem 7.1. Let $p > 1/2$ and $T > 0$. The sequence Q_n converges almost surely to a limit Q, and there exists a constant $C > 0$ that depends on p and T such that

$$\|Q - Q_n\|_{L^1(\Omega;\, C)} \leqslant \frac{C}{n^{p-1/2}},$$

$$\|Q - Q_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{C}{n^{p-1/2}}$$

Furthermore, the numerical solution $\mathbb{Q}_n$ converges (discretely) to Q_n. For the range of parameters $1/2 < p < 1$ there exists a constant $C > 0$ such that

$$\|r_h Q_n - \mathbb{Q}_n\|_{L^2(\Omega;\, L^2_h)} \leqslant C\, |\log h|\, h^{2-1/p}$$

Above and below the symbol C is used repeatedly to denote positive constants that depend on the parameters p, T (and possibly Q_0 and P_0), but are independent of n and h. The proof of Theorem 7.1 is based on a sequence of auxiliary results which are listed in the following proposition:

Proposition 7.1. Let $p > 1/2$ and $T > 0$. Then:

1. $K_n \to K$ in L^1 with

$$\|K - K_n\|_{L^1} \leqslant \begin{cases} C\,\dfrac{\log n}{n^{2p-1}} & \dfrac{1}{2} < p < 1 \\[2ex] \dfrac{C}{n^{p-1/2}} & p \geqslant 1 \end{cases}$$

(Proof given in Section 8.)

2. Let R_n and R be the resolvent kernels of K_n and K, respectively:

$$R_n = K_n + K_n * R_n$$
$$R = K + K * R$$

Then, for n sufficiently large

$$\|R - R_n\|_{L^1} \leqslant \frac{(1 + \|R\|_{L^1})\, \varepsilon_n}{1 - \varepsilon_n}$$

where

$$\varepsilon_n = (1 + \|R\|_{L^1})\, \|K - K_n\|_{L^1}$$

(Proof given in Section 9.)

3. $F_n \to F$ almost surely in C with

$$\|F - F_n\|_{L^1(\Omega;\, C)} \leqslant \frac{C}{n^{p-1/2}}$$

$$\|F - F_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{C}{n^{p-1/2}}$$

$f_n \to f$ in $L^2(\Omega;\, L^2)$ with

$$\|f - f_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{C}{n^{p-1/2}}$$

(Proofs given in Section 10.)

4. $Q_n \to Q$ almost surely in L^p with

$$\|Q - Q_n\|_{L^1(\Omega;\, C)} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \left[\|F - F_n\|_{L^1(\Omega;\, C)} + \varepsilon_n \, \|F\|_{L^1(\Omega;\, C)}\right]$$

$$\|Q - Q_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \left[\|F - F_n\|_{L^2(\Omega;\, L^2)} + \varepsilon_n \, \|F\|_{L^2(\Omega;\, L^2)}\right]$$

$P_n \to P$ in $L^2(\Omega;\, L^2)$ with

$$\|P - P_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \left[\|f - f_n\|_{L^2(\Omega;\, L^2)} + \varepsilon_n \, \|f\|_{L^2(\Omega;\, L^2)}\right]$$

(Proofs given in Section 11.)

5. The discrepancy between the exact n-particle solution, Q_n, and its underresolved numerical approximation, $\mathbb{Q}_n$, is given by an expression of the form:

$$r_h Q_n - \mathbb{Q}_n = \mathbb{L}_n^{-1}(\tau_1 + \tau_2)$$

where $\mathbb{L}_n$ is a linear operator defined by

$$(\mathbb{L}_n \mathbb{Q}_n)^k = \mathbb{Q}_n^k - h \sum_{\ell=0}^{k-1} \mathbb{K}_n^{k-\ell} \mathbb{Q}_n^\ell$$

and τ_1 and τ_2 are truncation errors associated with the approximation of the kernel and the forcing, respectively. (Details presented in Section 13.)

6. For $N, n \to \infty$, $h \to 0$, such that $n^p h \leqslant 1$, the approximation (18) is stable, i.e., $\|\mathbb{L}_n^{-1}\|$ is uniformly bounded. (Proof given in Section 14.)

7. For $1/2 < p < 1$,

$$\|\tau_1\|_{L^2(\Omega;\, L^2)} \leqslant C\, |\log h|\, h^{2-1/p}$$

(Proof given in Section 15.)

8. For $1/2 < p < 1$,

$$\|\tau_2\|_{L^2(\Omega;\, L^2)} \leqslant C h^{(4/3)(1-1/4p)}$$

(Proof given in Section 16.)

8. CONVERGENCE OF THE KERNEL

In this section we analyze the kernels K_n, given by (7), and show that they form a convergent sequence in L^1; we denote the limit by K. The convergence rate depends on p; different techniques are used for each of the ranges $1/2 < p < 1$, $p = 1$, and $p > 1$.

8.1. Case I: $p > 1$

Proposition 8.1. Let $p > 1$ and $T > 0$. Then,

$$\|K - K_n\|_{L^1} \leqslant \frac{C}{n^{p-1/2}}$$

Proof. We shall show that K_n is a Cauchy sequence in L^2, which by Cauchy–Schwarz, $\|K\|_{L^1} \leqslant \sqrt{T}\, \|K\|_{L^2}$, implies convergence in L^1.

Let $m < n$, then

$$\begin{aligned}
\|K_n - K_m\|_{L^2}^2 &= \int_0^T \left[\sum_{j=m+1}^{n} \frac{\sin(j^p t)}{j^p} \right] \left[\sum_{\ell=m+1}^{n} \frac{\sin(\ell^p t)}{\ell^p} \right] dt \\
&= \sum_{j=m+1}^{n} \frac{1}{j^{2p}} \left[\frac{T}{2} - \frac{1}{4j^p} \sin(2 j^p T) \right] \\
&\quad + \sum_{j=m+1}^{n} \sum_{\ell=j+1}^{n} \left[\frac{\sin[(j^p - \ell^p)\, T]}{j^p - \ell^p} - \frac{\sin[(j^p + \ell^p)\, T]}{j^p + \ell^p} \right] \\
&\leqslant \frac{1}{2} \sum_{j=m+1}^{n} \frac{1}{j^{2p}} \left(T + \frac{1}{4} \right) + \sum_{j=m+1}^{n} \sum_{\ell=j+1}^{n} \frac{1}{j^p \ell^p} \left(\frac{1}{\ell^p - j^p} + \frac{1}{2 j^p} \right)
\end{aligned}$$

where we have split $j = \ell$ and $j \neq \ell$ terms, bounded the sine functions by 1, and used $1/j^p \leqslant 1/2$.

The first sum can be bounded by an integral:

$$\frac{1}{2}\sum_{j=m+1}^{n}\frac{1}{j^{2p}}\left(T+\frac{1}{4}\right)\leqslant\frac{1}{2}\left(T+\frac{1}{4}\right)\int_{m}^{\infty}\frac{dx}{x^{2p}}\leqslant\frac{C_1}{m^{2p-1}}$$

where

$$C_1=\frac{T+1/4}{2(2p-1)}$$

The double sum is treated as follows: first,

$$\begin{aligned}\sum_{j=m+1}^{n}\sum_{\ell=j+1}^{n}\frac{1}{j^p\ell^p}\frac{1}{\ell^p-j^p}&=\sum_{j=m+1}^{n}\frac{1}{j^p}\left(\sum_{\ell=j+1}^{\min(n,\,2j)}\frac{1}{\ell^p}\frac{1}{\ell^p-j^p}+\sum_{\ell=2j+1}^{n}\frac{1}{\ell^{2p}}\frac{1}{1-(j/\ell)^p}\right)\\
&\leqslant\sum_{j=m+1}^{n}\frac{1}{j^p}\left(\sum_{v=1}^{j}\frac{1}{(j+v)^p}\frac{1}{(j+v)^p-j^p}+2\sum_{\ell=2j+1}^{n}\frac{1}{\ell^{2p}}\right)\\
&\leqslant\sum_{j=m+1}^{n}\frac{1}{j^p}\left(\frac{1}{j^{2p}}\sum_{v=1}^{j}\frac{1}{(1+v/j)^p-1}+\frac{2}{2p-1}\frac{1}{(2j)^{2p-1}}\right)\\
&\leqslant\sum_{j=m+1}^{n}\frac{1}{j^{3p}}\sum_{v=1}^{j}\frac{j}{pv}+\frac{4}{4^p(2p-1)}\sum_{j=m+1}^{n}\frac{1}{j^{3p-1}}\\
&\leqslant\frac{1}{p}\sum_{j=m+1}^{n}\frac{1+\log j}{j^{3p-1}}+\frac{4}{4^p(2p-1)(3p-2)}\frac{1}{m^{3p-2}}\\
&\leqslant\frac{(3p-2)\log m+(3p-1)}{p(3p-2)^2}\frac{1}{m^{3p-2}}\\
&\quad+\frac{4}{4^p(2p-1)(3p-2)}\frac{1}{m^{3p-2}}\\
&\leqslant\frac{C_2}{m^{2p-1}}\end{aligned}$$

where C_2 can be chosen, for example, as

$$C_2=\frac{6p-3}{p(3p-2)^2}+\frac{4}{4^p(2p-1)(3p-2)}$$

Finally,

$$\sum_{j=m+1}^{n}\sum_{\ell=j+1}^{n}\frac{1}{2j^{2p}\ell^p}\leqslant\frac{1}{2(p-1)}\sum_{j=m+1}^{n}\frac{1}{j^{3p-1}}\leqslant\frac{C_3}{m^{3p-2}}$$

where

$$C_3 = \frac{1}{2(p-1)(3p-2)}$$

Taking $C = \sqrt{C_1 + C_2 + C_3}$ we obtain the desired result. ∎

8.2. Case II: $p = 1$

Proposition 8.2. Let $p = 1$, then

$$\|K - K_n\|_{L^1} \leqslant \frac{C}{n^{1/2}}$$

Proof. We use again the $L^2 \subset L^1$ embedding: $\|K\|_{L^1} \leqslant \sqrt{T}\, \|K\|_{L^2}$.

For $p = 1$ the functions $\sin(j^p t)$ are Fourier basis functions. Let M be an integer such that

$$2\pi(M-1) < T \leqslant 2\pi M$$

then by the orthogonality of the Fourier basis,

$$\begin{aligned}
\|K_n - K_m\|_{L^2}^2 &= \int_0^T \left| \sum_{j=m+1}^{n} \frac{\sin(jt)}{j} \right|^2 dt \\
&\leqslant \int_0^{2\pi M} \left| \sum_{j=m+1}^{n} \frac{\sin(jt)}{j} \right|^2 dt \\
&= \frac{1}{2}\,(2\pi M) \sum_{j=m+1}^{n} \frac{1}{j^2} \\
&\leqslant \frac{T + 2\pi}{2m}
\end{aligned}$$

Thus,

$$\|K - K_n\|_{L^1} \leqslant \sqrt{\frac{T(T+2\pi)}{2}}\, \frac{1}{n^{1/2}} \qquad ∎$$

8.3. Case III: $1/2 < p < 1$

This is the most delicate case as $K_n(t)$ is not uniformly bounded. Lemmas 8.1–8.5 below provide pointwise estimates for $K_n(t)$, which are then used to obtain norm estimates. To simplify notations we write

$$K_n(t) = -t - \sum_{j=1}^{n} w_t(j)$$

where

$$w_t(x) = \frac{\sin(x^p t)}{x^p}$$

Lemma 8.1. Let $1/2 < p < 1$ and $0 \leqslant t \leqslant T$, then for $x \geqslant 1$,

$$|w_t^{(k)}(x)| \leqslant \frac{C_1(k, p, t)}{x^{(k-1)(1-p)+1}}, \qquad k = 1, 2,... \tag{23}$$

where

$$C_1(k, p, t) = (2k)^k \max(1, p^k t^k)$$

Proof. We examine the first two derivatives of $w_t(x)$:

$$\begin{aligned} w_t'(x) &= (-p)\, x^{-p-1} \sin(x^p t) + (pt)\, x^{-1} \cos(x^p t) \\ w_t''(x) &= (-p)(-p-1)\, x^{-p-2} \sin(x^p t) - p(pt)\, x^{-2} \cos(x^p t) \\ &\quad - (pt)\, x^{-2} \cos(x^p t) - (pt)^2\, x^{-2+p} \sin(x^p t), \end{aligned}$$

and observe that the kth derivative is a sum of 2^k terms, each consisting of a prefactor of the form $(-p)(-p-1)\cdots(-p-q) \times (pt)^r$, where $q, r \leqslant k$, times x to some power, the largest possible power being $(k-1)(p-1)-1$, times either $\sin(x^p t)$ or $\cos(x^p t)$. The bound (23) is obtained if one replace each of the 2^k terms by its largest possible value. ∎

Lemma 8.2. Let $1/2 < p < 1$ and $0 \leqslant t \leqslant T$, and set $r = \lceil \frac{p}{2(1-p)} \rceil$. Then,

$$\left| \sum_{j=m+1}^{n} \frac{\sin(j^p t)}{j^p} \right| \leqslant \left| \int_m^n \frac{\sin(x^p t)}{x^p}\, dx \right| + \frac{C_2(p, t)}{m^{2p-1}}$$

where

$$C_2(p,t) = 1 + 2 \sum_{k=1}^{r-1} \frac{|B_{2k}|}{(2k)!} C_1(2k-1, p, t) + \frac{|B_{2r}|}{(2r)!} \frac{C_1(2r, p, t)}{(2r-1)(1-p)}$$

with B_{2k} the Bernoulli numbers.

Proof. The proof is based on the Euler–Maclaurin summation formula:[17]

$$\sum_{j=m+1}^{n} w_t(j) = \int_m^n w_t(x)\,dx + \frac{1}{2}\left[w_t(n) - w_t(m)\right] + \sum_{k=1}^{r-1} \frac{B_{2k}}{(2k)!}\left[w_t^{(2k-1)}(n) - w_t^{(2k-1)}(m)\right] - \frac{B_{2r}}{(2r)!} \sum_{j=m+1}^{n} w_t^{(2r)}(j+\theta_j)$$

where $0 < \theta_j < 1$. Substituting $w_t(x) = \sin(x^p t)/x^p$, and using the bounds established in Lemma 8.1, we get

$$\left|\sum_{j=m+1}^{n} \frac{\sin(j^p t)}{j^p}\right| \leqslant \left|\int_m^n \frac{\sin(x^p t)}{x^p}\,dx\right| + \frac{1}{m^p} + \sum_{k=1}^{r-1} \frac{|B_{2k}|}{(2k)!} C_1(2k-1, p, t) \frac{2}{m^{(2k-2)(1-p)+1}} + \frac{|B_{2r}|}{(2r)!} C_1(2r, p, t) \sum_{j=m+1}^{n} \frac{1}{j^{(2r-1)(1-p)+1}}$$

For $1/2 < p < 1$ we have $2p-1 < p$, hence $1/m^p < 1/m^{2p-1}$. Similarly, $2p-1 < (2k-2)(1-p)+1$ for $k = 1, 2, \ldots, r-1$, hence, $1/m^{(2k-2)(1-p)+1} < 1/m^{2p-1}$. For the last term, we can bound the summation by an integral, extending the upper limit of integration to infinity. This yields a term proportional to $1/m^{(2r-1)(1-p)}$, which by our choice of r can be bounded by $1/m^{2p-1}$. This completes the proof. ∎

Lemma 8.3. Let $0 < a < b$ and $0 \leqslant \gamma \leqslant 1$. Then

$$\left|\int_a^b \frac{\sin y}{y^\gamma}\,dy\right| \leqslant 2$$

Proof. We first argue that for all a, b,

$$\left|\int_a^b \frac{\sin y}{y^\gamma}\,dy\right| \leqslant \int_0^\pi \frac{\sin y}{y^\gamma}\,dy \equiv g(\gamma)$$

the reason being that in each of the intervals $[0, \pi]$, $[\pi, 2\pi]$, etc., the integrand is the product of an oscillatory function, $\sin y$, and a positive, decreasing function, $y^{-\gamma}$. As a result, $\int_0^x y^{-\gamma} \sin y\,dy$ reaches local extrema at the points $x = k\pi$, the value of each extremum being between the values of the two preceding ones. The largest value is obtained when the range of integration coincides with the first interval, $[0, \pi]$.

We then consider the function $g(\gamma)$. It is convex for $0 \leqslant \gamma \leqslant 1$, hence $g(\gamma) \leqslant (1-\gamma)\, g(0) + \gamma g(1)$. It only remains to verify that $g(0) = 2$ and $g(1) = 1.85 < 2$. ∎

Lemma 8.4. Let $0 < a < b$ and $0 \leqslant \gamma \leqslant 1$. Then

$$\left|\int_a^b \frac{\sin y}{y^\gamma}\,dy\right| \leqslant \frac{2}{a^\gamma}$$

Proof. Integrating by parts,

$$\int_a^b \frac{\sin y}{y^\gamma}\,dy = \int_a^b \frac{(1-\cos y)'}{y^\gamma}\,dy$$
$$= \frac{1-\cos b}{b^\gamma} - \frac{1-\cos a}{a^\gamma} + \gamma \int_a^b y^{-\gamma-1}(1-\cos y)\,dy$$

from which readily follows

$$\frac{1-\cos b}{b^\gamma} - \frac{1-\cos a}{a^\gamma} \leqslant \int_a^b \frac{\sin y}{y^\gamma}\,dy \leqslant \frac{1+\cos a}{a^\gamma} - \frac{1+\cos b}{b^\gamma}$$

and

$$-\frac{2}{a^\gamma} \leqslant \int_a^b \frac{\sin y}{y^\gamma}\,dy \leqslant \frac{2}{a^\gamma}$$ ∎

Lemma 8.5. Let $1/2 < p < 1$, then

$$\left|\int_m^n \frac{\sin(x^p t)}{x^p}\,dx\right| \leqslant \frac{2}{p} \min\left(\frac{1}{t^{1/p-1}}, \frac{1}{t\, m^{2p-1}}\right)$$

Proof. By a change of variables, $y = x^p t$:

$$\int_m^n \frac{\sin(x^p t)}{x^p}\,dx = \frac{1}{p t^{1/p-1}} \int_{m^p t}^{n^p t} \frac{\sin y}{y^{2-1/p}}\,dy$$

To complete the proof we use Lemmas 8.3 and 8.4, with $a = m^p t$, $b = n^p t$, and $\gamma = 2 - 1/p$. ▮

Combining together Lemmas 8.1–8.5 we have the following result:

Corollary 8.1. Let $1/2 < p < 1$ and $0 \leqslant t \leqslant T$, then

$$|K_n(t) - K_m(t)| \leqslant \frac{C_2(p,t)}{m^{2p-1}} + \frac{2}{p} \min\left(\frac{1}{t^{1/p-1}}, \frac{1}{t\, m^{2p-1}}\right) \tag{24}$$

From this pointwise estimate follows the L^1-convergence of K_n:

Proposition 8.3. Let $1/2 < p < 1$, then that

$$\|K - K_n\|_{L^1} = C \frac{\log n}{n^{2p-1}}$$

Proof. Let $m < n$; integrating inequality (24), noting that $C_2(p,t)$ is monotonically increasing in t, and that the crossover of the minimum occurs at $t = 1/m^p$, we have

$$\begin{aligned}
\|K_n - K_m\|_{L^1} &\leqslant \frac{C_2(p,T)\,T}{m^{2p-1}} + \frac{2}{p}\int_0^{1/m^p} \frac{dt}{t^{1/p-1}} + \frac{2}{p}\int_{1/m^p}^T \frac{dt}{t m^{2p-1}} \\
&= \frac{C_2(p,T)\,T}{m^{2p-1}} + \frac{2}{p}\frac{1}{(2-1/p)\,m^{2p-1}} + \frac{2}{p m^{2p-1}} \log m^p T \\
&= C \frac{\log m}{m^{2p-1}}
\end{aligned}$$

where

$$C = C_2(p,T)\,T + \frac{2}{p(2-1/p)} + \frac{2(1+\log T)}{p}$$ ▮

In the following we will also need an estimate for the rate of convergence of the integral of K_n in L^2. We define

$$\mathscr{K}_n(t) = \int_0^t K_n(s)\, ds = -\frac{1}{2} t^2 - \sum_{j=1}^{n} \frac{1-\cos(j^p t)}{j^{2p}}$$

and correspondingly, $\mathscr{K}(t) = \int_0^t K(s)\, ds$.

Proposition 8.4. Let $p > 1/2$, then

$$\|\mathscr{K} - \mathscr{K}_n\|_{L^2} \leqslant \frac{C}{n^{2p-1}}$$

Proof. Let $n > m$, then

$$|\mathscr{K}_n(t) - \mathscr{K}_m(t)| = \left| \sum_{j=m+1}^{n} \frac{1-\cos(j^p t)}{j^{2p}} \right| \leqslant 2 \sum_{j=m+1}^{n} \frac{1}{j^{2p}} \leqslant \frac{2}{2p-1} \cdot \frac{1}{m^{2p-1}}$$

Thus,

$$\|\mathscr{K} - \mathscr{K}_n\|_{L^2} \leqslant \frac{2\sqrt{T}}{2p-1} \cdot \frac{1}{n^{2p-1}} \qquad \blacksquare$$

9. THE RESOLVENT KERNEL

Having established the convergence of K_n, we study next the convergence of the corresponding resolvent kernels. Some of the results in this section can be found, e.g., in ref. 18. It is convenient to introduce a shorthand notation for convolutions. Let $K \in L^1$ and $Q \in L^p$, $1 \leqslant p \leqslant \infty$, then we define

$$(K * Q)(t) = \int_0^t K(t-s)\, Q(s)\, ds$$

This convolution is commutative and associative. Young's inequality (see e.g., ref. 18, p. 39) states that $K * Q \in L^p$ and

$$\|K * Q\|_{L^p} \leqslant \|K\|_{L^1} \, \|Q\|_{L^p} \tag{25}$$

A similar inequality holds for $Q \in C$ with the corresponding maximum-norm. Note also that

$$(1_{[0,T]} * Q)(t) = \int_0^t Q(s)\, ds$$

Proposition 9.1. Let $K \in L^1$. Then the equation

$$R = K + K * R \tag{26}$$

has a unique solution $R \in L^1$, called the resolvent of K.

Proof. We first prove uniqueness. Suppose that $R, S \in L^1$ both satisfy

$$R = K + K * R$$
$$S = K + K * S$$

Then

$$\begin{aligned} R - S &= (K + K * R) - (K + K * S) \\ &= K * R - K * S \\ &= (S - K * S) * R - (R - K * R) * S \\ &= 0 \end{aligned}$$

To prove existence we first assume that $\|K\|_{L^1} < 1$. In this case we construct the resolvent by successive approximations:

$$R^{(0)} = K$$
$$R^{(m)} = K + K * R^{(m-1)}$$

The general term can be written as

$$R^{(m)} = \sum_{j=1}^{m+1} K^{*j}$$

where K^{*j} denotes a j-fold convolution of K by itself. By Young's inequality (25), $\|K^{*j}\|_{L^1} \leqslant \|K\|_{L^1}^j$, thus $R^{(m)}$ is a Cauchy sequence in L^1 and has a limit $R \in L^1$. It still remains to show that R satisfies Eq. (26):

$$\begin{aligned} \|R - K - K * R\|_{L^1} &= \|(R - R^{(m)}) - (K - K) - K * (R - R^{(m-1)})\|_{L^1} \\ &\leqslant \|R - R^{(m)}\|_{L^1} + \|K\|_{L^1}\, \|R - R^{(m-1)}\|_{L^1} \to 0 \end{aligned}$$

We proceed to show that the assumption $\|K\|_{L^1} < 1$ is not restrictive. It is always possible to find a real number $\gamma > 0$ such that

$$\kappa(t) = e^{-\gamma t} K(t)$$

satisfies $\|\kappa\|_{L^1} < 1$ (it follows, for example, from Lebesgue's dominated convergence theorem). Set $\rho \in L^1$ to be the resolvent (proven to exist) of κ,

$$\rho = \kappa + \kappa * \rho$$

then $R(t) = e^{\gamma t} \rho(t)$ is the resolvent of $K(t)$ as

$$R(t) = e^{\gamma t} \kappa(t) + \int_0^t e^{\gamma(t-s)} \kappa(t-s)\, e^{\gamma s} \rho(s)\, ds = K(t) + (K * R)(t)$$

This completes the proof. ▮

The next theorem establishes the role of the resolvent as the solution operator of the Volterra equation.

Proposition 9.2. Let $K \in L^1$, then for every $F \in L^p$ there is a unique solution $Q \in L^p$ to the Volterra equation,

$$Q = F + K * Q$$

given by

$$Q = F + R * F$$

where R is the resolvent of K. If $F \in C$ then $Q \in C$.

Proof. Let $F \in L^p$ and define

$$Q = F + R * F$$

which by Young's inequality (25) is in L^p. Now,

$$\begin{aligned} Q - K * Q &= Q - K * (F + R * F) \\ &= Q - (K + K * R) * F \\ &= Q - R * F \\ &= F \end{aligned}$$

hence Q is a solution of the Volterra equation.

Conversely, let $Q \in L^p$ be a solution of

$$Q = F + K * Q$$

then

$$\begin{aligned} Q &= F + (R - R * K) * Q \\ &= F + R * (Q - K * Q) \\ &= F + R * F \end{aligned}$$

which proves uniqueness. The same argument holds for $F \in C$. ▮

The next theorem shows that the resolvent R is continuous with respect to K in the L^1-norm topology:

Theorem 9.1. Let $K_n \to K$ in L^1, where the K_n have resolvents R_n and K has resolvent R. Then $R_n \to R$ and for sufficiently large n

$$\|R - R_n\|_{L^1} \leqslant \frac{(1 + \|R\|_{L^1})^2 \, \|K - K_n\|_{L^1}}{1 - (1 + \|R\|_{L^1}) \, \|K - K_n\|_{L^1}}$$

Proof. The resolvents R, R_n satisfy

$$\begin{aligned} R &= K + K * R \\ R_n &= K_n + K_n * R_n \end{aligned}$$

Subtracting one equation from the other,

$$\begin{aligned} (R - R_n) &= (K - K_n) + K * R - K_n * R_n \\ &= (K - K_n) + (K - K_n) * R_n + K * (R - R_n) \end{aligned}$$

This equation can be viewed as a Volterra equation for $R - R_n$ with kernel K and forcing $(K - K_n) + (K - K_n) * R_n$. By Proposition 9.2 the solution is

$$\begin{aligned} R - R_n = {} & [(K - K_n) + (K - K_n) * R_n] \\ & + R * [(K - K_n) + (K - K_n) * R_n] \end{aligned}$$

We define an "error,"

$$E_n = (K - K_n) + R * (K - K_n) \tag{27}$$

in terms of which

$$R - R_n = E_n + R * E_n - E_n * (R - R_n) \tag{28}$$

Taking norms and using the triangle inequality we obtain

$$\|R - R_n\|_{L^1} \leqslant \frac{(1 + \|R\|_{L^1})\, \|E_n\|_{L^1}}{1 - \|E_n\|_{L^1}} \leqslant \frac{(1 + \|R\|_{L^1})\, \varepsilon_n}{1 - \varepsilon_n} \tag{29}$$

where

$$\varepsilon_n = (1 + \|R\|_{L^1})\, \|K - K_n\|_{L^1} \geqslant \|E_n\|_{L^1}$$

and n is sufficiently large such that $\varepsilon_n < 1$. ∎

In the sequel we also need a bound for $\|R_n\|_{L^1}$. Equation (28) implies

$$R_n = R - E_n - E_n * R_n$$

hence for n sufficiently large

$$\|R_n\|_{L^1} \leqslant \frac{\|R\|_{L^1} + \|E_n\|_{L^1}}{1 - \|E_n\|_{L^1}} \leqslant \frac{\|R\|_{L^1} + \varepsilon_n}{1 - \varepsilon_n} \tag{30}$$

Finally, we consider the L^2 convergence of the integral of R_n:

Proposition 9.3. Let

$$\mathscr{R}_n(t) = \int_0^t R_n(s)\, ds$$

$$\mathscr{R}(t) = \int_0^t R(s)\, ds$$

then for n sufficiently large

$$\|\mathscr{R} - \mathscr{R}_n\|_{L^2} \leqslant \frac{(1 + \|R\|_{L^1})^2\, \|\mathscr{K} - \mathscr{K}_n\|_{L^2}}{1 - (1 + \|R\|_{L^1})\, \|K - K_n\|_{L^1}}$$

Proof. Let

$$\mathscr{E}_n(t) = \int_0^t E_n(s)\, ds$$

where E_n is given by (27). Recalling that integration is equivalent to a convolution by $1_{[0,T]}$, the integration of (27) yields

$$\mathscr{E}_n = (\mathscr{K} - \mathscr{K}_n) + R * (\mathscr{K} - \mathscr{K}_n)$$

and by Young's inequality:

$$\|\mathscr{E}_n\|_{L^2} \leqslant (1 + \|R\|_{L^1}) \, \|\mathscr{K} - \mathscr{K}_n\|_{L^2}$$

Similarly, if we integrate (28) we obtain

$$(\mathscr{R} - \mathscr{R}_n) = \mathscr{E}_n + R * \mathscr{E}_n - E_n * (\mathscr{R} - \mathscr{R}_n)$$

and after taking norms:

$$\|\mathscr{R} - \mathscr{R}_n\|_{L^2} \leqslant \frac{(1 + \|R\|_{L^1}) \, \|\mathscr{E}_n\|_{L^2}}{1 - \|E_n\|_{L^1}} \leqslant \frac{(1 + \|R\|_{L^1})^2 \, \|\mathscr{K} - \mathscr{K}_n\|_{L^2}}{1 - \varepsilon_n} \quad \blacksquare$$

10. CONVERGENCE OF THE FORCING

We next investigate the convergence of the forcing functions F_n and f_n.

Proposition 10.1. Let $p > \frac{1}{2}$, then F_n converges almost surely; we denote the limit by F. The convergence is uniform on $[0, T]$, hence $F \in C$.

Proof. Consider F_n given by (9). It is the sum of four series whose (almost sure) convergence needs to be established.

1. The series $\sum_{j=1}^{\infty} j^{-2p}[1 - \cos(j^p t)]$ is non-random and converges uniformly by Weierstrass' test for uniform convergence.

2. It is well known that $\xi_j, \eta_j \sim \mathscr{O}(j^\varepsilon)$ almost surely for any $\varepsilon > 0$, that is, for almost every $\omega \in \Omega$ there exists a constant $C_\varepsilon(\omega) > 0$ such that

$$|\xi_j|, |\eta_j| \leqslant C_\varepsilon(\omega) \, j^\varepsilon, \qquad j = 1, 2, \ldots$$

(see ref. 19, p. 139). Thus by Weierstrass' test, series $\sum_{j=1}^{\infty} \xi_j j^{-2p}[1 - \cos(j^p t)]$ and $\sum_{j=1}^{\infty} \eta_j j^{-2p} \sin(j^p t)$ converge with probability one.

3. The series $\sum_{j=1}^{\infty} \eta_j / j^p$ converges almost surely if $\sum_{j=1}^{\infty} \mathrm{Var}[\eta_j / j^p] < \infty$, which is an immediate consequence of Kolmogorov's inequality (see ref. 20, p. 296). Indeed, for $p > \frac{1}{2}$,

$$\sum_{j=1}^{\infty} \mathrm{Var}\left[\frac{\eta_j}{j^p}\right] = \sum_{j=1}^{\infty} \frac{1}{j^{2p}} < \infty \quad \blacksquare$$

Having established the (almost sure) convergence of F_n, the difference between F and F_n is given by the tail of the series:

$$F - F_n = Q_0 \sum_{j=n+1}^{\infty} \frac{1-\cos(j^p t)}{j^{2p}} + \sum_{j=n+1}^{\infty} \xi_j \frac{1-\cos(j^p t)}{j^{2p}}$$
$$+ t \sum_{j=n+1}^{\infty} \frac{\eta_j}{j^p} - \sum_{j=n+1}^{\infty} \eta_j \frac{\sin(j^p t)}{j^{2p}}$$

The next two theorems establish the rate of convergence of F_n in the $L^1(\Omega; C)$ and $L^2(\Omega; L^2)$ norms.

Proposition 10.2. $F_n \to F$ in $L^1(\Omega; C)$ and

$$\|F - F_n\|_{L^1(\Omega;\, C)} \leqslant \frac{C}{n^{p-1/2}}$$

Proof. We show that F_n is a Cauchy sequence in $L^1(\Omega; C)$. Let $n > m$, then

$$\|F_n - F_m\|_{L^1(\Omega;\, C)} \leqslant I_1 + I_2 + I_3 + I_4$$

where

$$I_1 = |Q_0| \sup_{0 \leqslant t \leqslant T} \left| \sum_{j=m+1}^{n} \frac{1-\cos(j^p t)}{j^{2p}} \right|$$

$$I_2 = E\left[\sup_{0 \leqslant t \leqslant T} \left| \sum_{j=m+1}^{n} \xi_j \frac{1-\cos(j^p t)}{j^{2p}} \right| \right]$$

$$I_3 = E\left[\sup_{0 \leqslant t \leqslant T} \left| t \sum_{j=m+1}^{n} \frac{\eta_j}{j^p} \right| \right]$$

$$I_4 = E\left[\sup_{0 \leqslant t \leqslant T} \left| \sum_{j=m+1}^{n} \eta_j \frac{\sin(j^p t)}{j^{2p}} \right| \right]$$

The first term involves no expectation values and is easy to bound:

$$I_1 \leqslant 2\,|Q_0| \sum_{j=m+1}^{n} \frac{1}{j^{2p}} \leqslant \frac{2\,|Q_0|}{2p-1} \cdot \frac{1}{m^{2p-1}}$$

If ξ is a standard Gaussian variable then $E[|\xi|] = \sqrt{2/\pi}$, hence

$$I_2 \leqslant E\left[\sup_{0 \leqslant t \leqslant T} \sum_{j=m+1}^{n} |\xi_j| \frac{|1-\cos(j^p t)|}{j^{2p}} \right] \leqslant \sum_{j=m+1}^{n} \frac{2E\,|\xi_j|}{j^{2p}} \leqslant \frac{2\sqrt{2/\pi}}{2p-1} \cdot \frac{1}{m^{2p-1}}$$

and

$$I_4 \leqslant E\left[\sup_{0\leqslant t\leqslant T} \sum_{j=m+1}^{n} |\eta_j| \frac{|\sin(j^p t)|}{j^{2p}}\right] \leqslant \sum_{j=m+1}^{n} \frac{E\,|\eta_j|}{j^{2p}} \leqslant \frac{\sqrt{2/\pi}}{2p-1} \cdot \frac{1}{m^{2p-1}}$$

To bound I_3 we use the following inequality: let $X_1, X_2,\ldots$ be a sequence of independent variables that have mean 0 and variance $\sigma_1^2, \sigma_2^2,\ldots$. It follows from Cauchy–Schwarz that

$$E\left[\left|\sum_{k=n+1}^{\infty} X_k\right|\right] \leqslant \sqrt{\sum_{k=n+1}^{\infty} \sigma_k^2}$$

thus,

$$I_3 \leqslant TE\left(\left|\sum_{j=m+1}^{n} \frac{\eta_j}{j^p}\right|\right) \leqslant T\sqrt{\sum_{j=m+1}^{n} \frac{1}{j^{2p}}} \leqslant \frac{T}{\sqrt{2p-1}} \cdot \frac{1}{m^{p-1/2}}$$

This is the term which has the slowest decay rate. Collecting all four terms, we obtain the desired result. ∎

Proposition 10.3. $F_n \to F$ in $L^2(\Omega; L^2)$ and

$$\|F - F_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{C}{n^{p-1/2}}$$

Proof. Let $n > m$, then

$$\|F_n - F_m\|_{L^2(\Omega;\, L^2)} \leqslant I_1 + I_2 + I_3 + I_4$$

where

$$I_1^2 = Q_0^2 \int_0^T \left[\sum_{j=m+1}^{n} \frac{1-\cos(j^p t)}{j^{2p}}\right]^2 dt$$

$$I_2^2 = E\left\{\int_0^T \left[\sum_{j=m+1}^{n} \xi_j \frac{1-\cos(j^p t)}{j^{2p}}\right]^2 dt\right\}$$

$$I_3^2 = E\left\{\int_0^T \left[t \sum_{j=m+1}^{n} \frac{\eta_j}{j^p}\right]^2 dt\right\}$$

$$I_4^2 = E\left\{\int_0^T \left[\sum_{j=m+1}^{n} \eta_j \frac{\sin(j^p t)}{j^{2p}}\right]^2 dt\right\}$$

For I_1 we have

$$I_1^2 \leqslant Q_0^2 \int_0^T \left(\frac{2}{2p-1} \cdot \frac{1}{m^{2p-1}} \right)^2 dt \leqslant \frac{4Q_0^2 T}{(2p-1)^2} \cdot \frac{1}{m^{4p-2}}$$

For I_2, I_3, I_4 we use Fubini's theorem to interchange expectation with time integration, and then use the independence of the $\xi_j, \eta_j \sim \mathcal{N}(0, 1)$:

$$I_2^2 \leqslant \int_0^T \sum_{j=m+1}^{n} \left[\frac{1-\cos(j^p t)}{j^{2p}} \right]^2 dt \leqslant \frac{4T}{4p-1} \cdot \frac{1}{m^{4p-1}}$$

$$I_3^2 \leqslant \frac{T^3}{3} E\left[\left(\sum_{j=m+1}^{n} \frac{\eta_j}{j^p} \right)^2 \right] = \frac{T^3}{3} \sum_{j=m+1}^{n} \frac{1}{j^{2p}} \leqslant \frac{T^3}{3(2p-1)} \cdot \frac{1}{m^{2p-1}}$$

$$I_4^2 \leqslant \int_0^T \sum_{j=m+1}^{n} \left[\frac{\sin(j^p t)}{j^{2p}} \right]^2 dt \leqslant \frac{T}{4p-1} \cdot \frac{1}{m^{4p-1}}$$

I_3 has the slowest convergence rate. Collecting all four terms we obtain the desired result. ∎

For the forcing function of the momentum equation, f_n, we can only prove convergence in $L^2(\Omega; L^2)$:

Proposition 10.4. f_n converges (to f) in $L^2(\Omega; L^2)$ and

$$\|f - f_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{C}{n^{p-1/2}}$$

Proof. Let $n > m$, then from (11)

$$f_n - f_m = \sum_{j=m+1}^{n} \xi_j \frac{\sin(j^p t)}{j^p} + \sum_{j=m+1}^{n} \eta_j \frac{1-\cos(j^p t)}{j^p}$$

Taking norms,

$$\|f_n - f_m\|_{L^2(\Omega;\, L^2)} \leqslant I_1 + I_2$$

where

$$I_1^2 = E\left\{ \int_0^T \left[\sum_{j=m+1}^{n} \xi_j \frac{\sin(j^p t)}{j^p} \right]^2 dt \right\}$$

$$I_2^2 = E\left\{ \int_0^T \left[\sum_{j=m+1}^{n} \eta_j \frac{1-\cos(j^p t)}{j^p} \right]^2 dt \right\}$$

Interchanging expectation and integration,

$$I_1^2 \leqslant \int_0^T \sum_{j=m+1}^{n} \left[\frac{\sin(j^p t)}{j^p}\right]^2 dt \leqslant \frac{T}{2p-1}\frac{1}{m^{2p-1}}$$

$$I_2^2 \leqslant \int_0^T \sum_{j=m+1}^{n} \left[\frac{1-\cos(j^p t)}{j^p}\right]^2 dt \leqslant \frac{4T}{2p-1}\frac{1}{m^{2p-1}} \quad \blacksquare$$

11. CONVERGENCE OF Q_n AND P_n

In the last three sections we have shown the convergence of K_n and R_n in L^1, of F_n in $L^1(\Omega; C)$ and $L^2(\Omega; L^2)$, and of f_n in $L^2(\Omega; L^2)$. These results imply the convergence of Q_n, P_n to the solutions Q, P of the Volterra equations

$$Q = F + K * Q$$

$$P = f + K * P$$

First, the almost sure convergence of F_n implies the almost sure convergence of Q_n:

Proposition 11.1. Let $K_n \to K$ in L^1 and $F_n \to F$ almost surely in L^p. Let Q and Q_n be the respective solutions of the Volterra equations

$$Q = F + K * Q$$

$$Q_n = F_n + K_n * Q_n$$

then $Q_n \to Q$ almost surely in L^p and for sufficiently large n

$$\|Q - Q_n\|_{L^p} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} [\|F - F_n\|_{L^p} + \varepsilon_n \|F\|_{L^p}] \tag{31}$$

where as in Section 9

$$\varepsilon_n = (1 + \|R\|_{L^1}) \|K - K_n\|_{L^1}$$

A similar inequality holds with $\|\cdot\|_{L^p}$ replaced by $\|\cdot\|_C$.

Proof. By Proposition 9.2 Q and Q_n are given by

$$Q = F + R * F$$

$$Q_n = F_n + R_n * F_n$$

Subtracting one equation from another,

$$(Q - Q_n) = (F - F_n) + R_n * (F - F_n) + (R - R_n) * F \tag{32}$$

Taking norms:

$$\begin{aligned}\|Q - Q_n\|_{L^p} &\leqslant (1 + \|R_n\|_{L^1}) \, \|F - F_n\|_{L^p} + \|R - R_n\|_{L^1} \, \|F\|_{L^p} \\ &\leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \, [\|F - F_n\|_{L^p} + \varepsilon_n \, \|F\|_{L^p}]\end{aligned}$$

where we have used (30) and (29) to bound $\|R_n\|_{L^1}$ and $\|R - R_n\|_{L^1}$. ∎

Quantitative error bounds are obtained within the spaces $L^1(\Omega; C)$ and $L^2(\Omega; L^2)$:

Proposition 11.2. $Q_n \to Q$ in $L^1(\Omega; C)$ and for sufficiently large n

$$\|Q - Q_n\|_{L^1(\Omega;\, C)} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \, [\|F - F_n\|_{L^1(\Omega;\, C)} + \varepsilon_n \, \|F\|_{L^1(\Omega;\, C)}] \tag{33}$$

Proof. This follows directly from (31), with $\|\cdot\|_{L^p}$ replaced by $\|\cdot\|_C$, and after taking expectation values. ∎

Proposition 11.3. $Q_n \to Q$ in $L^2(\Omega; L^2)$ and for sufficiently large n

$$\|Q - Q_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \, [\|F - F_n\|_{L^2(\Omega;\, L^2)} + \varepsilon_n \, \|F\|_{L^2(\Omega;\, L^2)}] \tag{34}$$

Proof. This follows from (31) after squaring, taking expectation values, and using the Cauchy–Schwarz inequality. ∎

Proposition 11.4. $P_n \to P$ in $L^2(\Omega; L^2)$ and for sufficiently large n

$$\|P - P_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{1 + \|R\|_{L^1}}{1 - \varepsilon_n} \, [\|f - f_n\|_{L^2(\Omega;\, L^2)} + \varepsilon_n \, \|f\|_{L^2(\Omega;\, L^2)}] \tag{35}$$

Proof. Same as Proposition 11.3 with the substitution $Q \mapsto P$ and $F \mapsto f$. ∎

Finally, an alternative expression can be derived for the convergence of Q_n in $L^2(\Omega; L^2)$. It will be used below to interpret numerical data.

Proposition 11.5. $Q_n \to Q$ in $L^2(\Omega; L^2)$ with

$$\|Q-Q_n\|_{L^2(\Omega;\,L^2)} \leqslant (1+\|R\|_{L^1})\,\|F-F_n\|_{L^2(\Omega;\,L^2)} \\ +(|Q_0|+|Q_0|\,\|K_n\|_{L^1}+\sqrt{T}\,\|f_n\|_{L^2(\Omega;\,L^2)})\,\|\mathscr{R}-\mathscr{R}_n\|_{L^2} \quad (36)$$

Proof. Equation (32) can also be written as

$$(Q-Q_n)=(F-F_n)+R*(F-F_n)+(R-R_n)*F_n \quad (37)$$

We then observe that F_n can be expressed as

$$F_n(t)=Q_0+\int_0^t [f_n(s)-Q_0K_n(s)]\,ds$$

or equivalently,

$$F_n=Q_0 1_{[0,T]}+1_{[0,T]}*(f_n-Q_0K_n)$$

Since $(1_{[0,T]}*f)*g=f*(1_{[0,T]}*g)$ it follows that

$$\begin{aligned}(R-R_n)*F_n &= Q_0(R-R_n)*1_{[0,T]}+(R-R_n)*1_{[0,T]}*(f_n-Q_0K_n)\\ &= Q_0(\mathscr{R}-\mathscr{R}_n)+(\mathscr{R}-\mathscr{R}_n)*(f_n-Q_0K_n)\end{aligned}$$

Substituting this back into (37), we take norms, and use Young's inequality to obtain

$$\|Q-Q_n\|_{L^2(\Omega;\,L^2)} \leqslant (1+\|R\|_{L^1})\,\|F-F_n\|_{L^2(\Omega;\,L^2)} \\ +(|Q_0|+|Q_0|\,\|K_n\|_{L^1}+\|f_n\|_{L^2(\Omega;\,L^1)})\,\|\mathscr{R}-\mathscr{R}_n\|_{L^2}$$

We recover the desired results by noting that

$$\|f_n\|_{L^2(\Omega;\,L^1)} \leqslant \sqrt{T}\,\|f_n\|_{L^2(\Omega;\,L^2)} \quad \blacksquare$$

12. NONLINEAR POTENTIAL

Our results can be extended to the case where the distinguished particle is driven by a non-harmonic potential force. Let the Hamiltonian of the system be

$$H(Q_n, P_n, q, p)=\frac{1}{2}(P_n^2+Q_n^2)+V(Q_n)+\frac{1}{2}\sum_{j=1}^{n}\left[\frac{p_j^2}{m_j}+k_j(q_j-Q_n)^2\right]$$

The equations of motion are

$$\ddot{Q}_n = -Q - V'(Q_n) + \sum_{j=1}^{n} (q_j - Q_n), \qquad Q_n(0) = Q_0, \quad \dot{Q}_n(0) = P_0$$
$$j^{-2p}\ddot{q}_j = -(q_j - Q_n), \qquad q_j(0) = Q_0 + \xi_j, \quad \dot{q}_j(0) = j^p \eta_j$$

giving rise to the nonlinear Volterra equation (Miller[21])

$$Q_n = F_n - t * V'(Q_n) + K_n * Q_n \tag{38}$$

where K_n and F_n are given by (7) and (9). The limiting equation as $n \to \infty$ is

$$Q = F - t * V'(Q) + K * Q \tag{39}$$

To prove that (39) has a unique solution we view $-t * V'(Q)$ as an additional forcing term as assume that V' is globally Lipschitz, i.e., $|V'(x) - V'(y)| \leqslant L\,|x-y|$. If (39) has a solution $Q \in C$, then Proposition 9.2 implies that

$$Q = F - t * V'(Q) + R * [F - t * V'(Q)] \tag{40}$$

Conversely, if Q is a solution of (40) with $Q, F \in C$, then Q satisfies (39).

Theorem 12.1. For almost all $\omega \in \Omega$, Eq. (40) has a unique solution $Q \in C$.

Proof. We solve Eq. (40) by successive approximation:

$$Q^{(k+1)} = F - t * V'(Q^{(k)}) + R * [F - t * V'(Q^{(k)})]$$
$$Q^{(0)} = F + R * F$$

Subtracting $Q^{(k)}$ from $Q^{(k+1)}$, taking norms, and using the global Lipschitz bound, we have

$$\|Q^{(k+1)} - Q^{(k)}\|_C \leqslant L\,\|t\|_{L^1}\,(1 + \|R\|_{L^1})\,\|Q^{(k)} - Q^{(k-1)}\|_C$$

which implies the convergence of $Q^{(k)}$ by a contraction argument, provided

$$L\,\|t\|_{L^1}\,(1 + \|R\|_{L^1}) < 1$$

If this is not the case we rewrite (40) as

$$e^{-\gamma t}Q(t) = e^{-\gamma t}F(t) - (e^{-\gamma t}t) * W(t, e^{-\gamma t}Q(t))$$
$$+ (e^{-\gamma t}R(t)) * [e^{-\gamma t}F(t) - (e^{-\gamma t}t) * W(t, e^{-\gamma t}Q(t))] \tag{41}$$

where $\gamma > 0$ and $W(t,x) = e^{-\gamma t} V'(e^{\gamma t} x)$. Since $|W(t,x) - W(t,y)| \leqslant L\,|x-y|$, we can apply the previous argument and get

$$\|e^{-\gamma t}(Q^{(k+1)} - Q^{(k)})\|_C \leqslant L\,\|e^{-\gamma t} t\|_{L^1}\,(1 + \|e^{-\gamma t} R\|_{L^1})\,\|e^{-\gamma t}(Q^{(k)} - Q^{(k-1)})\|_C$$

Note that $\|e^{-\gamma t} R\|_{L^1} \leqslant \|R\|_{L^1}$ and $\|e^{-\gamma t} t\|_{L^1} \leqslant 1/\gamma^2$. The method of successive approximations will therefore converge if $\gamma^2 > L(1 + \|R\|_{L^1})$.

Finally, suppose that (41) has two solutions Q, S. Then

$$\begin{aligned} \|e^{-\gamma t}(Q-S)\|_C &\leqslant L\,\|e^{-\gamma t} t\|_{L^1}\,(1 + \|e^{-\gamma t} R\|_{L^1})\,\|e^{-\gamma t}(Q-S)\|_C \\ &\leqslant \frac{1}{\gamma^2}\,L(1 + \|R\|_{L^1})\,\|e^{-\gamma t}(Q-S)\|_C \end{aligned}$$

i.e., $Q = S$. ∎

To estimate $Q - Q_n$ we use the fact that $R_n = K_n + K_n * R_n$ and rewrite (38) as

$$Q_n = F_n - t * V'(Q_n) + R_n * [F_n - t * V'(Q_n)]$$

Subtracting this from (40) gives

$$\begin{aligned} (Q - Q_n) = (F - F_n) - t * [V'(Q) - V'(Q_n)] + R_n * (F - F_n) \\ - R_n * t * [V'(Q) - V'(Q_n)] + (R - R_n) * [F - t * V'(Q)] \end{aligned} \tag{42}$$

Following the proof of Proposition 11.1 and using that V' is Lipschitz continuous we obtain

$$\begin{aligned} \|Q - Q_n\|_{L^1(\Omega;\,C)} \leqslant (1 + \|R_n\|_{L^1})[\|F - F_n\|_{L^1(\Omega;\,C)} + L\,\|t\|_{L^1}\,\|Q - Q_n\|_{L^1(\Omega;\,C)}] \\ + \|R - R_n\|_{L^1}\,\|F - t * V'(Q)\|_{L^1(\Omega;\,C)} \end{aligned}$$

The estimates for $\|R_n\|_{L^1}$ and $\|R - R_n\|_{L^1}$ in (30) and (28) then yield

$$\begin{aligned} \|Q - Q_n\|_{L^1(\Omega;\,C)} \leqslant \frac{1 + \|R_n\|_{L^1}}{1 - \|t\|_{L^1}\,(1 + \|R_n\|_{L^1})\,L - \varepsilon_n} \\ \times \{\|F - F_n\|_{L^1(\Omega;\,C)} + \varepsilon_n\,\|F - t * V'(Q)\|_{L^1(\Omega;\,C)}\} \end{aligned}$$

for T sufficiently small. If this is not the case we multiply both sides of (42) by $e^{-\gamma t}$. Since the structure is unchanged and $e^{-\gamma t} \leqslant 1$ it follows that

$$\|e^{-\gamma t}(Q-Q_n)\|_{L^1(\Omega;C)} \leqslant \frac{1+\|R_n\|_{L^1}}{1-L\,\|e^{-\gamma t}t\|_{L^1}\,(1+\|R_n\|_{L^1})-\varepsilon_n} \times \{\|F-F_n\|_{L^1(\Omega;C)}+\varepsilon_n\,\|F-t*V'(Q)\|_{L^1(\Omega;C)}\}$$

Using the bounds for $\|F-F_n\|_{L^1(\Omega;C)}$ and ε_n from Propositions 10.2 and 11.1, and letting γ and n be sufficiently large, we conclude

$$\|Q-Q_n\|_{L^1(\Omega;C)} \leqslant \frac{e^{\gamma T}(1+\|R_n\|_{L^1})}{1-\frac{1}{\gamma^2}\,L\,\|(1+\|R_n\|_{L^1})-\varepsilon_n} \cdot \frac{C}{n^{p-\frac{1}{2}}}$$

The nonlinear case therefore has the same rate of convergence as the linear case.

13. NUMERICAL ANALYSIS

We next analyze the discrete Volterra equation (18) that results from the symplectic Euler scheme (12). The limit under consideration is the following: we take $h \to 0$ and $n \to \infty$, such that $n^p h$ remains approximately fixed: $n = \lfloor (\xi/h)^{1/p} \rfloor$, $\xi \leqslant 1$.

We compare the numerical solution $\mathbb{Q}_n^k$, $k = 0, 1,..., N-1$, $Nh = T$, with the (exact) n-particle solution $Q_n(t)$. The non-standard aspect of this analysis is that n does not remain fixed as $h \to 0$; the equations change with step size.

It is very convenient to use similar notations for both continuous and discrete systems. The continuous Volterra equation is written as

$$L_n Q_n \equiv Q_n - K_n * Q_n = F_n \tag{43}$$

where the convolution is defined as before by

$$(K_n * Q_n)(t) = \int_0^t K_n(t-s)\, Q_n(s)\, ds$$

The discrete Volterra equation is written as

$$\mathbb{L}_n \mathbb{Q}_n \equiv \mathbb{Q}_n - \mathbb{K}_n * \mathbb{Q}_n = \mathbb{F}_n \tag{44}$$

where the discrete convolution is defined analogously by

$$(\mathbb{K}_n * \mathbb{Q}_n)^k = h \sum_{\ell=0}^{k-1} \mathbb{K}_n^{k-\ell} \mathbb{Q}_n^{\ell}$$

We carry out our analysis in $L^2(\Omega; L^2)$ and $L^2(\Omega; L^2_h)$ and use mapping operators to connect the continuous and the discrete spaces; see Aubin[22] and Linz[23] for related techniques.

Definition 13.1. The restriction operator $r_h: L^2(\Omega; L^2) \mapsto L^2(\Omega; L^2_h)$ is defined by

$$(r_h Q)^k = \frac{1}{h} \int_0^T \chi_k(t)\, Q(t)\, dt, \qquad k = 0, 1, \ldots, N-1$$

where $Q \in L^2(\Omega; L^2)$, and $\chi_k(t)$ is the indicator function of the interval $[t_k, t_{k+1})$. The random variable $(r_h Q)^k$ is the cell-average of $Q(t)$ in the kth subinterval.

Definition 13.2. The prolongation operator $p_h: L^2(\Omega; L^2_h) \mapsto L^2(\Omega; L^2)$ is defined by

$$(p_h \mathbb{Q})(t) = \sum_{k=0}^{N-1} \mathbb{Q}^k \chi_k(t)$$

where $\mathbb{Q} \in L^2(\Omega; L^2_h)$. The range of p_h consists of piecewise-constant random functions.

We now establish a number of properties satisfied by the r_h and p_h:

Lemma 13.1. The restriction and prolongation operators satisfy the following properties:

1. $\|r_h\| = 1$.
2. $\|p_h\| = 1$.
3. $r_h p_h$ is the identity in $L^2(\Omega; L^2_h)$.
4. For $Q(t) = \int_0^t P(s)\, ds$, $P \in L^2(\Omega; L^2)$,

$$\|p_h r_h Q - Q\|_{L^2(\Omega; L^2)} \leqslant \|P\|_{L^2(\Omega; L^2)}\, h \tag{45}$$

Proof.

1. For all $Q \in L^2(\Omega; L^2)$:

$$\|r_h Q\|^2_{L^2(\Omega;\, L^2_h)} = E\left[h \sum_{k=0}^{N-1} [(r_h Q)^k]^2 \right]$$

$$= E\left[h \sum_{k=0}^{N-1} \frac{1}{h^2} \left(\int_0^T Q(t)\, \chi_k(t)\, dt \right)^2 \right]$$

$$\leqslant E\left[\frac{1}{h} \sum_{k=0}^{N-1} \left(\int_0^T \chi_k(t)\, dt \right) \left(\int_0^T Q^2(t)\, \chi_k(t)\, dt \right) \right]$$

$$= E\left[\sum_{k=0}^{N-1} \int_0^T Q^2(t)\, \chi_k(t)\, dt \right]$$

$$= E\left[\int_0^T Q^2(t)\, dt \right]$$

$$= \|Q\|^2_{L^2(\Omega;\, L^2)}$$

hence $\|r_h\| \leqslant 1$. Equality holds if $Q(t)$ is piecewise-constant.

2. For all $\mathbb{Q} \in L^2(\Omega; L^2_h)$:

$$\|p_h \mathbb{Q}\|^2_{L^2(\Omega;\, L^2)} = \left(E\left[h \sum_{k=0}^{N-1} (\mathbb{Q}^k)^2 \right] \right)^{1/2} = \|\mathbb{Q}\|^2_{L^2(\Omega;\, L^2_h)}$$

that is $\|p_h\| = 1$.

3. The third property is obvious.

4. Let $Q(t) = \int_0^t P(s)\, ds$, $P \in L^2(\Omega; L^2)$. The difference $p_h r_h Q - Q$ can be written in the following form:

$$(p_h r_h Q - Q)(t) = \frac{1}{h} \sum_{k=0}^{N-1} \chi_k(t) \int_{t_k}^{t_{k+1}} [Q(s) - Q(t)]\, ds$$

$$= \frac{1}{h} \sum_{k=0}^{N-1} \chi_k(t) \int_{t_k}^{t_{k+1}} \int_t^s P(\tau)\, d\tau\, ds$$

Taking norms and using Cauchy–Schwarz:

$$\begin{aligned}
\|p_h r_h Q - Q\|^2_{L^2(\Omega;\, L^2)} &= \frac{1}{h^2} E \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \left(\int_{t_k}^{t_{k+1}} \int_t^s P(\tau)\, d\tau\, ds \right)^2 dt \\
&\leqslant \frac{1}{h^2} E \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} h^2 \int_{t_k}^{t_{k+1}} \int_t^s P^2(\tau)\, d\tau\, ds\, dt \\
&\leqslant h^2 E \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} P^2(\tau)\, d\tau \\
&= h^2\, \|P\|^2_{L^2(\Omega;\, L^2)} \quad \blacksquare
\end{aligned}$$

Consider now Q_n and $\mathbb{Q}_n$ given by (43) and (44), respectively. We apply r_h to (43) and then add and subtract $\mathbb{K}_n * (r_h Q_n)$,

$$\begin{aligned}
\mathbb{L}_n * (r_h Q_n) &= r_h Q_n - \mathbb{K}_n * (r_h Q_n) \\
&= r_h (K_n * Q_n) - \mathbb{K}_n * (r_h Q_n) + r_h F_n
\end{aligned}$$

Subtracting $\mathbb{L}_n \mathbb{Q}_n = \mathbb{F}_n$ we obtain

$$\mathbb{L}_n * (r_h Q_n - \mathbb{Q}_n) = \tau_1 + \tau_2$$

where

$$\begin{aligned}
\tau_1 &= r_h (K_n * Q_n) - \mathbb{K}_n * (r_h Q_n) \\
\tau_2 &= r_h F_n - \mathbb{F}_n
\end{aligned}$$

If $\mathbb{L}_n$ is invertible then:

$$\|r_h Q_n - \mathbb{Q}_n\|_{L^2(\Omega;\, L^2_h)} \leqslant \|\mathbb{L}_n^{-1}\| \left[\|\tau_1\|_{L^2(\Omega;\, L^2_h)} + \|\tau_2\|_{L^2(\Omega;\, L^2_h)} \right]$$

The right hand side can be interpreted by the standard terminology of numerical analysis. The two terms inside the brackets are truncation errors. τ_1 is the truncation error associated with the approximation of the integral operator, and τ_2 is the truncation error associated with the forcing. The total truncation error is amplified by the discrete solution operator $\mathbb{L}_n^{-1}$. The scheme is said to be stable if $\mathbb{L}_n^{-1}$ is uniformly bounded.

14. STABILITY ANALYSIS

In this section we show that the scheme is stable, i.e., that $\mathbb{L}_n^{-1}$ is uniformly bounded. We concentrate on the range of parameters $1/2 < p < 1$ where we expect order reduction.

Proposition 14.1. Let $\mathbb{L}_n \colon L^2(\Omega; L_h^2) \mapsto L^2(\Omega; L_h^2)$ be a sequence of operators of the form

$$\mathbb{L}_n \mathbb{Q}_n = \mathbb{Q}_n - \mathbb{K}_n * \mathbb{Q}_n$$

where $\mathbb{K}_n$ is uniformly bounded in L_h^1, i.e., $\|\mathbb{K}_h\|_{L_h^1} \leqslant C < \infty$. Then the sequence $\mathbb{L}_n$ is stable.

Proof. We need to show that $\mathbb{L}_n^{-1}$ exists and has bounded norm. The proof is similar to the existence proof for the resolvent in Section 9. The equation $\mathbb{L}_n \mathbb{Q}_n = \mathbb{F}_n$ is solved by successive approximations:

$$\mathbb{Q}_n = \mathbb{F}_n + \mathbb{K}_n * \mathbb{F}_n + \mathbb{K}_n * \mathbb{K}_n * \mathbb{F}_n + \cdots$$

Suppose first that

$$\|\mathbb{K}_n\|_{L_h^1} \leqslant C < 1$$

Using the discrete Young inequality,

$$\|\mathbb{K}_n * \mathbb{Q}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant \|\mathbb{K}_n\|_{L_h^1} \, \|\mathbb{Q}_n\|_{L^2(\Omega;\, L_h^2)} \tag{46}$$

the sequence of successive approximations forms a Cauchy sequence in $L^2(\Omega; L_h^2)$, and

$$\|\mathbb{Q}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant \sum_{j=1}^{\infty} \|\mathbb{K}_n\|_{L_h^1}^j \, \|\mathbb{F}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant (1-C)^{-1} \, \|\mathbb{F}_n\|_{L^2(\Omega;\, L_h^2)}$$

that is,

$$\|\mathbb{L}_n^{-1}\| \leqslant (1-C)^{-1}$$

If $C > 1$, then there exists a $\gamma > 0$ such $\kappa_n^k = \mathbb{K}_n^k e^{-\gamma hk}$ satisfies

$$\|\kappa_n\|_{L_h^1} \leqslant C' < 1$$

Let $\mathbb{S}_n^k = \mathbb{Q}_n^k e^{-\gamma hk}$ and $\mathbb{G}_n^k = \mathbb{F}_n^k e^{-\gamma hk}$, then,

$$\mathbb{S}_n = \mathbb{G}_n + \kappa_n * \mathbb{G}_n + \kappa_n * \kappa_n * \mathbb{G}_n + \cdots$$

from which follows that

$$\|\mathbb{S}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant (1-C')^{-1} \, \|\mathbb{G}_n\|_{L^2(\Omega;\, L_h^2)}$$

and

$$\|\mathbb{Q}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant e^{\gamma T}\, \|\mathbb{S}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant (1-C')^{-1}\, e^{\gamma T}\, \|\mathbb{F}_n\|_{L^2(\Omega;\, L_h^2)}$$

hence

$$\|\mathbb{L}_h^{-1}\| \leqslant (1-C')^{-1}\, e^{\gamma T} \quad \blacksquare$$

Thus, stability boils down to whether $\mathbb{K}_n$ is a bounded sequence in L_h^1. To prove that this is indeed the case we need the following three lemmas:

Lemma 14.1. For all $0 \leqslant y < 1$ and $k = 1, 2,...,$

$$|y^2 U'_{k-1}(1-y^2)| \leqslant 2(k-1)$$

Proof. Starting from the definition of the Chebyshev polynomials,

$$U_{k-1}(x) = \frac{\sin(k \cos^{-1} x)}{\sin(\cos^{-1} x)}$$

explicit differentiation gives

$$U'_{k-1}(x) = \frac{-1}{1-x^2}\, [(k-1)\, T_k(x) - U_{k-2}(x)]$$

For $0 < x \leqslant 1$:

$$|(1-x)\, U'_{k-1}(x)| \leqslant \frac{1}{1+x}\, [(k-1)\, |T_k(x)| + |U_{k-2}(x)|] \leqslant (k-1) + (k-1)$$

where we have used bounds for $|T_k(x)|$ and $|U_{k-2}(x)|$ (see Appendix B). Setting $x = 1 - y^2$ we recover the desired result. $\blacksquare$

Lemma 14.2. For all $0 \leqslant y < 1$ and $k = 1, 2,...,$

$$|y^4 U''_{k-1}(1-y^2)| \leqslant 6(k-1) + (k^2-1)\, y$$

Proof. Let $0 < x \leqslant 1$. Differentiating $U'_{k-1}(x)$ we get

$$U''_{k-1}(x) = \frac{-3x}{(1-x^2)^2}\, [(k-1)\, T_k(x) - U_{k-2}(x)] - \frac{k^2-1}{1-x^2}\, U_{k-1}(x)$$

which immediately implies

$$|U''_{k-1}(x)| \leqslant \frac{6(k-1)}{(1-x)^2} + \frac{k^2-1}{(1-x)^{3/2}}$$

Setting $x = 1 - y^2$ and multiplying both sides by y^4 we obtain the desired result. ∎

Lemma 14.3. For all $0 \leqslant y_0 < 1$, $0 \leqslant \gamma < 1$, and $k = 1, 2, \ldots,$

$$|I_k(\gamma, y_0)| = \left| \int_0^{y_0} \frac{U_{k-1}(1-y)}{y^\gamma} \, dy \right| \leqslant \frac{\pi^2}{2^{1+\gamma}(1-\gamma)} k^{2\gamma-1}$$

Proof. Changing variables into $x = \cos^{-1}(1-y)$, this integral reduces to

$$I_k(\gamma, y_0) = \int_0^{x_0} \frac{\sin(kx)}{(1-\cos x)^\gamma} \, dx$$

where $x_0 = \cos^{-1}(1-y_0) \in [0, \pi/2)$. The integrand is the product of an oscillatory function, $\sin(kx)$, and a positive, decreasing, and convex function $(1-\cos x)^{-\gamma}$. This structure implies that $I_k(\gamma, y_0)$ reaches its maximum value after half a period of the sine function, i.e., at $x_0 = \pi/k$. Thus,

$$\begin{aligned}
|I_k(\gamma, y_0)| &\leqslant \int_0^{\pi/k} \frac{\sin(kx)}{(1-\cos x)^\gamma} \, dx \\
&= \int_0^{\pi/k} \frac{\sin(kx)}{2^\gamma \sin^{2\gamma}(x/2)} \, dx \\
&\leqslant \int_0^{\pi/k} \frac{kx}{2^\gamma (x/\pi)^{2\gamma}} \, dx \\
&= \frac{\pi^2}{2^{1+\gamma}(1-\gamma)} k^{2\gamma-1}
\end{aligned}$$

where we have estimated $\sin(kx)$ upward by kx and $\sin(x/2)$ downward by x/π. ∎

Lemma 14.4. Let $\frac{1}{2} < p < 1$, then $\mathbb{K}_n$ satisfies the pointwise estimate:

$$|\mathbb{K}_n^k| \leqslant t_k + \frac{\pi^2}{t_k^{1/p-1}} + t_k + \frac{B_2}{2} \left[64 p^2 t_k + 2\sqrt{2}\, p^2 \frac{2-p}{1-p} t_k^2 \right]$$

where B_2 is a Bernoulli number.

Proof. We write the discrete kernel as

$$\mathbb{K}_n^k = -t_k - \sum_{j=1}^{n} w_k(j)$$

where

$$w_k(x) = h\, U_{k-1}(1 - \tfrac{1}{2} x^{2p} h^2)$$

The Euler–Maclaurin formula truncated after one term is

$$\sum_{j=1}^{n} w_k(j) = \int_0^n w_k(x)\, dx + \frac{1}{2}\,[w_k(n) - w_k(0)] - \frac{B_2}{2} \sum_{j=1}^{n} w_k''(j+\theta_j)$$

where $0 < \theta_j < 1$.

We estimate the right hand side term-by-term: $w_k(n)$ and $w_k(0)$ are bounded by

$$\sup_{0 \leqslant j \leqslant n} |w_k(j)| = h \sup_{0 < x \leqslant 1} |U_{k-1}(x)| = hk = t_k \tag{47}$$

The first two derivatives of $w_k(x)$ are given by

$$w_k'(x) = -ph^3 x^{2p-1} U_{k-1}'(1 - \tfrac{1}{2} x^{2p} h^2)$$
$$w_k''(x) = -p(2p-1)\, h^3 x^{2p-2} U_{k-1}'(1 - \tfrac{1}{2} x^{2p} h^2) + p^2 h^5 x^{4p-2} U_{k-1}''(1 - \tfrac{1}{2} x^{2p} h^2)$$

Setting $\frac{1}{2} x^{2p} h^2 = y^2$ and using Lemmas 14.1 and 14.2, we find

$$\begin{aligned} |w_k''(x)| &\leqslant 2p(2p-1)\, \frac{h}{x^2}\, |y^2 U_{k-1}'(1-y^2)| + 4p^2\, \frac{h}{x^2}\, |y^4 U_{k-1}''(1-y^2)| \\ &\leqslant 2p(2p-1)\, \frac{h}{x^2}\, 2(k-1) + 4p^2\, \frac{h}{x^2}\, [6(k-1) + (k^2-1)\, 2^{-1/2} x^p h] \\ &\leqslant 32 p^2\, \frac{t_k}{x^2} + 2\sqrt{2}\, p^2\, \frac{t_k^2}{x^{2-p}} \end{aligned}$$

Thus

$$\begin{aligned} \left| \sum_{j=1}^{n} w_k''(j+\theta_j) \right| &\leqslant 32 p^2 t_k \left[1 + \int_1^\infty \frac{dx}{x^2} \right] + 2\sqrt{2}\, p^2 t_k^2 \left[1 + \int_1^\infty \frac{dx}{x^{2-p}} \right] \\ &= 64 p^2 t_k + 2\sqrt{2}\, p^2 t_k^2 \cdot \frac{2-p}{1-p} \end{aligned} \tag{48}$$

It remains to bound the integral:

$$\int_0^n w_k(x)\,dx = h\int_0^n U_{k-1}(1-\tfrac{1}{2}x^{2p}h^2)\,dx$$
$$= \frac{2^{1/2p-1}}{p}\frac{1}{h^{1/p-1}}\int_0^{\frac{1}{2}n^{2p}h^2}\frac{U_{k-1}(1-y)}{y^{1-1/2p}}\,dy$$

Lemma 14.3 with $\gamma = 1-1/2p$ gives

$$\left|\int_0^x \frac{U_{k-1}(1-y)}{y^{1-1/2p}}\,dy\right| \leqslant \frac{2p\pi^2}{2^{2-1/2p}k^{1/p-1}}$$

hence,

$$\left|\int_0^n w_k(x)\,dx\right| \leqslant \frac{\pi^2}{t_k^{1/p-1}} \tag{49}$$

Combining (47), (48), and (49) we obtain the desired bound. ∎

An immediate consequence is:

Theorem 14.1. The discrete kernels $\mathbb{K}_n$ form a bounded sequence in L_h^1, hence the sequence of discrete operators $\mathbb{L}_n$ is stable.

15. CONSISTENCY ANALYSIS: THE KERNEL

In this section we evaluate the truncation error associated with the integral operator:

$$\tau_1 = r_h(K_n * Q_n) - \mathbb{K}_n * (r_h Q_n)$$

Adding and subtracting $r_h[K_n * (p_h r_h Q_n)]$, τ_1 splits into

$$\tau_1 = \tau_{1a} + \tau_{1b}$$

where

$$\tau_{1a} = r_h[K_n * (p_h r_h Q_n)] - \mathbb{K}_n * (r_h Q_n)$$

and

$$\tau_{1b} = r_h[K_n * (Q_n - p_h r_h Q_n)]$$

The second term, τ_{1b}, can be estimated as follows:

$$\begin{aligned}\|\tau_{1b}\|_{L^2(\Omega;\, L^2_h)} &\leqslant \|r_h\|\ \|K_n\|_{L^1}\ \|Q_n - p_h r_h Q_n\|_{L^2(\Omega;\, L^2)}\\ &\leqslant \|K_n\|_{L^1}\ \|P_n\|_{L^2(\Omega;\, L^2)} h\end{aligned}$$

where we have used Lemma 13.1. Both $\|K_n\|_{L^1}$ and $\|P_n\|_{L^2(\Omega;\, L^2)}$ are uniformly bounded, thus, the convergence of τ_{1b} is first-order, which is the convergence rate of the symplectic Euler method for non-stiff systems.

To evaluate τ_{1a} we first write it in explicit form:

$$\tau_{1a}^k = \frac{1}{h}\int_{t_k}^{t_{k+1}}\int_0^t K_n(t-s)\sum_{\ell=0}^{N-1}\chi_\ell(s)(r_h Q_n)^\ell\, ds\, dt - h\sum_{\ell=0}^{k-1}\mathbb{K}_n^{k-\ell}(r_h Q_n)^\ell$$

Note that the summation in the first term can be truncated at $\ell = k$. Separating the $\ell = k$ term from the other terms,

$$\tau_{1a}^k = \Delta(r_h Q_n)^k + h\sum_{\ell=0}^{k-1}\Delta\mathbb{K}_n^{\ell-k}(r_h Q_n)^\ell$$

where

$$\Delta = \frac{1}{h}\int_{t_k}^{t_{k+1}}\int_{t_k}^t K_n(t-s)\, ds\, dt = -\frac{h^2}{6} - \sum_{j=1}^n \frac{1}{j^{3p}h}\left[\sin(j^p h) - j^p h\right]$$

and

$$\begin{aligned}\Delta\mathbb{K}_n^{k-\ell} &= \frac{1}{h^2}\int_{t_k}^{t_{k+1}}\int_{s_\ell}^{s_{\ell+1}} K_n(t-s)\, ds\, dt - \mathbb{K}_n^{k-\ell}\\ &= \sum_{j=1}^n\left[\frac{1}{j^p}\frac{\sin[(k-\ell)\,\phi_j]}{\cos(\frac{1}{2}\phi_j)} - \frac{4\sin^2(\frac{1}{2}j^p h)}{j^{3p}h^2}\sin[j^p(t_k - t_\ell)]\right]\end{aligned}$$

Using the triangle inequality, the discrete Young inequality (46), and the boundedness of r_h, we obtain

$$\|\tau_{1a}\|_{L^2(\Omega;\, L^2_h)} \leqslant (|\Delta| + \|\Delta\mathbb{K}_n\|_{L^1_h})\ \|Q_n\|_{L^2(\Omega;\, L^2)}$$

By Taylor's expansion $|\sin(j^p h) - j^p h| \leqslant \frac{1}{6}j^{3p}h^3$, hence

$$|\Delta| \leqslant \frac{h^2}{6} + \sum_{j=1}^n \frac{1}{j^{3p}h}\frac{j^{3p}h^3}{6} = \frac{h^2}{6} + \frac{nh^2}{6} \leqslant Ch^{2-1/p}$$

It remains to evaluate $\|\varDelta\mathbb{K}_n\|_{L^1_h}$ which is what we undertake next. To simplify notations, we write $\varDelta\mathbb{K}_n$ as

$$\varDelta\mathbb{K}_n^k = \sum_{j=1}^{n} w_k(j) = w_k(1) + \sum_{j=2}^{n} w_k(j)$$

where

$$w_k(x) = \frac{1}{x^p}\left\{\frac{\sin[2k\sin^{-1}(\frac{1}{2}x^p h)]}{\sqrt{1-(\frac{1}{2}x^p h)^2}} - \frac{\sin^2(\frac{1}{2}x^p h)}{(\frac{1}{2}x^p h)^2}\sin(kx^p h)\right\} \tag{50}$$

and use the Euler–Maclaurin formula:

$$\sum_{j=1}^{n} w_k(j) = \int_1^n w_k(x)\,dx + \frac{1}{2}[w_k(n) + w_k(1)]$$
$$+\sum_{m=1}^{r-1}\frac{B_{2m}}{(2m)!}[w_k^{(2m-1)}(n) - w_k^{(2m-1)}(1)] - \frac{B_{2r}}{(2r)!}\sum_{j=2}^{n} w_k^{(2r)}(j+\theta_j) \tag{51}$$

where $0 < \theta_j < 1$ and r is determined below. We have separated $w_k(1)$ from the rest of the sum to avoid function evaluations at the origin.

We now make the following observation: the functions

$$\frac{1}{\sqrt{1-z^2}} \quad \text{and} \quad \frac{\sin^2 z}{z^2}$$

are both of the form $1 + g_2(z)$, where $g_2(z)$ represents a generic expression for a function that is analytic at $|z| < 1$ and has a double root at the origin. In particular, for every function $g_2(z)$ in this class there exists a constant $C > 0$ such that

$$|g_2(z)| \leqslant C\,|z|^2 \tag{52}$$

for $|z| \leqslant 1/2$. This abstract notation implies the following algebraic equivalences: $g_2(z) \pm g_2(z) \sim g_2(z)$, $\alpha g_2(z) \sim g_2(z)$, and $zg_2'(z) \sim g_2(z)$. Also, let the function trig(z) represent any of the trigonometric functions $\pm\sin(z)$ or $\pm\cos(z)$. Then, $w_k(x)$, given by (50), is of the form

$$w_k(x) = w_{k,1}(x) + w_{k,2}(x) + w_{k,3}(x)$$

where

$$w_{k,1}(x) = x^{-\alpha p}\{\text{trig}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] - \text{trig}[kx^p h]\}$$
$$w_{k,2}(x) = x^{-\alpha p}\, \text{trig}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] \cdot g_2(\tfrac{1}{2}x^p h)$$
$$w_{k,3}(x) = x^{-\alpha p}\, \text{trig}(kx^p h) \cdot g_2(\tfrac{1}{2}x^p h)$$

and $\alpha = 1$. We have introduced the parameter $\alpha \in [1, 2]$ to exploit the present analysis in the next section as well.

By Taylor's expansion

$$2 \sin^{-1}(\tfrac{1}{2}z) = z + \frac{\theta z}{4(1 - \frac{1}{4}\theta^2 z^2)^{3/2}} \frac{z^2}{2}$$

for some $0 < \theta < 1$, hence

$$|2 \sin^{-1}(\tfrac{1}{2}z) - z| \leqslant \tfrac{1}{4}|z|^3, \qquad |z| \leqslant 1$$

Combined with the trigonometric identity,

$$\text{trig}(a) - \text{trig}(b) = 2\, \text{trig}'[\tfrac{1}{2}(a+b)] \cdot \sin[\tfrac{1}{2}(a-b)]$$

we get

$$|\text{trig}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] - \text{trig}(kx^p h)| \leqslant \min(2, \tfrac{1}{4}kx^{3p}h^3) \tag{53}$$

We proceed to evaluate the various terms in the Euler–Maclaurin formula (51). Using (52), (53), and the boundedness of trig(x),

$$|w_{k,1}(1)| \leqslant 1 \cdot \tfrac{1}{4}kh^3 \leqslant Ch^2$$
$$|w_{k,1}(n)| \leqslant n^{-\alpha p} \cdot 2 \leqslant 2h^\alpha$$
$$|w_{k,2}(1)|, |w_{k,3}(1)| \leqslant 1 \cdot 1 \cdot Ch^2 \leqslant Ch^2$$
$$|w_{k,2}(n)|, |w_{k,3}(n)| \leqslant n^{-\alpha p} \cdot 1 \cdot C \leqslant Ch^\alpha$$

hence,

$$|w_k(n)| + |w_k(1)| \leqslant Ch^\alpha \tag{54}$$

Next we evaluate the derivatives of $w_k(x)$. We start with $w_{k,3}(x)$ and note that its first derivative can be recast in the following form:

$$w'_{k,3}(x) = \frac{1}{x^{\alpha p}} \left\{ \frac{1}{x}\, \text{trig}(kx^p h) \cdot g_2(\tfrac{1}{2}x^p h) + \frac{t_k}{x^{1-p}}\, \text{trig}'(kx^p h) \cdot g_2(\tfrac{1}{2}x^p h) \right\} \tag{55}$$

where we have used the properties of the class of functions $g_2(z)$. One can prove by induction that

$$w_{k,3}^{(m)}(x) = \frac{1}{x^{\alpha p}} \sum_{s=0}^{m} \binom{m}{s} \frac{t_k^s}{x^{s(1-p)+(m-s)}} \operatorname{trig}^{(s)}(kx^p h) \cdot g_2(\tfrac{1}{2}x^p h)$$

which leads to the following estimate:

$$|w_{k,3}^{(m)}(x)| \leqslant \frac{1}{x^{\alpha p}} \sum_{s=0}^{m} \binom{m}{s} \frac{t_k^s \cdot 1 \cdot C x^{2p} h^2}{x^{s(1-p)+(m-s)}} \leqslant C(1+t_k)^m \frac{x^{2p}h^2}{x^{m(1-p)+\alpha p}} \tag{56}$$

where we have used the fact that $m(1-p) \leqslant s(1-p)+(m-s)$ for $s \leqslant m$ and $1/2 < p < 1$.

Examining $w_{k,2}(x)$ we see that it has the same structure as $w_{k,3}(x)$, hence by the same arguments,

$$w_{k,2}^{(m)}(x) = \frac{1}{x^{\alpha p}} \sum_{s=0}^{m} \binom{m}{s} \frac{t_k^s}{x^{s(1-p)+(m-s)}} \operatorname{trig}^{(s)}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] \cdot g_2(\tfrac{1}{2}x^p h)$$

and

$$|w_{k,2}^{(m)}(x)| \leqslant C(1+t_k)^m \frac{x^{2p}h^2}{x^{m(1-p)+\alpha p}} \tag{57}$$

The term $w_{k,1}(x)$ requires more attention. Differentiating it once we obtain

$$\begin{aligned} w'_{k,1}(x) = {} & -\alpha p x^{-\alpha p-1}\{\operatorname{trig}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] - \operatorname{trig}(kx^p h)\} \\ & + p t_k x^{-\alpha p+(p-1)} \operatorname{trig}'[2k \sin^{-1}(\tfrac{1}{2}x^p h)] \cdot [1 - \tfrac{1}{4}x^{2p}h^2]^{-1/2} \\ & - p t_k x^{-\alpha p+(p-1)} \operatorname{trig}'(kx^p h) \end{aligned}$$

Noting that $[1-\frac{1}{4}x^{2p}h^2]^{-1/2} = 1 + g_2(\frac{1}{2}x^p h)$, this can be rewritten as

$$\begin{aligned} w'_{k,1}(x) = {} & -\alpha p x^{-\alpha p-1}\{\operatorname{trig}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] - \operatorname{trig}(kx^p h)\} \\ & + p t_k x^{-\alpha p+(p-1)}\{\operatorname{trig}'[2k \sin^{-1}(\tfrac{1}{2}x^p h)] - \operatorname{trig}'(kx^p h)\} + w'_{k,2}(x) \end{aligned}$$

where the last term represents an expression *of the same form* as one of the terms in $w'_{k,2}(x)$. By induction,

$$\begin{aligned} w_{k,1}^{(m)}(x) = {} & \frac{1}{x^{\alpha p}} \sum_{s=0}^{m} \binom{m}{s} C_s \frac{t_k^s}{x^{s(1-p)+(m-s)}} \\ & \times \{\operatorname{trig}^{(s)}[2k \sin^{-1}(\tfrac{1}{2}x^p h)] - \operatorname{trig}^{(s)}(kx^p h)\} + w_{k,2}^{(m)}(x) \end{aligned}$$

where the C_s are constants that depend on α, p, and s. Using (53) and (56),

$$|w_{k,1}^{(m)}(x)| \leqslant C(1+t_k)^m \frac{1}{x^{m(1-p)+\alpha p}} \min(1, kx^{3p}h^3) + |w_{k,2}^{(m)}(x)|$$

which combined with (56) and (57) gives

$$|w_k^{(m)}(x)| \leqslant C(1+t_k)^m \frac{1}{x^{m(1-p)+\alpha p}} [x^{2p}h^2 + \min(1, kx^{3p}h^3)] \tag{58}$$

and in particular,

$$|w_k^{(m)}(1)| \leqslant C(1+t_k)^{m+1} h^2 \leqslant Ch^\alpha$$

$$|w_k^{(m)}(n)| \leqslant C(1+t_k)^m h^{\alpha+m(1/p-1)} \leqslant Ch^\alpha$$

Let r be fixed, then there exists a constant $C > 0$ such that

$$\left| \sum_{m=1}^{r-1} \frac{B_{2m}}{(2m)!} [w_k^{(2m-1)}(n) - w_k^{(2m-1)}(1)] \right| \leqslant Ch^\alpha \tag{59}$$

Setting now $m = 2r$ and $x \geqslant 1$,

$$|w_k^{(2r)}(x)| \leqslant C(1+t_k)^{2r} \frac{x^{2p}h^2 + kx^{3p}h^3}{x^{2r(1-p)+\alpha p}} \leqslant C(1+t_k)^{2r+1} \frac{x^{3p}h^2}{x^{2r(1-p)+\alpha p}}$$

If $r > [1+p(3-\alpha)]/2(1-p)$ then a crude estimate gives

$$\frac{B_{2r}}{(2r)!} \left| \sum_{j=2}^{n} w_k^{(2r)}(j+\theta_j) \right| \leqslant C(1+t_k)^{2r+1} h^2 \sum_{j=2}^{n} \frac{1}{j^{2r(1-p)+(\alpha-3)p}}$$

$$\leqslant C(1+t_k)^{2r+1} h^2 \tag{60}$$

It remains to evaluate $\int_1^n w_k(x)\,dx$. Changing variables into $y = \frac{1}{2}x^p h$ we get

$$\int_1^n w_{k,1}(x)\,dx + \int_1^n w_{k,2}(x)\,dx + \int_1^n w_{k,3}(x)\,dx \equiv I_1 + I_2 + I_3$$

where

$$I_1 = Ch^{\alpha-1/p} \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \frac{1}{y^{1+\alpha-1/p}} \{\mathrm{trig}[2k \sin^{-1}(y)] - \mathrm{trig}[2ky]\}\, dy$$

$$I_2 = Ch^{\alpha-1/p} \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \frac{g_2(y)}{y^{1+\alpha-1/p}} \mathrm{trig}[2k \sin^{-1}(y)]\, dy$$

$$I_3 = Ch^{\alpha-1/p} \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \frac{g_2(y)}{y^{1+\alpha-1/p}} \mathrm{trig}(2ky)\, dy$$

We start with I_3. Using $\mathrm{trig}''(x) = -\mathrm{trig}(x)$ we write it as follows:

$$I_3 = Ch^{\alpha-1/p} \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \frac{g_2(y)}{y^{1+\alpha-1/p}} \left[-\frac{\mathrm{trig}'(2ky)}{2k} \right]' dy$$

Integrating by parts we find

$$I_3 = -\frac{C}{2k} h^{\alpha-1/p} \left[\frac{g_2(y)}{y^{1+\alpha-1/p}} \mathrm{trig}'(2ky) \right]_{\frac{1}{2}h}^{\frac{1}{2}n^p h} + \frac{C}{2k} h^{\alpha-1/p} \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \left[\frac{g_2(y)}{y^{1+\alpha-1/p}} \right]' \mathrm{trig}'(2ky)\, dy$$

Since $y^{-(1+\alpha-1/p)} g_2(y)$ is uniformly bounded on $(0, 1/2]$, and $|[y^{-(1+\alpha-1/p)} g_2(y)]'|$ is integrable,

$$|I_3| \leqslant \frac{C}{2k} h^{\alpha-1/p}$$

Consider next I_2: changing variables, $z = \sin^{-1}(y)$, we obtain

$$I_2 = Ch^{\alpha-1/p} \int_{\sin^{-1}(\frac{1}{2}h)}^{\sin^{-1}(\frac{1}{2}n^p h)} \frac{g_2(\sin z) \cos z}{(\sin z)^{1+\alpha-1/p}} \mathrm{trig}(2kz)\, dz$$

Noting that

$$g_2(\sin z) \sim g_2(z)$$

$$\cos z \sim 1 + g_2(z)$$

$$(\sin z)^{-(1+\alpha-1/p)} \sim z^{-(1+\alpha-1/p)}[1 + g_2(z)]$$

we can write

$$I_2 = Ch^{\alpha-1/p} \int_{\sin^{-1}(\frac{1}{2}h)}^{\sin^{-1}(\frac{1}{2}n^p h)} \frac{g_2(z)}{z^{1+\alpha-1/p}} \mathrm{trig}(2kz)\, dz$$

Since $[\sin^{-1}(\frac{1}{2}h), \sin^{-1}(\frac{1}{2}n^p h)] \subset [h/2, \pi/6]$ then I_2 has the same structure as I_3 and

$$|I_2| \leqslant \frac{C}{k}\, h^{\alpha-1/p}$$

Consider I_1: changing variables $z = \sin^{-1}(y)$ only in the first term and using again the equivalence relations of functions in the class $g_2(z)$, we get

$$I_1 = Ch^{\alpha-1/p}\left\{\int_{\sin^{-1}(\frac{1}{2}h)}^{\sin^{-1}(\frac{1}{2}n^p h)} \frac{\mathrm{trig}(2kz)}{z^{1+\alpha-1/p}}\, dz - \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \frac{\mathrm{trig}(2ky)}{y^{1+\alpha-1/p}}\, dz\right\}$$

$$+ Ch^{\alpha-1/p} \int_{\frac{1}{2}h}^{\frac{1}{2}n^p h} \frac{g_2(y)}{y^{1+\alpha-1/p}}\, \mathrm{trig}(2ky)\, dz$$

The last term is of the same form as I_3; the first two terms differ only in their ranges of integration, hence

$$I_1 = Ch^{\alpha-1/p}\left\{\int_{\sin^{-1}(\frac{1}{2}h)}^{\frac{1}{2}h} \frac{\mathrm{trig}(2kz)}{z^{1+\alpha-1/p}}\, dz + \int_{\frac{1}{2}n^p h}^{\sin^{-1}(\frac{1}{2}n^p h)} \frac{\mathrm{trig}(2kz)}{z^{1+\alpha-1/p}}\, dz\right\} + I_3$$

The first integral can be estimated directly, using $|\frac{1}{2}h - \sin^{-1}(\frac{1}{2}h)| \leqslant Ch^3$,

$$\left| h^{\alpha-1/p} \int_{\sin^{-1}(\frac{1}{2}h)}^{\frac{1}{2}h} \frac{\mathrm{trig}(2kz)}{z^{1+\alpha-1/p}}\, dz \right| \leqslant Ch^3 \frac{h^{\alpha-1/p}}{h^{1+\alpha-1/p}} \leqslant Ch^2$$

The second integral can be bounded using integration by parts:

$$\left| h^{\alpha-1/p} \int_{\sin^{-1}(\frac{1}{2}n^p h)}^{\frac{1}{2}n^p h} \frac{\mathrm{trig}(2kz)}{z^{1+\alpha-1/p}}\, dz \right| \leqslant \frac{C}{k}\, h^{\alpha-1/p}$$

Combining I_1, I_2, and I_3,

$$\left| \int_1^n w_k(x)\, dx \right| \leqslant \frac{C}{k}\, h^{\alpha-1/p} \tag{61}$$

We collect (54), (59), (60), and (61), which we substitute into the Euler–Maclaurin summation formula (51). Since for $p < 1$

$$h^\alpha = h^{\alpha-1/p} \frac{h^{1/p} k}{k} \leqslant C\, \frac{h^{\alpha-1/p}}{k}$$

we end up with a simple pointwise estimate:

$$\left|\sum_{j=1}^{n} w_k(j)\right| \leqslant C \frac{h^{\alpha-1/p}}{k} \tag{62}$$

The corresponding L_h^1 norm satisfies:

$$\left\|\sum_{j=1}^{n} w_k(j)\right\|_{L_h^1} \leqslant Ch^{\alpha-1/p} \cdot h \sum_{k=1}^{N-1} \frac{1}{k} \leqslant Ch^{1+\alpha-1/p}(1+\log N)$$

Setting $\alpha = 1$ we conclude:

Proposition 15.1. Let $1/2 < p < 1$, then for h sufficiently small

$$\|\varDelta \mathbb{K}_n\|_{L_h^1} \leqslant Ch^{2-1/p} \, |\log h|$$

16. CONSISTENCY ANALYSIS: THE FORCING

In this section we evaluate the truncation error associated with the forcing:

$$\tau_2 = r_h F_n - \mathbb{F}_n$$

Substituting F_n, given by (9), we obtain

$$\begin{aligned}
(r_h F_n)^k = {} & Q_0 + P_0 \frac{(t_k+h)^2 - t_k^2}{2h} \\
& + Q_0 \sum_{j=1}^{n} \frac{1 - \frac{2}{j^p h} \cos[(k+\frac{1}{2})\, j^p h] \sin(\frac{1}{2} j^p h)}{j^{2p}} \\
& + \sum_{j=1}^{n} \xi_j \frac{1 - \frac{2}{j^p h} \cos[(k+\frac{1}{2})\, j^p h] \sin(\frac{1}{2} j^p h)}{j^{2p}} \\
& + \sum_{j=1}^{n} \eta_j \left[\frac{(t_k+h)^2 - t_k^2}{2 j^p h} - \frac{2}{j^{3p} h} \sin[(k+\tfrac{1}{2})\, j^p h] \sin(\tfrac{1}{2} j^p h) \right]
\end{aligned}$$

$k = 0, 1, \ldots, N-1$, from which we subtract $\mathbb{F}_n^k$, given by (20). Using relations (15) to express the Chebyshev polynomials in terms of trigonometric functions, we can write τ_2 as the sum of five terms:

$$\tau_2 = \varDelta_1 + \varDelta_2 + \varDelta_3 + \varDelta_4 + \varDelta_5$$

where

$$\Delta_1^k = -\frac{1}{2}\, h P_0$$

$$\Delta_2^k = 2Q_0 \sum_{j=1}^{n} \frac{1}{j^{3p}h} \{\cos[(k+\tfrac{1}{2})\, j^p h] \sin(\tfrac{1}{2} j^p h) - \cos[(k+\tfrac{1}{2})\, \phi_j] \tan(\tfrac{1}{2}\phi_j)\}$$

$$\Delta_3^k = 2 \sum_{j=1}^{n} \xi_j \frac{1}{j^{3p}h} \{\cos[(k+\tfrac{1}{2})\, j^p h] \sin(\tfrac{1}{2} j^p h) - \cos[(k+\tfrac{1}{2})\, \phi_j] \tan(\tfrac{1}{2}\phi_j)\}$$

$$\Delta_4^k = \frac{h}{2} \sum_{j=1}^{n} \frac{\eta_j}{j^p}$$

$$\Delta_5^k = 2 \sum_{j=1}^{n} \eta_j \frac{1}{j^{3p}h} \{\sin[(k+\tfrac{1}{2})\, j^p h] \sin(\tfrac{1}{2} j^p h) - \sin(k\phi_j) \tan(\tfrac{1}{2}\phi_j)\}$$

and $\phi_j = 2 \sin^{-1}(\tfrac{1}{2} j^p h)$.

The first and fourth terms are easy to evaluate:

$$\|\Delta_1\|_{L^2(\Omega;\, L_h^2)} = \left[h \sum_{k=1}^{N-1} (\Delta_1^k)^2 \right]^{1/2} = Ch \tag{63}$$

and

$$\|\Delta_4\|_{L^2(\Omega;\, L_h^2)} = \left[h \sum_{k=1}^{N-1} E(\Delta_4^k)^2 \right]^{1/2} = \left[T \frac{h^2}{4} \sum_{j=1}^{n} \frac{1}{j^{2p}} \right]^{1/2}$$
$$\leqslant Ch \left[1 + \int_1^\infty \frac{dx}{x^{2p}} \right]^{1/2} = Ch \tag{64}$$

where we have used the independence of the Gaussian variables η_j.

Consider now Δ_2^k, which we split as follows,

$$\Delta_2^k = Q_0 \sum_{j=1}^{n} \frac{1}{j^{2p}} \{\cos[(k+\tfrac{1}{2})\, j^p h] - \cos[(k+\tfrac{1}{2})\, \phi_j]\}$$
$$+ Q_0 \sum_{j=1}^{n} \frac{1}{j^{2p}} \cos[(k+\tfrac{1}{2})\, j^p h] \cdot \left[\frac{\sin(\tfrac{1}{2} j^p h)}{\tfrac{1}{2} j^p h} - 1 \right]$$
$$+ Q_0 \sum_{j=1}^{n} \frac{1}{j^{2p}} \cos[(k+\tfrac{1}{2})\, \phi_j] \cdot \left[1 - \frac{1}{\sqrt{1 - (\tfrac{1}{2} j^p h)^2}} \right]$$

and identify as being of the form $\sum_{j=1}^{n} w_k(j)$, where $w_k(j)$ has the same structure as in the previous section but with $\alpha = 2$. Thus, we can use the pointwise estimate (62) to deduce

$$|\Delta_2^k| \leqslant C\,\frac{h^{2-1/p}}{k}$$

and consequently,

$$\|\Delta_2\|_{L^2(\Omega;\, L_h^2)} \leqslant Ch^{2-1/p} \cdot \left(h \sum_{k=1}^{N-1} \frac{1}{k^2} \right)^{1/2} \leqslant Ch^{2-1/p+1/2} \tag{65}$$

We next consider Δ_3, which we split in a similar way:

$$\begin{aligned}
\Delta_3^k = {} & \sum_{j=1}^{n} \xi_j \frac{1}{j^{2p}} \{\cos[(k+\tfrac{1}{2})\, j^p h] - \cos[(k+\tfrac{1}{2})\, \phi_j]\} \\
& + \sum_{j=1}^{n} \xi_j \frac{1}{j^{2p}} \cos[(k+\tfrac{1}{2})\, j^p h] \cdot \left[\frac{\sin(\frac{1}{2} j^p h)}{\frac{1}{2} j^p h} - 1 \right] \\
& + \sum_{j=1}^{n} \xi_j \frac{1}{j^{2p}} \cos[(k+\tfrac{1}{2})\, \phi_j] \cdot \left[1 - \frac{1}{\sqrt{1-(\frac{1}{2} j^p h)^2}} \right] \\
= {} & \Delta_{3a}^k + \Delta_{3b}^k + \Delta_{3c}^k
\end{aligned}$$

Using the fact that the ξ_j are independent and normally distributed,

$$\begin{aligned}
\|\Delta_{3a}\|^2_{L^2(\Omega;\, L_h^2)} &= h \sum_{k=0}^{N-1} \sum_{j=1}^{n} \left[\frac{1}{j^{2p}} \{\cos[(k+\tfrac{1}{2})\, j^p h] - \cos[(k+\tfrac{1}{2})\, \phi_j]\} \right]^2 \\
&\leqslant h \sum_{k=0}^{N-1} \sum_{j=1}^{n} \left\{ \frac{1}{j^{2p}} \min[2, \tfrac{1}{4}(k+\tfrac{1}{2})\, j^{3p} h^3] \right\}^2
\end{aligned}$$

where we have used (53). We can break this summation, say, at $n^{2/3}$, which gives

$$\begin{aligned}
\|\Delta_{3a}\|^2_{L^2(\Omega;\, L_h^2)} &\leqslant h \sum_{k=0}^{N-1} \sum_{j=1}^{n^{2/3}} [\tfrac{1}{4}(k+\tfrac{1}{2})\, j^p h^3]^2 + h \sum_{k=0}^{N-1} \sum_{j=n^{2/3}+1}^{n} \left(\frac{2}{j^{2p}} \right)^2 \\
&\leqslant Ch^4 \left(\int_0^{n^{2/3}} x^{2p}\, dx \right) + C \left(\int_{n^{2/3}}^{\infty} \frac{dx}{x^{4p}} \right) \\
&= Ch^4 n^{(2/3)(2p+1)} + C\, \frac{1}{n^{(2/3)(4p-1)}} \leqslant Ch^{(4/3)(2-1/2p)}
\end{aligned}$$

thus

$$\|\Delta_{3a}\|_{L^2(\Omega;\,L_h^2)} \leqslant Ch^{(4/3)(1-1/4p)}$$

The terms Δ_{3b} and Δ_{3c} are even easier to estimate:

$$\|\Delta_{3b}\|_{L^2(\Omega;\,L_h^2)},\ \|\Delta_{3c}\|_{L^2(\Omega;\,L_h^2)} \leqslant \left\{ h \sum_{k=1}^{N-1} \sum_{j=1}^{n} \left[\frac{1}{j^{2p}} \cdot Cj^{2p}h^2 \right]^2 \right\}^{1/2}$$

$$= C(h^4 n)^{1/2} \leqslant Ch^{2(1-1/4p)}$$

Collecting Δ_{3a}, Δ_{3b}, and Δ_{3c}:

$$\|\Delta_3\|_{L^2(\Omega;\,L_h^2)} \leqslant Ch^{(4/3)(1-1/4p)} \tag{66}$$

It remains to evaluate Δ_5, which we split again as follows:

$$\begin{aligned}
\Delta_5^k &= \sum_{j=1}^{n} \eta_j \frac{1}{j^{2p}} \{\sin[(k+\tfrac{1}{2})\, j^p h] - \sin(k\phi_j)\} \\
&\quad + \sum_{j=1}^{n} \eta_j \frac{1}{j^{2p}} \sin[(k+\tfrac{1}{2})\, j^p h] \cdot \left[\frac{\sin(\frac{1}{2} j^p h)}{\frac{1}{2} j^p h} - 1 \right] \\
&\quad + \sum_{j=1}^{n} \eta_j \frac{1}{j^{2p}} \sin(k\phi_j) \cdot \left[1 - \frac{1}{\sqrt{1-(\frac{1}{2} j^p h)^2}} \right] \\
&= \Delta_{5a}^k + \Delta_{5b}^k + \Delta_{5c}^k
\end{aligned}$$

The terms Δ_{5b} and Δ_{5c} are similar to Δ_{3b} and Δ_{3c}, hence

$$\|\Delta_{5b}\|_{L^2(\Omega;\,L_h^2)},\ \|\Delta_{5c}\|_{L^2(\Omega;\,L_h^2)} \leqslant Ch^{2(1-1/4p)}$$

To evaluate Δ_{5a} we have to split it once more. Using the trigonometric identity,

$$\sin[(k+\tfrac{1}{2})\, x] = \sin(kx) - 2\sin(kx)\sin^2(\tfrac{1}{4}x) + \cos(kx)\sin(\tfrac{1}{2}x)$$

we get

$$\begin{aligned}
\Delta_{5a}^k &= \sum_{j=1}^{n} \eta_j \frac{1}{j^{2p}} [\sin(kj^p h) - \sin(k\phi_j)] - 2 \sum_{j=1}^{n} \eta_j \frac{1}{j^{2p}} \sin(kj^p h) \sin^2(\tfrac{1}{4} j^p h) \\
&\quad + \sum_{j=1}^{n} \eta_j \frac{1}{j^{2p}} \cos(kj^p h) \sin(\tfrac{1}{2} j^p h) \\
&= \Delta_{5a_1}^k + \Delta_{5a_2}^k + \Delta_{5a_3}^k
\end{aligned}$$

Each of these three terms is now straightforward to estimate, yielding

$$\|\Delta_{5a}\|_{L^2(\Omega;\, L_h^2)} \leqslant Ch^{(4/3)(1-1/4p)}$$

which together with Δ_{5b} and Δ_{5c} implies

$$\|\Delta_5\|_{L^2(\Omega;\, L_h^2)} \leqslant Ch^{(4/3)(1-1/4p)} \tag{67}$$

Collecting (63), (64), (65), (66), and (67) we can summarize this section as follows:

Proposition 16.1. Let $1/2 < p < 1$ and $T > 0$, then there exists a constant $C > 0$ such that

$$\|\tau_2\|_{L^2(\Omega;\, L_h^2)} = \|r_h F_n - \mathbb{F}_n\|_{L^2(\Omega;\, L_h^2)} \leqslant Ch^{(4/3)(1-1/4p)}$$

Note that for $1/2 < p < 1$,

$$2 - 1/p < (4/3)(1 - 1/4p)$$

hence the total truncation error is dominated by τ_1.

17. NUMERICAL VALIDATION

We turn now to a numerical validation of our convergence estimates for Q_n and P_n. The numerical data reported in Refs. 6–8 refers to single realizations of systems as large as $n = 32000$ particles. All our estimates, however, are for mean convergence, hence we must average over an ensemble of solutions. This, in turn, limits us to much smaller systems.

The system of Eqs. (4) is linear, which we write as $\dot{x}(t) = A_n x(t)$, with $x = (Q, P, a_1, \ldots, a_n, b_1, \ldots, b_n)$; its solution is $x(t) = x_n(t) = \exp(A_n t)\, x(0)$. In comparison, we consider a system of m particles, $\dot{x}(t) = A_m x(t)$, $m < n$, whose solution is $x(t) = x_m(t) = \exp(A_m t)\, x(0)$. In the smaller system $x(t)$ is still a vector of $2n+2$ entries; the decoupling of the last $2(n-m)$ degrees of freedom from the rest of the system lies in the structure of the matrix A_m. This construction is necessary in order to allow a path-by-path comparison of the two systems, as required by the probabilistic setting of our analysis.

The difference between the two solutions is

$$x_n(t) - x_m(t) = [\exp(A_n t) - \exp(A_m t)]\, x(0) \equiv S(t)\, x(0)$$

hence,

$$Q_n(t) - Q_m(t) = \sum_{j=1}^{2n+1} S_{1,j}(t)\, x_j(0)$$

$$P_n(t) - P_m(t) = \sum_{j=1}^{2n+1} S_{2,j}(t)\, x_j(0)$$

Finally, since $x(0)$ is a vector of independent normal variables, then $E[x_j(0)\, x_k(0)] = \delta_{j,k}$ and

$$E\,|Q_n(t) - Q_m(t)|^2 = \sum_{j=1}^{2n+2} S_{1,j}^2(t)$$

$$E\,|P_n(t) - P_m(t)|^2 = \sum_{j=1}^{2n+2} S_{2,j}^2(t)$$

For moderate values of n these functions are easy to compute.

In Figs. 1–3 we plot the mean square deviations, $E|Q_n(t) - Q_{2n}(t)|^2$ and $E|P_n(t) - P_{2n}(t)|^2$, as function of n for $t = 1$. The solid lines corresponds to the predicted asymptotic slopes. Figure 1 is for a value of p above 1, Fig. 2 is for a value of p slightly below 1, and Fig. 3 is for a value of p close to critical value of $p = 1/2$ where our analysis breaks down.

The first two sets of data show the validity of the predicted convergence rate for system sizes as small as 10–80. Note, however, the less smooth behavior of the curves that correspond to the momentum coordinate. Figure 3 shows that as p approaches the critical value of $1/2$ the asymptotic scaling does not show up for such small systems.

18. DISCUSSION

The results presented in this paper are divided into two main categories. (1) Estimates for the rate at which the trajectory of the distinguished particle in an n-particle heat bath converges to the infinite heat bath limit. In the two norms under consideration the rate of convergence was found to be $1/n^{p-1/2}$. (2) Estimates for the rate at which a numerical solution computed by the symplectic Euler scheme approaches the exact n-particle solution when the highest frequencies are underresolved, i.e., when the step size h is of the order of the inverse of the highest frequency. In this case, order reduction occurs; for $1/2 < p < 1$ the order of the method is $|\log h|\, h^{2-1/p}$, which in terms of n amounts to a convergence rate of $\log n/n^{2p-1}$. Thus, if one uses underresolved computation as an approximation to the infinite system, then the dominant part of the error arises from the truncation of the heat bath rather than from the underresolution

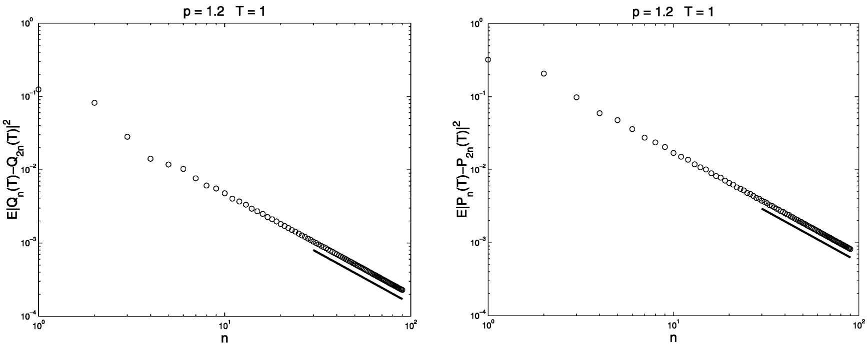

Fig. 1. Log–log plot of the mean square deviations, $E\,|Q_{2n}(t)-Q_n(t)|^2$ (left) and $E\,|P_{2n}(t)-P_n(t)|^2$ (right), versus n for $p=1.2$ and $t=1$. The solid lines have the expected slope of decay of $2p-1$.

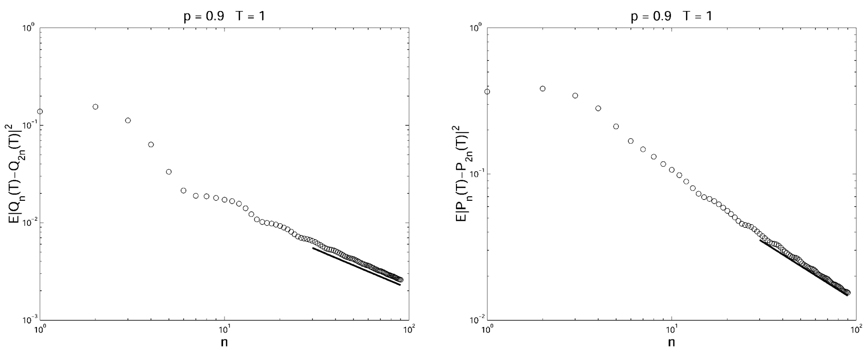

Fig. 2. Same as Fig. 1 for $p=0.9$.

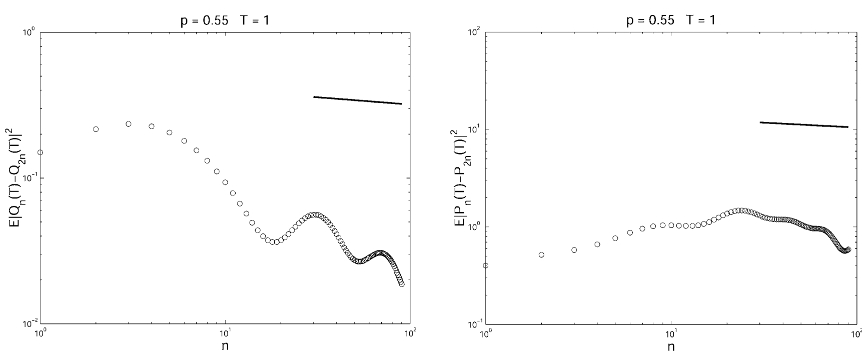

Fig. 3. Same at Fig. 1 for $p=0.55$.

of the high frequencies. In particular, the accuracy cannot be improved by resorting to higher-order integration schemes.

We compare our estimates with the numerical results of Cano and Stuart.[8] For $p=1$ they compare the trajectory $\mathbb{Q}_n$ of the distinguished particle for underresolved computations with $n=1000\cdot 2^m$, $m=0, 1, 2, 3$, with an "exact" solution, which is a well-resolved, $n=32000$ particle solution. Their measured rate of convergence is roughly 1, which seems contradictory to our predicted convergence rate of $p-1/2=1/2$. The reason for this apparent contradiction is their different choice of random initial data, which in our notations corresponds to $\xi_j \sim \mathcal{N}(0, 1)$, and $\eta_j \equiv 0$. Re-examining Proposition 10.3 we see that in this particular case $F-F_n$ decays at a faster rate:

$$\|F-F_n\|_{L^2(\Omega;\, L^2)} \leqslant \frac{C}{n^{2p-1}} = \frac{C}{n}$$

Combining this result with (36) we obtain that $\|Q-Q_n\|_{L^2(\Omega;\, L^2)} \leqslant C/n$. Assuming that our estimates for the convergence rate of underresolved computations can be extrapolated to $p=1$, we conclude that the expected rate of convergence is indeed 1, up to a possible logarithmic correction, that is,

$$\|r_h Q - \mathbb{Q}_n\|_{L^2(\Omega;\, L^2_h)} \leqslant C\,\frac{\log n}{n}$$

Another question of interest is how sensitive are our results to the specific details of the model. Since our choice of masses and spring constants is artificial, estimates must be robust with respect to slight modifications in the parameters for the results to be of physical relevance. An examination of our estimates indicates that the crucial ingredient is the summability of $\sum_{j=1}^{\infty} \omega_j^{-2}$. Any mass distribution that satisfies this summability constraint can be expected to lead to similar estimates. This does not include, however, the case of random frequencies, which requires a separate analysis (see ref. 9).

APPENDIX A. ELIMINATION OF THE DISCRETE HEAT BATH VARIABLES

Consider Eqs. (13). The equations for a_j^k, b_j^k, can be written as independent 2×2 systems

$$\begin{pmatrix} 1 & -j^p h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a_j^{k+1} \\ b_j^{k+1} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -j^p h & 1 \end{pmatrix} \begin{pmatrix} a_j^k \\ b_j^k \end{pmatrix} - \begin{pmatrix} \mathbb{Q}_n^{k+1} - \mathbb{Q}_n^k \\ 0 \end{pmatrix}$$

easily inverted into an explicit form,

$$\begin{pmatrix} a_j^{k+1} \\ b_j^{k+1} \end{pmatrix} = A \begin{pmatrix} a_j^k \\ b_j^k \end{pmatrix} - \begin{pmatrix} \mathbb{Q}_n^{k+1} - \mathbb{Q}_n^k \\ 0 \end{pmatrix} \tag{A.1}$$

where

$$A = \begin{pmatrix} 1 - j^{2p}h^2 & j^p h \\ -j^p h & 1 \end{pmatrix}$$

The eigenvalues of A can be written as

$$\lambda_1 = \exp(+\imath\phi_j), \qquad \lambda_2 = \exp(-\imath\phi_j)$$

where

$$\cos\phi_j = 1 - \tfrac{1}{2} j^{2p}h^2, \qquad \text{and} \qquad \sin\phi_j = j^p h \sqrt{1 - \tfrac{1}{4} j^{2p}h^2}$$

and it has been assumed that $1 - \frac{1}{2} j^{2p}h^2 > 0$ for all j, i.e., that $hn^p < \sqrt{2}$. The corresponding eigenvectors can be written as

$$u_1 = \begin{pmatrix} 1 \\ +\imath\exp(-\tfrac{1}{2}\imath\phi_j) \end{pmatrix}, \qquad u_2 = \begin{pmatrix} 1 \\ -\imath\exp(+\tfrac{1}{2}\imath\phi_j) \end{pmatrix}$$

where

$$\cos(\tfrac{1}{2}\phi_j) = \sqrt{1 - \tfrac{1}{4} j^{2p}h^2} \qquad \text{and} \qquad \sin(\tfrac{1}{2}\phi_j) = \tfrac{1}{2} j^p h$$

The diagonalizing transformation is

$$A = T\Lambda T^{-1}$$

where

$$\Lambda = \begin{pmatrix} \exp(\imath\phi_j) & 0 \\ 0 & \exp(-\imath\phi_j) \end{pmatrix} \qquad T = \begin{pmatrix} 1 & 1 \\ \imath\exp(-\tfrac{1}{2}\imath\phi_j) & -\imath\exp(\tfrac{1}{2}\imath\phi_j) \end{pmatrix}$$

Thus, A can be represented as

$$A = \frac{1}{\cos(\tfrac{1}{2}\phi_j)} \begin{pmatrix} \cos[(1+\tfrac{1}{2})\,\phi_j] & \sin\phi_j \\ -\sin\phi_j & \cos[(1-\tfrac{1}{2})\,\phi_j] \end{pmatrix}$$

and its kth power as

$$A^k = \frac{1}{\cos(\frac{1}{2}\phi_j)} \begin{pmatrix} \cos[(k+\frac{1}{2})\,\phi_j] & \sin k\phi_j \\ -\sin k\phi_j & \cos[(k-\frac{1}{2})\,\phi_j] \end{pmatrix} \tag{A.2}$$

By Duhammel's principle, the solution to Eq. (A.1) is:

$$\begin{pmatrix} a_j^k \\ b_j^k \end{pmatrix} = A^k \begin{pmatrix} \xi_j \\ \eta_j \end{pmatrix} - \sum_{m=1}^{k} A^{k-m} \begin{pmatrix} \mathbb{Q}_n^m - \mathbb{Q}_n^{m-1} \\ 0 \end{pmatrix}$$

which upon substitution of (A.2) read,

$$\begin{aligned} \begin{pmatrix} a_j^k \\ b_j^k \end{pmatrix} = & \frac{1}{\cos(\frac{1}{2}\phi_j)} \begin{pmatrix} \cos[(k+\frac{1}{2})\,\phi_j] & \sin k\phi_j \\ -\sin k\phi_j & \cos[(k-\frac{1}{2})\,\phi_j] \end{pmatrix} \begin{pmatrix} \xi_j \\ \eta_j \end{pmatrix} \\ & - \sum_{m=1}^{k} \frac{1}{\cos(\frac{1}{2}\phi_j)} \begin{pmatrix} \cos[(k-m+\frac{1}{2})\,\phi_j] & \sin[(k-m)\,\phi_j] \\ -\sin[(k-m)\,\phi_j] & \cos[(k-m-\frac{1}{2})\,\phi_j] \end{pmatrix} \\ & \times \begin{pmatrix} \mathbb{Q}_n^m - \mathbb{Q}_n^{m-1} \\ 0 \end{pmatrix} \end{aligned}$$

APPENDIX B. THE CHEBYSHEV POLYNOMIALS

The Chebyshev polynomials[24] of the first kind are defined by

$$T_k(x) = \cos(k \cos^{-1} x), \qquad -1 \leqslant x \leqslant 1$$

They satisfy the recurrence relation

$$T_k(x) = 2x\, T_{k-1}(x) - T_{k-2}(x)$$

and are bounded by $|T_k(x)| \leqslant 1$. Their derivative satisfies the recurrence relation

$$(1-x^2)\, T'_k(x) = k[T_{k-1}(x) - xT_k(x)]$$

The Chebyshev polynomials of the second kind are defined by

$$U_{k-1}(x) = \frac{\sin(k \cos^{-1} x)}{\sin(\cos^{-1} x)} = \frac{1}{k} T'_k(x)$$

and are bounded by $|U_{k-1}(x)| \leqslant k$. Other useful relations are

$$\frac{\cos[(k+\frac{1}{2})\cos^{-1} x]}{\cos(\frac{1}{2}\cos^{-1} x)} = U_k(x) - U_{k-1}(x)$$

$$\frac{\sin[(k+\frac{1}{2})\cos^{-1} x]}{\sin(\frac{1}{2}\cos^{-1} x)} = U_k(x) + U_{k-1}(x)$$

APPENDIX C. DERIVATION OF THE DISCRETE VOLTERRA EQUATION

In this appendix we derive the discrete Volterra equation (18) from the discrete second-order integro-differential equation (16). The procedure is analogous to its continuous counterpart, described in Section 4.

Multiply (16) by h and summing up over k from 1 to ℓ, we obtain an equation of the form

$$A_1^\ell = A_2^\ell + A_3^\ell + A_4^\ell + A_5^\ell \tag{C.1}$$

where

$$\begin{aligned} A_1^\ell &= h \sum_{k=1}^{\ell} \frac{\mathbb{Q}_n^{k+1} - 2\mathbb{Q}_n^k + \mathbb{Q}_n^{k-1}}{h^2} \\ &= \frac{(\mathbb{Q}_n^{\ell+1} - \mathbb{Q}_n^\ell) - (\mathbb{Q}_n^1 - Q_0)}{h} \\ &= \frac{\mathbb{Q}_n^{\ell+1} - \mathbb{Q}_n^\ell}{h} - P_0 + hQ_0 - h \sum_{j=1}^{n} \xi_j \end{aligned}$$

$$A_2^\ell = -h \sum_{k=1}^{\ell} \mathbb{Q}_n^k$$

$$A_3^\ell = h \sum_{j=1}^{n} \xi_j \sum_{k=1}^{\ell} [U_k(x_j) - U_{k-1}(x_j)] = h \sum_{j=1}^{n} \xi_j \, [U_\ell(x_j) - 1]$$

$$A_4^\ell = h \sum_{j=1}^{n} \eta_j \sum_{k=1}^{\ell} (j^p h)\, U_{k-1}(x_j) = \sum_{j=1}^{n} \eta_j \frac{1}{j^p} [1 - U_\ell(x_j) + U_{\ell-1}(x_j)]$$

and

$$
\begin{aligned}
A_5^\ell &= -h \sum_{j=1}^{n} \sum_{k=1}^{\ell} \sum_{m=1}^{k} [U_{k-m}(x_j) - U_{k-m-1}(x_j)](\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1}) \\
&= -h \sum_{j=1}^{n} \sum_{m=1}^{\ell} (\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1}) \sum_{k=m}^{\ell} [U_{k-m}(x_j) - U_{k-m-1}(x_j)] \\
&= -h \sum_{j=1}^{n} \sum_{m=1}^{\ell} (\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1}) \sum_{k=0}^{\ell-m} [U_k(x_j) - U_{k-1}(x_j)] \\
&= -h \sum_{j=1}^{n} \sum_{m=1}^{\ell} (\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1})\, U_{\ell-m}(x_j)
\end{aligned}
$$

where we have used the following identity:

$$
\begin{aligned}
\sum_{k=1}^{\ell} U_{k-1}(x_j) &= \frac{1}{2(1-x_j)} [1 - U_\ell(x_j) + U_{\ell-1}(x_j)] \\
&= \frac{1}{j^{2p} h^2} [1 - U_\ell(x_j) + U_{\ell-1}(x_j)]
\end{aligned}
$$

Equation (C.1) is a first-order difference equation for $\mathbb{Q}_n^{\ell+1}$, $\ell = 1, 2, \ldots$. Note that expression (17) for $\mathbb{Q}_n^1$ coincides with (C.1) for $\ell = 0$, thus (C.1) holds for all $\ell = 0, 1, 2, \ldots$.

We multiply Eq. (C.1) by h and perform a second summation over ℓ ranging from 0 to $s-1$, $s = 1, 2, \ldots, N-1$. The resulting equation is of the form

$$
B_1^s = B_2^s + B_3^s + B_4^s + B_5^s \tag{C.2}
$$

where

$$
\begin{aligned}
B_1^s &= \sum_{\ell=0}^{s-1} hA_1^\ell = \mathbb{Q}_n^s - Q_0 - P_0 t_s + h\, Q_0 t_s - h t_s \sum_{j=1}^{n} \xi_j \\
B_2^s &= \sum_{\ell=0}^{s-1} hA_2^\ell = -h \sum_{k=1}^{s} t_{s-k} \mathbb{Q}_n^k = hQ_0 t_s - h \sum_{k=0}^{s-1} t_{s-k} \mathbb{Q}_n^k \\
B_3^s &= \sum_{\ell=0}^{s-1} hA_3^\ell = \sum_{j=1}^{n} \xi_j \frac{1 - U_s(x_j) + U_{s-1}(x_j)}{j^{2p}} - h t_s \sum_{j=1}^{n} \xi_j \\
B_4^s &= \sum_{\ell=0}^{s-1} hA_4^\ell = \sum_{j=1}^{n} \eta_j \left[\frac{t_s}{j^p} - \frac{h}{j^p} U_{s-1}(x_j) \right]
\end{aligned}
$$

and

$$\begin{aligned}
B_5^s &= \sum_{\ell=0}^{s-1} hA_5^\ell \\
&= -h^2 \sum_{j=1}^{n} \sum_{\ell=0}^{s-1} \sum_{m=1}^{\ell} (\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1})\, U_{\ell-m}(x_j) \\
&= -h^2 \sum_{j=1}^{n} \sum_{m=1}^{s-1} \sum_{\ell=m}^{s-1} (\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1})\, U_{\ell-m}(x_j) \\
&= -h^2 \sum_{j=1}^{n} \sum_{m=1}^{s-1} (\mathbb{Q}_n^m - \mathbb{Q}_n^{m-1}) \sum_{k=0}^{s-m-1} U_k(x_j)
\end{aligned}$$

Using summation by parts,

$$\sum_{m=1}^{s-1} (a_m - a_{m-1}) \sum_{k=0}^{s-m-1} b_k = -a_0 \sum_{k=0}^{s-1} b_k + \sum_{k=0}^{s-1} a_k b_{s-k-1}$$

we obtain

$$\begin{aligned}
B_5^s &= -h^2 \sum_{j=1}^{n} \left[-Q_0 \sum_{k=0}^{s-1} U_k(x_j) + \sum_{k=0}^{s-1} \mathbb{Q}_n^k U_{s-k-1}(x_j) \right] \\
&= Q_0 \sum_{j=1}^{n} \frac{1 - U_s(x_j) + U_{s-1}(x_j)}{j^{2p}} - h^2 \sum_{j=1}^{n} \sum_{k=0}^{s-1} \mathbb{Q}_n^k U_{s-k-1}(x_j)
\end{aligned}$$

Substituting B_1^s–B_5^s into (C2) we obtain the discrete Volterra equation (18).

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