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Stiff Oscillatory Systems, Delta Jumps and White Noise

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Abstract. Two model problems for stiff oscillatory systems are introduced. Both comprise a linear superposition of $N \gg 1$ harmonic oscillators used as a forcing term for a scalar ODE. In the first case the initial conditions are chosen so that the forcing term approximates a delta function as $N \to \infty$ and in the second case so that it approximates white noise. In both cases the fastest natural frequency of the oscillators is $\mathcal{O}(N)$. The model problems are integrated numerically in the stiff regime where the time-step Δt satisfies $N\Delta t = \mathcal{O}(1)$. The convergence of the algorithms is studied in this case in the limit $N \to \infty$ and $\Delta t \to 0$. For the white noise problem both strong and weak convergence are considered. Order reduction phenomena are observed numerically and proved theoretically.

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1. Introduction

In the field of computational statistical mechanics, stiff oscillatory systems with broad frequency spectra often arise. It is hence of interest to develop a theory of the numerical analysis for such problems. In the area of stiff dissipative systems the understanding of numerical algorithms has been greatly enhanced by the study of a variety of simple model problems [**6**]; here we introduce, and then study numerical methods for, several model problems in stiff oscillatory systems. A review of existing literature in this area may be found in [**14**] and in Section 6 of [**15**].

The context for the models we study is as follows. Many problems arising from the molecular modeling of materials may be written in the form

$$\begin{aligned} \frac{dx}{dt} &= a(x, y), \qquad x(0) = x_0, \\ \frac{dy}{dt} &= b(x, y), \qquad y(0) = y_0, \end{aligned} \tag{1.1}$$

where $x \in \mathbb{R}^m$ and $y \in \mathbb{R}^p$ with $p \gg m$. We think of x as representing variables of intrinsic interest (observables) and of y as representing variables of interest only inasmuch as they effect the evolution of x. For such problems (x_0, y_0) is often incompletely known and it is natural to think of a probability measure μ on $\mathbb{R}^{m+p}$ which governs this initial data. In principle, we may write

$$y(t) = \mathcal{F}(y_0, \{x(s)\}_{0 \le s \le t})$$

so that

$$\frac{dx}{dt} = a(x, \mathcal{F}(y_0, \{x(s)\}_{0 \le s \le t})), \qquad x(0) = x_0.$$

It is often the case that in some limit (such as $p \to \infty$) this equation simplifies to yield a relatively simple stochastic process for the variable $x(s)$; furthermore, this process is sometimes Markovian. If the limiting stochastic process is known explicitly it is therefore natural to approximate it directly to find information about x, rather than to simulate the large system (1.1). However, in many situations some form of stochastic process for x is believed to exist but its form is either unknown or not explicitly computable (see [**9**] for example). In such a situation it is natural to approximate (1.1) directly and to ask what is the minimal resolution of the y variable necessary to accurately approximate x. In order to make headway with this question we will consider two simple models where the limiting process for x *is known* but study its approximation through under-resolved simulation of (1.1). Of course if the limit process *is* known explicitly it should be approximated directly; we consider approximation of (1.1) simply to shed light on the general case where the limit process is not known explicitly, or not even known to exist.

A related, but different, approach may be found in the work of Chorin et al. [**3**], [**4**], [**5**]. They attempt to develop an equation for $X(t) = \mathbb{E}x(t)$, where $\mathbb{E}$ is with respect to μ on (x_0, y_0). By *assuming* that μ is stationary for (1.1) they consider the equation

$$\frac{dX}{dt} = A(X),$$

where $A(X) = \mathbb{E}(a(x, y) \mid x = X)$ and now $\mathbb{E}(\cdot \mid x = X)$ is, with respect to μ on (x, y), conditional on $x = X$. This approach has had some success and further analytical justification may be forthcoming through the study of its application to models such as those studied here and in [**15**], [**11**].

We recognize that the models we consider are somewhat artificial since, as the limits are known explicitly, the numerical methods studied would never be used in practice. However, the analysis sheds light on what may be expected in the general case when the limit is not explicitly known and may hence be viewed as a (hopefully) useful first step in the numerical analysis of stiff oscillatory systems with random data.

Section 2 introduces two basic models, both motivated by a simple mechanical description of a heat bath. In the first, a family of harmonic oscillators is used to construct an approximate delta function, through Fourier analysis, and this is used as a forcing term for a scalar ODE. In the second, a family of harmonic oscillators is used to construct an approximation to white noise, again through Fourier analysis, and this is used as a forcing term for a scalar ODE. For both models the fastest natural frequency of the oscillators is $\mathcal{O}(N)$, where N is the number of oscillators. The approximation to a delta function or to white noise becomes exact as $N \to \infty$; theorems making this precise are given. See also [**2**].

Our aim is to study the convergence of numerical methods for these models in the regime

$$N\Delta t \text{ fixed}; \qquad \Delta t \to 0, \quad N \to \infty. \tag{1.2}$$

In statistical mechanics, the interaction of an observable with a heat bath can be modeled by a purely mechanical system with random data [**7**], [**16**]. That work motivates the choice of constructing a delta function and white noise through families of oscillators since there Fourier-based approximations of delta-function induced jumps arise in the modeling of the energy-loss mechanism from the observable to the heat bath, whilst the Fourier-based white noise models the (expected) energy gain mechanism, given a random distribution on the initial data. Numerical experiments in [**15**] study the observable–heat bath interaction numerically under the limit (1.2). The purpose of this paper is to further understand the numerical analysis of such problems by isolating, and then studying separately, the approximation of delta functions and white noise through numerically approximated Fourier series. Section 3 contains a preliminary discussion of the situation where the equation for the observable is discretized, but exact samples of the rapidly varying heat bath are used; this helps to place subsequent analysis in context.

Section 4 contains an analysis of the delta jump model and the numerical approximation is studied in a discrete L^2-norm under the limit process (1.2). In Section 5 the white noise problem is studied in a discrete L^∞-norm in time, from the point of view of strong convergence of the numerical approximation (with respect to an appropriate probability measure) under (1.2). In Section 6 the white noise problem is again studied, but from the viewpoint of weak convergence of the numerical approximation under (1.2). Here we construct pathwise approximations to SDEs, through Fourier analysis. This necessarily requires that the dimension of the model problems grows to infinity in the limit. It would also be of interest to study numerical aspects of weak approximations of SDEs through deterministic problems with random data as outlined in [**1**]; for such constructions the system size is fixed and a separation of time-scales facilitates the construction of white noise.

Our results show that:

- For the delta jump model, only certain special methods exhibit convergence to the correct limit under (1.2). Other methods accurately approximate an *incorrect* limit.
- For the delta jump model convergence under (1.2) is at a reduced rate when compared with the fixed N, $\Delta t \to 0$ behavior—an order reduction phenomenon [**6**].
- For the white noise model, similar reduced rates of convergence (order reduction) are again observed, both for strong and weak convergence.
- For the white noise model the rates of convergence are better for weak than for strong convergence, a situation familiar from standard approximation theory for SDEs [**12**].

2. Model Problems

Consider the equations

$$\begin{aligned} \ddot{u}_j + j^2 u_j &= 0, \\ u_j(0) = a_j, \qquad \dot{u}_j(0) &= 0, \qquad j = 0, \ldots, N, \end{aligned} \tag{2.1}$$

and

$$\begin{aligned} \dot{z}_{\mathrm{N}} &= f(z_{\mathrm{N}}) + H_{\mathrm{N}}(t), \\ z_{\mathrm{N}}(0) &= z_0, \end{aligned} \tag{2.2}$$

where

$$H_{\mathrm{N}}(t) := \sum_{j=0}^{N} u_j(t).$$

We consider two choices for the $\{a_j\}_{j=0}^{N}$: the first is

$$a_0 = \tfrac{1}{2}, \qquad a_j = 1, \qquad j \geq 1. \tag{MP1}$$

The second is

$$a_0 = \frac{1}{\sqrt{\pi}}\eta_0, \qquad a_j = \sqrt{\frac{2}{\pi}}\eta_j, \qquad j \geq 1; \tag{MP2}$$

here the η_j are i.i.d. Gaussian random variables with mean 0 and variance 1.

Throughout the following we assume that $f \in C^\infty(\mathbb{R}, \mathbb{R})$ and satisfies the global Lipschitz condition

$$|f(x) - f(y)| \le L|x - y| \qquad \forall x, y \in \mathbb{R}.$$

Formal calculations indicate that for [MP1], $0 \le t \le \pi$ and N large, $z_{\rm N}$ should behave like z solving

$$\dot{z} = f(z), \qquad z(0) = z_0 + \frac{\pi}{2}. \tag{2.3}$$

For [MP2] the analogous formal limit is the SDE:

$$dz = f(z)\,dt + dW, \qquad z(0) = z_0, \tag{2.4}$$

where W is a standard Brownian motion on $0 \le t \le \pi$. The following three results make this intuition precise:

Theorem 2.1. *Consider $z_{\rm N}(t)$ solving* [MP1] *and $z(t)$ solving* (2.3). *Then, for $T \in (0, \pi]$:*

$$\|z(\cdot) - z_{\rm N}(\cdot)\|^2_{L^2(0,T)} \le \frac{C(T)}{N}.$$

Theorem 2.2. *Consider $z_{\rm N}(t)$ solving* [MP2] *and $z(t)$ solving* (2.4). *Then, for $T \in (0, \pi]$:*

$$\sup_{t\in(0,T)} \mathbb{E}|z(t) - z_{\rm N}(t)|^2 \le \frac{C(T)}{N}.$$

It is often the case that weak convergence results can be obtained at faster rates than strong convergence and we now demonstrate this. We consider expectations of functions $g\colon \mathbb{R} \to \mathbb{R}$ whose Fourier transform $\hat{g}$ satisfies:

Hypothesis H. *There exists a real number $\beta > 1$ and a positive constant C_1 such that*

$$|\hat{g}(k)| \le C_1(1 + |k|)^{-\beta} \qquad \forall k \in \mathbb{R}.$$

In the following theorem, in Proposition 2.5, and in Section 6, we consider the case $f \equiv 0$. Thus z solving (2.4) is a pure Brownian motion. This allows relatively straightforward analysis using Fourier techniques; more sophisticated methods would be required to analyze the case of nonzero f.

Theorem 2.3. *Let $f(z) \equiv 0$ and let $g\colon \mathbb{R} \to \mathbb{R}$ satisfy Hypothesis* H. *Consider $z_{\rm N}(t)$ solving* [MP2] *and $z(t)$ solving* (2.4). *Then, for $T \in [0, \pi]$:*

$$\sup_{z_0\in R} |\mathbb{E}g(z(T)) - \mathbb{E}g(z_{\rm N}(T))| \le \begin{cases} CN^{(1-\beta)/2}, & 1 < \beta < 3, \\ CN^{-1}\log(1 + N), & \beta = 3, \\ CN^{-1}, & \beta > 3, \end{cases}$$

where $C = C(\beta, C_1)$, *with* β *and* C_1 *as in Hypothesis* H, *is independent of* $T \in [0, \pi]$.

These theorems are proved at the end of the section.

Since, when $f \equiv 0$, $z_{\mathrm{N}}(t)$ is a Gaussian random variable for each T, theorems similar to Theorem 2.3 could be proved directly by use of limit theorems for sums of Gaussian random variables. Our proof, though less direct, explicitly calculates the time evolution of the probability density function (pdf) for $z_{\mathrm{N}}(t)$, which may be of independent interest, and hence yields convergence rates which are independent of $T \in [0, \pi]$. Estimates for the difference between $p(z, t)$, the pdf for $z(t)$ solving (2.4), and $\bar{p}_{\mathrm{N}}(z, t)$ the pdf for $z_{\mathrm{N}}(t)$ solving [MP2] may be found after the proof of Theorem 2.3.

In Section 3 we briefly consider the numerical solution of (2.2) by the θ-method, taking the *exact* solution of (2.1) as input data. The results are stated in order to enable comparison with the fully discrete problems considered in subsequent sections: in Sections 4, 5, and 6 we consider numerical solutions of (2.1), (2.2) in the regime (1.2) and address the question of whether the numerical approximations identify the correct limiting behavior, as given in Theorems 2.1, 2.2, and 2.3. We solve (2.1) by a family of parametrized energy conserving methods,[1] namely, for $\alpha \in [0, 1]$,

$$\begin{aligned} &U_j^{n+1} - 2U_j^n + U_j^{n-1} + j^2 \Delta t^2 U_j^n = 0, \\ &U_j^0 = a_j, \qquad U_j^1 = a_j[1 - \alpha j^2 \Delta t^2], \end{aligned} \tag{2.5}$$

and (2.2) by the θ-method, $\theta \in [0, 1]$, for $t^n = n\Delta t$:

$$\begin{aligned} Z^{n+1} - Z^n \;=\; &\Delta t[\theta f(Z^{n+1}) + (1-\theta) f(Z^n)] \\ &+ \Delta t[\theta H_{\mathrm{N}}^{\Delta t}(t^{n+1}) + (1-\theta) H_{\mathrm{N}}^{\Delta t}(t^n)] \end{aligned} \tag{2.6}$$

with $Z^0 = z_0$ and where $H_{\mathrm{N}}^{\Delta t}(t^n)$ is the approximation to $H_{\mathrm{N}}(t^n)$ with the $u_j(t^n)$ computed through (2.5).

The following lemma will be useful in the study of (2.5), (2.6). The first statement is taken from [**15**]; the second is proved by a minor modification of the techniques in [**15**].

Lemma 2.4. (*i*) *Let* $N\Delta t < 2$. *The sequence* $\{Z^n\}_{n \ge 0}$ *generated by* (2.6) *satisfies*

$$\begin{aligned} Z^n \;=\; &z_0 + \Delta t \sum_{m=0}^{n}{}' f(Z^m) + (n\Delta t) a_0 + \sum_{j=1}^{N} a_j \gamma_j \sin(\varphi_j n) \\ &+ (1 - \theta - \alpha)\Delta t \sum_{j=1}^{N} 2a_j \sin^2(\varphi_j n/2), \end{aligned} \tag{2.7}$$

[1] For $j\Delta t \in (0, 2)$ the method (2.5) conserves a small perturbation of the energy of the underlying harmonic oscillator.

where $\sum_{m=0}^{n}{}'$ *denotes a sum with weight* $(1-\theta)$ *on* $m = 0$, θ *on* $m = n$, *and* 1 *otherwise. Furthermore,* φ_j *and* γ_j *are given by*

$$\cos\varphi_j = 1 - \tfrac{1}{2} j^2 \Delta t^2$$

and

$$\gamma_j = \frac{\sqrt{1 - \frac{1}{4} j^2 \Delta t^2}}{j} + \frac{(\alpha - \frac{1}{2})(\frac{1}{2} - \theta) j \Delta t^2}{\sqrt{1 - \frac{1}{4} j^2 \Delta t^2}}.$$

(*ii*) *Let* $N\Delta t < 2\pi$. *If* $H_{\mathrm{N}}^{\Delta t}(\cdot)$ *is replaced by* $H_{\mathrm{N}}(\cdot)$ *in* (2.6), *then*

$$\begin{aligned} Z^n \;=\; & z_0 + \Delta t \sum_{m=0}^{n}{}' f(Z^m) + (n\Delta t)a_0 + \sum_{j=1}^{N} a_j \gamma_j' \sin(jn\Delta t) \\ & + (1-2\theta)\Delta t \sum_{j=1}^{N} a_j \sin^2(jn\Delta t/2), \end{aligned} \tag{2.8}$$

where

$$\gamma_j' = \frac{\Delta t}{2\tan(j\Delta t/2)}.$$

The constraint $N\Delta t < 2\pi$ is required to avoid the resonances which arise if the denominator of γ_j' passes through zero.

We now prove Theorems 2.1–2.3.

Proof of Theorem 2.1. In this case

$$H_{\mathrm{N}}(t) = \frac{dh_{\mathrm{N}}}{dt}(t),$$

where

$$h_{\mathrm{N}}(t) = \frac{t}{2} + \sum_{j=1}^{N} \frac{\sin(jt)}{j}.$$

Straightforward Fourier analysis shows that

$$\left\| \left(h_{\mathrm{N}}(\cdot) - \frac{\cdot}{2}\right) - \left(\frac{\pi - \cdot}{2}\right) \right\|^2_{L^2(0,\pi)} \le \frac{C}{N}. \tag{2.9}$$

Writing (2.2), (2.3) as integral equations gives

$$z_{\mathrm{N}}(t) = z_0 + \int_0^t f(z_{\mathrm{N}}(s))\,ds + h_{\mathrm{N}}(t), \tag{2.10}$$

$$z(t) = z_0 + \int_0^t f(z(s))\,ds + \frac{\pi}{2}. \tag{2.11}$$

Subtracting and defining $e_{\mathrm{N}}(t) = z_{\mathrm{N}}(t) - z(t)$ gives

$$e_{\mathrm{N}}(t) = \int_0^t [f(z_{\mathrm{N}}(s)) - f(z(s))]\,ds + \left[h_{\mathrm{N}}(t) - \frac{\pi}{2}\right].$$

Taking L^2-norms and using (2.9) gives, for $t \in [0, \pi]$:

$$\|e_{\mathrm{N}}(\cdot)\|^2_{L^2(0,t)} \leq \frac{2C}{N} + 2\pi L^2 \int_0^t \|e_{\mathrm{N}}(\cdot)\|^2_{L^2(0,s)}\,ds.$$

A Gronwall argument gives the desired result. □

Proof of Theorem 2.2. In the case of [MP2] it follows that

$$h_{\mathrm{N}}(t) = \frac{\eta_0 t}{\sqrt{\pi}} + \sum_{j=1}^{N} \sqrt{\frac{2}{\pi}}\eta_j \frac{\sin(jt)}{j}. \tag{2.12}$$

From [**13**, Chapter 2, Theorem 2.5] it is known that, with probability one, as $N \to \infty$,

$$h_{\mathrm{N}}(t) \to W(t)$$

uniformly for $t \in [0, \pi]$, where $W(t)$ is standard Brownian motion. Hence, almost surely,

$$W(t) = \frac{\eta_0 t}{\sqrt{\pi}} + \sum_{j=1}^{\infty} \sqrt{\frac{2}{\pi}}\eta_j \frac{\sin(jt)}{j} \tag{2.13}$$

from which it follows that, for each $t \in [0, \pi]$:

$$\begin{aligned} \mathbb{E}|h_{\mathrm{N}}(t) - W(t)|^2 &= \mathbb{E} \sum_{j,k \geq N+1} \frac{2}{\pi}\eta_j\eta_k \frac{\sin(jt)\sin(kt)}{jk} \\ &= \sum_{j \geq N+1} \frac{2}{\pi} \frac{\sin^2(jt)}{j^2} \\ &\leq \frac{2C}{\pi N}. \end{aligned}$$

Rewriting (2.4) as an integral equation gives

$$z(t) = z_0 + \int_0^t f(z(s))\,ds + W(t). \tag{2.14}$$

Subtracting from (2.10) and defining $e_{\mathrm{N}}(t) = z_{\mathrm{N}}(t) - z(t)$ gives

$$e_{\mathrm{N}}(t) = \int_0^t [f(z_{\mathrm{N}}(s)) - f(z(s))]\,ds + [h_{\mathrm{N}}(t) - W(t)].$$

Thus

$$\mathbb{E}|e_{\mathrm{N}}(t)|^2 \;\le\; 2\mathbb{E}\left\{\int_0^t [\,f(z_{\mathrm{N}}(s)) -\, f(z(s))]\,ds\right\}^2 + \frac{4C}{\pi N}$$
$$\le\; 2\pi L^2 \int_0^t \mathbb{E}|e_{\mathrm{N}}(s)|^2\,ds + \frac{4C}{\pi N}.$$

A Gronwall argument gives the desired result. □

Proof of Theorem 2.3. We wish to study the rate of convergence of the quantity

$$|\mathbb{E}g(z(t)) - \mathbb{E}g(z_{\mathrm{N}}(t))| \tag{2.15}$$

to 0 as $N \to \infty$ in the case when

$$f(\cdot) \equiv 0. \tag{2.16}$$

The pdf $p(z,t)$ for the problem (2.4) under (2.16) is the solution of the parabolic initial-value problem

$$\begin{cases} \dfrac{\partial p}{\partial t} = \dfrac{1}{2}\dfrac{\partial^2 p}{\partial z^2}, \\ p(z,0) = \delta(z - z_0). \end{cases}$$

Similarly, for each fixed $\omega := \{\eta_j\}_{j\ge 0}$, the pdf $p_{\mathrm{N}}(z,t;\omega)$ for the problem (2.2) satisfies the hyperbolic initial-value problem

$$\begin{cases} \dfrac{\partial p_{\mathrm{N}}}{\partial t} + \dfrac{\partial}{\partial z}\left(\dfrac{dh_{\mathrm{N}}}{dt}\, p_{\mathrm{N}}\right) = 0, \\ p_{\mathrm{N}}(z,0;\omega) = \delta(z - z_0), \end{cases} \tag{2.17}$$

where $h_{\mathrm{N}}(t) = h_{\mathrm{N}}(t;\omega)$ is given by (2.12). We set

$$\bar{p}_{\mathrm{N}}(z,t) = \mathbb{E}p_{\mathrm{N}}(z,t;\omega),$$

and note that

$$\mathbb{E}g(z(t)) \;=\; \int_{-\infty}^{\infty} p(z,t)g(z)\,dz, \tag{2.18}$$

$$\mathbb{E}g(z_{\mathrm{N}}(t)) \;=\; \int_{-\infty}^{\infty} \bar{p}_{\mathrm{N}}(z,t)g(z)\,dz. \tag{2.19}$$

Thus we shall first estimate the closeness of $\bar{p}_{\mathrm{N}}$ to p, and thereby derive bounds on the quantity (2.15).

We define

$$\hat{p}_{\mathrm{N}}(k,t;\omega) = \int_{-\infty}^{\infty} e^{ikz}\, p_{\mathrm{N}}(z,t;\omega)\,dz.$$

Applying the Fourier transform to (2.17), it is a straightforward matter to check that

$$\frac{\partial}{\partial t}\hat{p}_{\mathrm{N}} - ik\frac{dh_{\mathrm{N}}}{dt}\hat{p}_{\mathrm{N}} = 0, \qquad \hat{p}_{\mathrm{N}}(k,0;\omega) = e^{ikz_0},$$

and therefore

$$\hat{p}_{\mathrm{N}}(k,t;\omega) = e^{ikz_0}e^{ikh_{\mathrm{N}}(t;\omega)},$$

where we have made use of the fact that $h_{\mathrm{N}}(0;\omega) = 0$. Hence,

$$p_{\mathrm{N}}(z,t;\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(z_0-z)}e^{ikh_{\mathrm{N}}(t;\omega)}\,dk,$$

so that

$$\bar{p}_{\mathrm{N}}(z,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(z_0-z)}\psi_{\mathrm{N}}(k,t)\,dk,$$

where $\psi_{\mathrm{N}}(k,t)$ is the characteristic function for $h_{\mathrm{N}}(t;\omega)$; i.e.,

$$\begin{aligned}
\psi_{\mathrm{N}}(k,t) &= \mathbb{E}\ \exp\{ikh_{\mathrm{N}}(t;\omega)\}\\
&= \exp\left\{-\frac{k^2t^2}{2\pi} - \frac{k^2}{\pi}\sum_{j=1}^{N}\frac{\sin^2 jt}{j^2}\right\}\\
&= \exp\left\{-\frac{k^2}{2}\left[\frac{t^2}{\pi} + \frac{2}{\pi}\sum_{j=1}^{N}\frac{\sin^2 jt}{j^2}\right]\right\}\\
&= \exp\left\{-\frac{k^2}{2}\left[\frac{t^2}{\pi} + \frac{2}{\pi}\sum_{j=1}^{N}\frac{1-\cos(2jt)}{2j^2}\right]\right\}\\
&= \exp\left\{-\frac{k^2}{2}\left[\frac{t^2}{\pi} + \frac{1}{\pi}\sum_{j=1}^{N}\frac{1}{j^2} - \frac{1}{\pi}\sum_{j=1}^{N}\frac{\cos(2jt)}{j^2}\right]\right\}. \qquad (2.20)
\end{aligned}$$

As

$$\sum_{j=1}^{\infty}\frac{1}{j^2} = \frac{\pi^2}{6}$$

and, by straightforward Fourier series expansion,

$$\frac{t^2}{\pi} - t = -\frac{\pi}{6} + \frac{1}{\pi}\sum_{j=1}^{\infty}\frac{\cos(2jt)}{j^2}, \qquad (2.21)$$

we deduce (formally, at least) that, as $N \to \infty$:

$$\begin{aligned}
\psi_{\mathrm{N}}(k,t) &\to \exp\left\{-\frac{1}{2}k^2t\right\},\\
\bar{p}_{\mathrm{N}}(z,t) &\to \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(z-z_0)}e^{-\frac{1}{2}k^2t}\,dk = p(z,t).
\end{aligned}$$

We now aim to make these statements precise.

Since the Fourier series on the right-hand side of (2.21) converges uniformly for $t \in [0, \pi]$ to the function on the left-hand side of (2.21):

$$\mathrm{e}^{-\frac{1}{2}k^2 t} = \exp\left\{-\tfrac{1}{2}k^2\left[\frac{t^2}{\pi} + \frac{\pi}{6} - \frac{1}{\pi}\sum_{j=1}^{\infty}\frac{\cos(2jt)}{j^2}\right]\right\} \qquad \forall\, t \in [0, \pi].$$

Also, from (2.20) we have that

$$\psi_{\mathrm{N}}(k, t) = \exp\left\{-\tfrac{1}{2}k^2\left[\frac{t^2}{\pi} + \frac{1}{\pi}\sum_{j=1}^{N}\frac{1}{j^2} - \frac{1}{\pi}\sum_{j=1}^{N}\frac{\cos(2jt)}{j^2}\right]\right\}.$$

Alternatively, the last two lines can be rewritten as, respectively,

$$\mathrm{e}^{-\frac{1}{2}k^2 t} \;=\; \exp\left\{-\tfrac{1}{2}k^2\left[\frac{t^2}{\pi} + S_1^{\infty}\right]\right\}, \tag{2.22}$$

$$\psi_{\mathrm{N}}(k, t) \;=\; \exp\left\{-\tfrac{1}{2}k^2\left[\frac{t^2}{\pi} + S_1^{N}\right]\right\}, \tag{2.23}$$

where

$$S_1^{\infty} = \frac{2}{\pi}\sum_{j=1}^{\infty}\frac{\sin^2 jt}{j^2}, \qquad S_1^{N} = \frac{2}{\pi}\sum_{j=1}^{N}\frac{\sin^2 jt}{j^2}.$$

On subtracting (2.23) from (2.22) and noting that

$$|e^{-a} - e^{-b}| \le [1 - e^{-|a-b|}], \qquad a, b \ge 0, \tag{2.24}$$

we deduce that

$$|e^{-\frac{1}{2}k^2 t} - \psi_{\mathrm{N}}(k, t)| \le e^{-k^2 t^2/2\pi}\left[1 - \exp\left(-\frac{k^2}{\pi}\sum_{j \ge N+1}\frac{\sin^2 jt}{j^2}\right)\right]. \tag{2.25}$$

Further, since

$$\sum_{j \ge N+1}\frac{\sin^2 jt}{j^2} \le \sum_{j \ge N+1}\frac{1}{j^2} \le \frac{1}{N},$$

it follows from (2.25) that

$$|e^{-\frac{1}{2}k^2 t} - \psi_{\mathrm{N}}(k, t)| \le e^{-k^2 t^2/2\pi}[1 - e^{-k^2/\pi N}]. \tag{2.26}$$

Now we consider (2.18) and (2.19). By virtue of Parseval's identity

$$\begin{aligned} \mathbb{E}g(z(t)) - \mathbb{E}g(z_{\mathrm{N}}(t)) \;&=\; \int_{-\infty}^{\infty} [p(z, t) - \bar{p}_{\mathrm{N}}(z, t)]\, g(z)\, dz \\ &=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(z_0 - z)}[e^{-\frac{1}{2}k^2 t} - \psi_{\mathrm{N}}(k, t)]\hat{g}(k) dk. \end{aligned}$$

Thus,

$$|\mathbb{E}g(z(t)) - \mathbb{E}g(z_{\mathrm{N}}(t))| \le \frac{1}{2\pi}\int_{-\infty}^{\infty} |e^{-\frac{1}{2}k^2 t} - \psi_{\mathrm{N}}(k,t)|\,|\hat{g}(k)|\,dk. \tag{2.27}$$

Applying Hypothesis H in (2.27) and recalling (2.26), it follows that

$$|\mathbb{E}g(z(t)) - \mathbb{E}g(z_{\mathrm{N}}(t))| \le \frac{C_1}{\pi}\int_0^{\infty} e^{-k^2t^2/2\pi}[1-e^{-k^2/\pi N}](1+k)^{-\beta}\,dk. \tag{2.28}$$

In order to complete the analysis, it remains to bound the right-hand side in (2.28). First, we note that

$$1 - e^{-a} \le \min(1,a), \qquad a \ge 0.$$

Applying this in (2.28) with $a = k^2/(\pi N)$, it follows that

$$|\mathbb{E}g(z(t)) - \mathbb{E}g(z_{\mathrm{N}}(t))| \le \frac{C_1}{\pi}\int_0^{\infty} e^{-k^2t^2/2\pi}(1+k)^{-\beta}\min\left(1, \frac{k^2}{\pi N}\right)dk. \tag{2.29}$$

In Appendix A we show that

$$\int_0^{\infty} e^{-k^2t^2/2\pi}(1+k)^{-\beta}\min\left(1,\frac{k^2}{\pi N}\right)dk \le \begin{cases} CN^{(1-\beta)/2}, & 1<\beta<3,\\ CN^{-1}\log(1+N), & \beta = 3,\\ CN^{-1}, & \beta>3, \end{cases} \tag{2.30}$$

where $C = C(\beta)$ is a positive constant. Finally, inserting (2.30) into (2.29), we arrive at the required bound. □

By using the estimates from the proof of Theorem 2.3, some simple calculations given in Appendix B enable the proof of the following:

Proposition 2.5. *Let $f(z) \equiv 0$. Consider $\bar{p}_{\mathrm{N}}(z,t)$, the pdf for $z_{\mathrm{N}}(t)$ solving* [MP2], *and $p(z,t)$, the pdf for $z(t)$ solving* (2.4)*. Then, for $T \in [0,\pi]$:*

$$\int_0^T t^{\alpha}\|\bar{p}_{\mathrm{N}}(\cdot,t) - p(\cdot,t)\|_{L_\infty(\mathbb{R})}\,dt \le C\begin{cases} N^{-\alpha/2} & \text{for } 0<\alpha<2,\\ N^{-1}\log(1+N) & \text{for } \alpha = 2,\\ N^{-1} & \text{for } \alpha>2, \end{cases} \tag{2.31}$$

where $C = C(\alpha)$ is a positive constant. Furthermore,

$$\int_0^T t^{\alpha}\|\bar{p}_{\mathrm{N}}(\cdot,t) - p(\cdot,t)\|_{L^2(\mathbb{R})}\,dt \le C\begin{cases} N^{-(\alpha/2+1/4)} & \text{for } -\frac{1}{2}<\alpha<\frac{3}{2},\\ N^{-1}\log(1+N) & \text{for } \alpha=\frac{3}{2},\\ N^{-1} & \text{for } \alpha>\frac{3}{2}, \end{cases} \tag{2.32}$$

where, again, $C = C(\alpha)$ is a positive constant.

3. Sampling versus Under-Resolved Approximation

In this section we address the issue of what features arise simply through the *sampling* of $H_{\mathrm{N}}(t)$, which is rapidly varying, rather than through the *approximation* of $H_{\mathrm{N}}(t)$ through under-resolved simulation of (2.1). We approximate (2.2) by the θ-method, taking the exact solution for the u_j as input data. By use of the second part of Lemma 2.4 we deduce that the approximation Z^n to $z(n\Delta t)$ is given by (2.8). No proofs will be given in this section as they are very similar to, but simpler than, those appearing in subsequent sections; they rely on the use of (2.8) rather than (2.7).

To state our basic result it will be useful to introduce some notation. Given a vector $(v_0, \ldots, v_{m-1})^T$ we define

$$v = (v_0, \ldots, v_{m-1})^T;$$

this notation will be extended to vectors other than v, specifically to w, z, and Z and to vectors indexed by superscripts. We make $\mathbb{R}^m$ a Hilbert space, defining

$$\begin{aligned} \langle v, w\rangle_m &= \Delta t \sum_{n=0}^{m-1} v_n w_n, \\ \|w\|^2_{L^2(0,m\Delta t)} &= \langle w, w\rangle_m. \end{aligned}$$

For purposes of comparison with the numerical method, it will be useful to project the solutions of (2.3) or (2.4) onto the grid by defining $z^n = z(n\Delta t)$.

For the first result we define w by

$$\dot{w} = f(w), \qquad w(0) = z_0 + \frac{\pi}{2} + \frac{r}{2}(1 - 2\theta),$$

noting that if $\theta = \frac{1}{2}$ this reduces to (2.3).

Theorem 3.1. *Consider* $\{Z^n\}_{n\geq 0}$ *solving* (2.2), [MP1] *by the* θ*-method, with* $H_{\mathrm{N}}(t)$ *given exactly and* $N\Delta t = r < 2\pi$, *and* $\{w^n\}_{n\geq 0}$ *the projection of* $w(t)$ *solving* (2.3) *onto the grid. Then, for* $n\Delta t \in [0, \pi]$, *and all* Δt *sufficiently small*

$$\|w - Z\|^2_{L^2(0,n\Delta t)} \leq C(n\Delta t)\Delta t.$$

This result should be compared with Theorem 2.1. It shows that if $\theta = \frac{1}{2}$ we loose no accuracy by approximating (2.2) numerically, whilst for $\theta \neq \frac{1}{2}$ we approximate the wrong problem—the jump in the initial condition is incorrectly represented. Recall that the condition $r < 2\pi$ arises in Lemma 2.4 to avoid resonances due to sampling. When we also approximate the $H_{\mathrm{N}}(t)$ by solving for the $u_j(t)$ numerically in the under-resolved regime (see (1.2)) the basic picture will remain, although theoretical bounds on the rate of convergence are diminished and the nature of the shifted initial condition will depend upon α as well as θ. Furthermore, it will be necessary to restrict $r < 2$ to avoid numerical instability; see Section 4.

Theorem 3.2. *Consider* $\{Z^n\}_{n\geq 0}$ *solving* (2.2), [MP2] *by the* θ*-method, with* $H_{\mathrm{N}}(t)$ *given exactly and* $N\Delta t = r < 2\pi$. *Then, for* $n\Delta t \in [0, \pi]$, *and all* Δt *sufficiently small*

$$\sup_{0\leq m\leq n-1} \mathbb{E}|z^m - Z^m|^2 \leq C(n\Delta t)\Delta t.$$

This should be compared with Theorem 2.2. The convergence rate is unaffected by the numerical approximation of (2.2). Note, however, that in contrast to the approximation of jumps, the value of θ does not affect the basic convergence result here. This basic picture will remain when we approximate the $u_j(t)$, and hence $H_{\mathrm{N}}(t)$, numerically, but the rates of convergence obtained will be reduced; see Section 5. It is interesting to note at this point that the issue of regaining optimal rates of convergence to solutions of ODEs forced by rough functions of time is addressed in paper [**10**]; that work does not apply directly to the problems considered here, though modifications might well do.

4. Numerical Approximation of Jumps

In this section it is useful to define the vectors $s^{(j)}, \bar{s}^{(j)}$ by

$$s_n^{(j)} = \sin(jn\Delta t)$$

and

$$\bar{s}^{(j)} = \sin(n\varphi_j).$$

Using the notational conventions established in the last section we see that, if $M\Delta t = \pi$ and using discrete orthogonality,

$$\langle s^{(k)}, s^{(j)}\rangle_M = \delta_{jk}\frac{\pi}{2}. \tag{4.1}$$

The following theorem should be compared with Theorems 2.1 and 3.1. By "solving numerically" we mean use of the fully discrete method (2.5), (2.6). Note that the theoretical bound on the rate of convergence is reduced when compared with Theorems 2.1 and 3.1, although numerical evidence indicates that this situation might be improved by more careful analysis.

Theorem 4.1. *Consider* $\{Z^n\}_{n\geq 0}$ *solving* [MP1] *numerically with* $\theta + \alpha = 1$ *and* $N\Delta t = r < 2$ *and* $\{z^n\}_{n\geq 0}$ *the projection of* $z(t)$ *solving* (2.3) *onto the grid. Then, for* $n\Delta t \in [0, \pi]$, *and all* Δt *sufficiently small*

$$\|z - Z\|^2_{L^2(0,n\Delta t)} \leq C(n\Delta t)\log|\Delta t^{-1}|\Delta t^{2/3}.$$

Proof. For simplicity we assume that there is an integer M such that $M\Delta t = \pi$. Other choices of Δt can be handled by approximation. By (2.9) we may write (2.11) as

$$z(t) = z_0 + \int_0^t f(z(s))\,ds + \frac{t}{2} + \sum_{j=1}^{\infty}\frac{\sin(jt)}{j}.$$

By Lemma 2.4 we obtain

$$\begin{aligned} z^n - Z^n \;=\; & \int_0^t f(z(s))ds - \Delta t {\sum_{m=0}^{n}}' f(Z^m) \\ & + \sum_{j \geq N+1} a_j \frac{\sin(jn\Delta t)}{j} + \sum_{j=1}^{N} a_j (j^{-1} - \gamma_j) \sin(jn\Delta t) \\ & + \sum_{j=1}^{N} a_j \gamma_j [\sin(jn\Delta t) - \sin(\varphi_j n)] \\ & + (\theta + \alpha - 1)\Delta t \sum_{j=1}^{N} 2a_j \sin^2(\varphi_j n/2), \end{aligned} \tag{4.2}$$

where for [MP1], $a_j = 1,\ j \geq 1$. Henceforth in this proof we set $\theta + \alpha = 1$. Now the regularity of solutions to ODEs implies that

$$\sup_{t \in [0,\pi]} \left| \int_0^t f(z(s))\, ds - \Delta t {\sum_{m=0}^{n}}' f(z^m) \right| \leq C\Delta t.$$

Defining $e^n = z^n - Z^n$, we have from (4.2), with $|q_n| \leq C\Delta t$:

$$\begin{aligned} e^n \;=\; & \Delta t {\sum_{m=0}^{n}}' [f(z^m) - f(Z^m)] + q_n \\ & + \sum_{j \geq N+1} \frac{s_n^{(j)}}{j} + \sum_{j=1}^{N} (j^{-1} - \gamma_j) s_n^{(j)} \\ & + \sum_{j=1}^{N} \gamma_j [s_n^{(j)} - \bar{s}_n^{(j)}]. \end{aligned}$$

Thus

$$\begin{aligned} |e^n|^2 \;\leq\; & 5\Delta t^2 \left[{\sum_{m=0}^{n}}' |f(z^m) - f(Z^m)| \right]^2 + 5C^2 \Delta t^2 \\ & + 5 \sum_{j,k \geq N+1} \frac{s_n^{(j)} s_n^{(k)}}{jk} + 5 \sum_{j,k=1}^{N} (j^{-1} - \gamma_j)(k^{-1} - \gamma_k) s_n^{(j)} s_n^{(k)} \\ & + 5 \left| \sum_{j=1}^{N} \gamma_j [s_n^{(j)} - \bar{s}_n^{(j)}] \right|^2. \end{aligned}$$

Now, using $n\Delta t \leq M\Delta t = \pi$, $n + 1 \leq 2n$, and $\theta \in [0, 1]$, we deduce that

$$\Delta t^2 \left[{\sum_{m=0}^{n}}' |f(z^m) - f(Z^m)| \right]^2 \;\leq\; \Delta t^2 L^2 \left[\sum_{m=0}^{n} |e^m| \right]^2$$

$$
\begin{aligned}
&\le \Delta t^2 L^2 (n+1) \sum_{m=0}^{n} |e^m|^2 \\
&\le 2\pi\, \Delta t L^2 \sum_{m=0}^{n} |e^m|^2 \\
&= 2\pi L^2 \|e\|^2_{L^2(0,n\Delta t)} + 2\pi\, \Delta t L^2 |e^n|^2.
\end{aligned}
$$

Thus, choosing Δt sufficiently small so that $(1 - 10\pi\, \Delta t L^2)^{-1} \le 2$, we obtain

$$
\begin{aligned}
|e^n|^2 \;\le\; & 20\pi L^2 \|e\|^2_{L^2(0,n\Delta t)} + 10C^2 \Delta t^2 \\
& + 10 \sum_{j,k \ge N+1} \frac{s_n^{(j)} s_n^{(k)}}{jk} + 10 \sum_{j,k=1}^{N} (j^{-1} - \gamma_j)(k^{-1} - \gamma_k) s_n^{(j)} s_n^{(k)} \\
& + 10 \left| \sum_{j=1}^{N} \gamma_j [s_n^{(j)} - \bar{s}_n^{(j)}] \right|^2 .
\end{aligned}
$$

Summing over $n \le M$ and using (4.1) we obtain

$$
\begin{aligned}
\|e\|^2_{L^2(0,n\Delta t)} \;\le\; & 20\pi\, \Delta t L^2 \left[\sum_{m=0}^{n-1} \|e\|^2_{L^2(0,m\Delta t)} \right] + 10\pi C^2 \Delta t^2 \\
& + 5\pi \sum_{j \ge N+1} \frac{1}{j^2} + 5\pi \sum_{j=1}^{N} (j^{-1} - \gamma_j)^2 \\
& + 10\Delta t \sum_{m=0}^{M-1} \left| \sum_{j=1}^{N} \gamma_j [s_m^{(j)} - \bar{s}_m^{(j)}] \right|^2 .
\end{aligned}
$$

By using

$$
1 - (1-x)^{1/2} \le x \qquad \forall\, x \in [0,1]
$$

we obtain

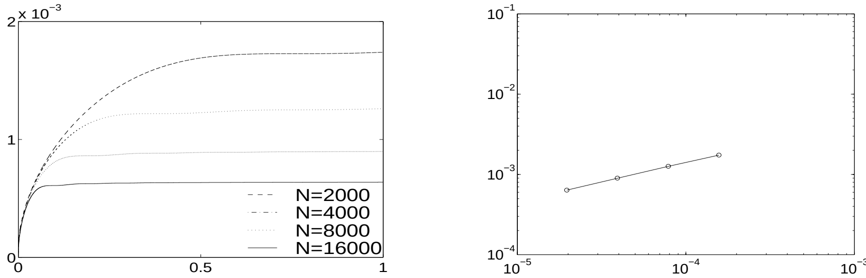
$$
\left| \gamma_j - \frac{1}{j} \right| = \mathcal{O}(\Delta t^2 j), \qquad |\gamma_j| = \mathcal{O}(j^{-1}), \tag{4.3}
$$

so that, since $N\Delta t = r$:

$$
\sum_{j \ge N+1} \frac{1}{j^2} = \mathcal{O}(\Delta t), \qquad \sum_{j=1}^{N} (j^{-1} - \gamma_j)^2 = \mathcal{O}(\Delta t). \tag{4.4}
$$

Hence

$$
\begin{aligned}
\|e\|^2_{L^2(0,n\Delta t)} \;\le\; & 20\pi\, \Delta t L^2 \left[\sum_{m=0}^{n-1} \|e\|^2_{L^2(0,m\Delta t)} \right] \\
& + \mathcal{O}(\Delta t) + 10\Delta t \sum_{m=0}^{M-1} \left| \sum_{j=1}^{N} \gamma_j [s_m^{(j)} - \bar{s}_m^{(j)}] \right|^2 .
\end{aligned}
$$



(a) (b)

Fig. 4.1. (a) $L^2(0,t)$ error curves from [MP1] with $f \equiv 0$ using method (2.5), (2.6) with $N\Delta t = \pi/10$ and $\theta = 0$, $\alpha = 1$. (b) Log–log plot for the convergence rate of $L^2(0,1)$ error as a function of Δt; the approximate slope is 0.4831.

The near-orthogonality of the $s^{(j)}$ and the $\bar{s}^{(k)}$ enables a bound on the final term (use Appendix C with $\beta_j = \gamma_j$) and the required result follows from a Gronwall argument.[2] $\square$

To verify this result numerically we performed a simulation for [MP1] with $f \equiv 0$ using method (2.5), (2.6). The parameters for the experiment were $\alpha = 1$, $\theta = 0$, and $N\Delta t = \pi/10$ for $N = 2000$, 4000, 8000, and 16,000. We observed that the $L^2(0,t)$ error converged at a rate of $\mathcal{O}(\Delta t^{0.4831})$, an improvement over the proven bound $\mathcal{O}(\sqrt{\log \Delta t^{-1}}\Delta t^{1/3})$; see Figure 4.1. To close the gap between theory and experiment will require a more careful analysis of the term estimated in Appendix C.

Note that the convergence rate was determined as the slope of the least-squares fit line through the log–log data points in Figure 4.1. This methodology is employed for determining all numerical convergence rates in this paper.

We now comment on what happens to the numerical method if $\theta + \alpha \neq 1$. In this case, Z^n has an extra contribution

$$(1 - \theta - \alpha)\Delta t \sum_{j=1}^{N} [1 - \cos(\varphi_j n)].$$

By use of Appendix C with $\beta_j = \Delta t = \zeta/N \leq \zeta/j$ it follows that

$$\Delta t \sum_{j=1}^{N} \cos(\varphi_j n) = \Delta t \sum_{j=1}^{N} \cos(jn\Delta t) + \delta_1,$$

where

$$\|\delta_1\|^2_{L^2(0,M\Delta t)} = \mathcal{O}(\log|\Delta t^{-1}|\Delta t^{2/3}).$$

[2] In the proof of Theorem 3.1 the final term does not appear, thus improving the rate of convergence.

Summing the resulting geometric series found by writing the cosine as the real part of a complex exponential (by use of [**8**, 1.342(2)]) shows that Z^n has an extra contribution

$$(1 - \theta - \alpha)\{r + \delta_2\},$$

where

$$\|\delta_2\|^2_{L^2(0,M\Delta t)} = \mathcal{O}(\log|\Delta t^{-1}|\Delta t^{2/3}).$$

From this it follows that for $\theta + \alpha \neq 1$ and under (1.2), the numerical method approximates the ODE

$$\dot{y} = f(y), \qquad y(0) = z_0 + \frac{\pi}{2} + (1 - \theta - \alpha)r \tag{4.5}$$

instead of the true limiting equation (2.3). Thus the numerical method accurately computes the wrong limit. More precisely we have:

Theorem 4.2. *Consider* $\{Z^n\}_{n\geq 0}$ *solving* [MP1] *numerically with* $\theta + \alpha \neq 1$ *and* $N\Delta t = r < 2$ *and* $\{y^n\}_{n\geq 0}$ *the projection of* $y(t)$ *solving* (4.5) *onto the grid. Then, for* $n\Delta t \in [0, \pi]$:

$$\|y - Z\|^2_{L^2(0,n\Delta t)} \leq C(n\Delta t)\log|\Delta t^{-1}|\Delta t^{2/3}.$$

This result has been verified via simulation analogous to the experiment illustrated in Figure 4.1. Again we observed that the $L^2(0, t)$ error converged at rate approximately $\mathcal{O}(\Delta t^{1/2})$, suggesting the theoretical upper bounds from Theorems 4.1 and 4.2 may be improved.

5. Strong Numerical Approximation of White Noise

We employ the notation introduced in Section 3. The following theorem should be compared with Theorems 2.2 and 3.2. By "solving numerically" we mean use of the fully discrete method (2.5), (2.6). Note that the theoretical bound on the rate of convergence is reduced when compared with Theorems 2.2 and 3.2; numerical evidence is inconclusive as to whether this situation might be improved by more careful analysis.

Theorem 5.1. *Consider* $\{Z^n\}_{n\geq 0}$ *solving* [MP2] *numerically with* $N\Delta t = r < 2$. *Then, for* $n\Delta t \in [0, \pi]$, *and all* Δt *sufficiently small*

$$\sup_{0\leq m\leq n-1} \mathbb{E}|z^m - Z^m|^2 \leq C(n\Delta t)\Delta t^{2/3}.$$

Proof. By (2.13) we can almost surely rewrite (2.14) as

$$z(t) = z_0 + \int_0^t f(z(s))\,ds + \frac{\eta_0 t}{\sqrt{\pi}} + \sqrt{\frac{2}{\pi}} \sum_{j=1}^{\infty} \eta_j \frac{\sin(jt)}{j}.$$

Using the limited regularity of solutions $z(t)$ to the SDE (2.4) it follows that

$$\mathbb{E}\left|\int_0^t f(z(s))\,ds - \Delta t {\sum_{m=0}^{n}}' f(z^m)\right|^2 \le C\Delta t.$$

By techniques similar to those employed in the previous section, but with $a_j = \eta_j$, we obtain from (4.2):

$$\begin{aligned}\mathbb{E}|e^n|^2 \;\le\; & 6(n+1)\Delta t^2 L^2 \sum_{m=0}^{n} \mathbb{E}|e^m|^2 + 6C\Delta t \\ & + 6\sum_{j\ge N+1}\frac{1}{j^2} + 6\sum_{j=1}^{N}(j^{-1}-\gamma_j)^2 \\ & + 6\sum_{j=1}^{N}\gamma_j^2[\sin(jn\Delta t) - \sin(\varphi_j n)]^2 \\ & + 24N\Delta t^2(\theta+\alpha-1)^2.\end{aligned}$$

In this proof we use the fact that $a_j = \eta_j$ are i.i.d. random variables distributed as $\mathcal{N}(0,1)$ so that they are orthogonal under $\mathbb{E} : \mathbb{E}\eta_i\eta_j = \delta_{ij}$.

Now

$$\begin{aligned}\sum_{j=1}^{N}\gamma_j^2[\sin(jn\Delta t) - \sin(\varphi_j n)]^2 \;\le\; & \mathcal{O}\left[\sum_{j=1}^{N^\alpha} j^4\Delta t^4 + \sum_{j\ge N^\alpha}\frac{1}{j^2}\right] \\ =\; & \mathcal{O}(\Delta t^4 N^{5\alpha} + N^{-\alpha}).\end{aligned}$$

Choosing $\alpha = \frac{2}{3}$ we obtain, also using (4.4) and $(n+1)\Delta t \le 2n\Delta t \le 2\pi$:

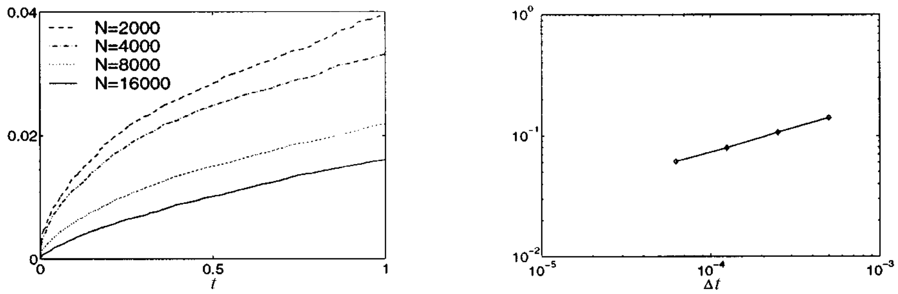
$$\mathbb{E}|e^n|^2 \le 12\pi\,\Delta t L^2 \sum_{m=0}^{n}\mathbb{E}|e^m|^2 + \mathcal{O}(\Delta t^{2/3})$$

and the required result follows by a Gronwall argument.[3] □

Once again we verified our result numerically, solving [MP2] with $\theta = \alpha = 0$, $f(z) = -z$, and $N\Delta t = 1$ for $N = 2000$, 4000, 8000, and 16,000. Due to the highly oscillatory behavior of a single realization path, we depict the $L^2(0,t)$ error, observing an approximate convergence rate of $\mathcal{O}(\Delta t^{0.3997})$ for this single realization; see Figure 5.1. Note that Theorem 5.1 estimates the average error over all paths, whilst our experiment is for a single path.

---

[3] In Theorem 3.2 the final term does not appear in the analysis and hence the improved rate of convergence.



(a) (b)

Fig. 5.1. (a) $L^2(0, t)$ error curves from [MP2] with $f(z) = -z$ using method (2.5), (2.6) with $N\Delta t = 1$ and $\theta = \alpha = 0$. (b) Log–log plot for the convergence rate of $L^2(0, 1)$ as a function of Δt; the approximate slope is 0.3997.

6. Weak Numerical Approximation of White Noise

Our analysis is confined to the simple case where $f \equiv 0$ so that the desired weak convergence properties of [MP2] solved numerically should approximate those of pure diffusion. This enables us to use Fourier techniques. After the analysis some experiments will be presented to show that the result is more general than that presented in the following theorem and can be extended to nonzero f. To analyze the case of nonzero f would require more sophisticated techniques, such as those described in [**2**].

The following theorem should be compared with Theorem 2.3. By "solving numerically" we mean use of the fully discrete method (2.5), (2.6). Numerical evidence indicates that the rate of convergence in this theorem might be improved by more careful analysis.

Theorem 6.1. *Consider* $\{Z^n\}_{n\geq 1}$ *solving* [MP2] *numerically with* $N\Delta t = r < 2$. *Then, for* $n\Delta t \in [0, \pi]$, *and all* Δt *sufficiently small,*

$$\sup_{z_0 \in R} |\mathbb{E}g(z(n\Delta t)) - \mathbb{E}g(Z^n)| \leq C \begin{cases} N^{(1-\beta)/3}, & 1 < \beta < 3, \\ N^{-2/3}\log(1+N), & \beta = 3, \\ N^{-2/3}, & \beta > 3, \end{cases}$$

where $C = C(\beta, C_1)$ *with* β *and* C_1 *as in Hypothesis* H.

Proof. We let $p^n_{\mathrm{N},\Delta t}(z; \omega)$ denote the pdf for Z^n solving (2.6), for each fixed ω, and

$$\bar{p}^n_{\mathrm{N},\Delta t}(z) = \mathbb{E}p^n_{\mathrm{N},\Delta t}(z; \omega).$$

Since $f(\cdot) \equiv 0$ we have, by Lemma 2.4,

$$Z^n = z_0 + s^n,$$

where

$$s^n = \frac{1}{\pi}\eta_0(n\Delta t) + \sum_{j=1}^{N}\sqrt{\frac{2}{\pi}}\eta_j\{\gamma_j \sin(\varphi_j n) + 2\Delta t(1-\theta-\alpha)\sin^2(\varphi_j n/2)\}.$$

If $p^0_{\mathrm{N},\Delta t}(z;\omega) = p_0(z)$ then $p^n_{\mathrm{N},\Delta t}(z;\omega) = p_0(z - s^n)$; assuming that $p_0(z) = \delta(z - z_0)$ we obtain

$$\bar{p}^n_{\mathrm{N},\Delta t}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(z_0 - z)}\psi^n_{\mathrm{N},\Delta t}(k)\,dk,$$

where $\psi^n_{\mathrm{N},\Delta t}(k)$ is the characteristic function for $s^n = s^n(\omega)$; i.e.,

$$\begin{aligned}\psi^n_{\mathrm{N},\Delta t}(k) &= \mathbb{E}\,\exp\{iks^n(t;\omega)\}\\ &= \exp\left\{-\tfrac{1}{2}k^2\left[\frac{(n\Delta t)^2}{\pi} + S_2^N\right]\right\},\end{aligned}$$

where

$$S_2^N = \frac{2}{\pi}\sum_{j=1}^{N}[\gamma_j\sin(n\varphi_j) + 2\Delta t(1-\theta-\alpha)\sin^2(\varphi_j n/2)]^2.$$

By (2.23) and (2.24) we deduce that

$$|\psi_{\mathrm{N}}(k, n\Delta t) - \psi^n_{\mathrm{N},\Delta t}(k)| \le e^{-k^2(n\Delta t)^2/2\pi}[1 - e^{-k^2|S_1^N - S_2^N|}].$$

But

$$\begin{aligned}\frac{\pi}{2}|S_1^N - S_2^N| = \Bigg|&\sum_{j=1}^{N}\left[\gamma_j^2 - \frac{1}{j^2}\right]\sin^2(jn\Delta t)\\ &+ \sum_{j=1}^{N}\gamma_j^2[\sin^2(n\varphi_j) - \sin^2(jn\Delta t)]\\ &+ \sum_{j=1}^{N}4\Delta t(1-\theta-\alpha)\gamma_j\sin(n\varphi_j)\sin^2(n\varphi_j/2)\\ &+ \sum_{j=1}^{N}4\Delta t^2(1-\theta-\alpha)^2\sin^4(n\varphi_j/2)\Bigg|.\end{aligned}$$

Thus, by (4.3),

$$\begin{aligned}\frac{\pi}{2}|S_1^N - S_2^N| &\le \sum_{j=1}^{N}\frac{C}{j}\left|\gamma_j - \frac{1}{j}\right| + \sum_{j=1}^{N}\frac{C}{j^2}|\sin(n\varphi_j) - \sin(jn\Delta t)|\\ &\quad + \sum_{j=1}^{N}\frac{C\Delta t}{j} + \sum_{j=1}^{N}C\Delta t^2\\ &\le \mathcal{O}(\log|\Delta t^{-1}|\Delta t) + \sum_{j=1}^{N}\frac{C}{j^2}|\sin(n\varphi_j) - \sin(jn\Delta t)|.\end{aligned}$$

But $\varphi_j = j\Delta t + \mathcal{O}(j^3\Delta t^3)$ and so, by choosing $\beta = \frac{2}{3}$ and noting that $n\Delta t = \mathcal{O}(1)$,

$$\sum_{j=1}^{N} \frac{C}{j^2} |\sin(n\varphi_j) - \sin(jn\Delta t)| \leq \mathcal{O}\left(\sum_{j=1}^{N^\beta} j\Delta t^2 + \sum_{j\geq N^\beta} \frac{1}{j^2}\right) = \mathcal{O}(\Delta t^{2/3}).$$

Thus

$$|\psi_{\mathrm{N}}(k, n\Delta t) - \psi^n_{\mathrm{N},\Delta t}(k)| \leq e^{-k^2(n\Delta t)^2/2\pi}[1 - e^{-Ck^2/N^{2/3}}].$$

Now, by Parseval's identity,

$$\begin{aligned} \mathbb{E}g(z_{\mathrm{N}}(n\Delta t)) - \mathbb{E}g(Z^n) &= \int_{-\infty}^{\infty} \left[\bar{p}_{\mathrm{N}}(z, n\Delta t) - \bar{p}^n_{\mathrm{N},\Delta t}(z)\right] g(z) dz \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(z_0 - z)}[\psi_{\mathrm{N}}(k, n\Delta t) - \psi^n_{\mathrm{N},\Delta t}(k)]\hat{g}(k)\, dk. \end{aligned}$$

Thus, by Hypothesis H,

$$|\mathbb{E}g(z_{\mathrm{N}}(n\Delta t)) - \mathbb{E}g(Z^n)| \leq \frac{C_1}{\pi} \int_0^{\infty} e^{-k^2(n\Delta t)^2/2\pi}[1 - e^{-Ck^2/N^{2/3}}](1 + k)^{-\beta} dk.$$

Analysis analogous to that at the end of the proof of Theorem 2.3 (using Appendix A) but with N^{-1} replaced by $N^{-2/3}$ gives the required result. □

For our first numerical experiment we solved [MP2] with $f \equiv 0$ and chose $g(z) = z^2$. Thus z is simply Brownian motion and $\mathbb{E}g(z(t)) = t$. However, calculating $\mathbb{E}g(Z^n)$ accurately is a computationally intense task since, by Theorem 5.1, for sufficiently smooth g:

$$|\mathbb{E}g(z(n\Delta t)) - \mathbb{E}g(Z^n)| \leq \mathcal{O}(N^{-2/3}).$$

Hence to determine the rate of convergence, the statistical error in estimating the expectation $\mathbb{E}g(Z^n)$ must be insignificant compared to this bound. Furthermore, the variance of $g(Z^n)$ increases as n increases, thus requiring more realizations to accurately estimate this expectation. [4]

Figure 6.1 shows the difference in numerical estimates of the expectations up to time $t = 0.1$, using eight million and ten million realizations with $N = 1600$. Note that the curves differ for $t > 0.05$ in the two cases, even for $\mathcal{O}(10^7)$ realizations (though the relative error $|t - \mathbb{E}g(Z^n)|/t$ is better behaved). Moreover, for large t ($t \approx 1$), this statistical error overwhelms the quantity of interest $|\mathbb{E}g(z(n\Delta t)) - \mathbb{E}g(Z^n)|$. This suggests that to examine the rate of weak convergence numerically we are restricted to small time intervals and a large number of realizations. Note that for $t \leq 0.05$ both estimates of $\mathbb{E}g(Z^n)$ are fairly well converged and, in fact,

[4] Variance reduction techniques could, perhaps, be used to relieve this problem; we have not chosen to pursue this here as the data required to illustrate our point can be easily found by intensive simulation.

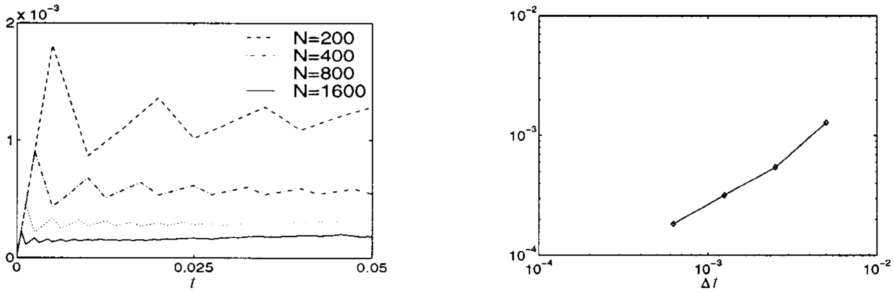


Fig. 6.1. $|t - \mathbb{E}g(Z^n)|$ up to time $t = 0.1$ for $N = 1600$ and $\mathbb{E}g(Z^n)$ approximated with eight million and ten million realizations.

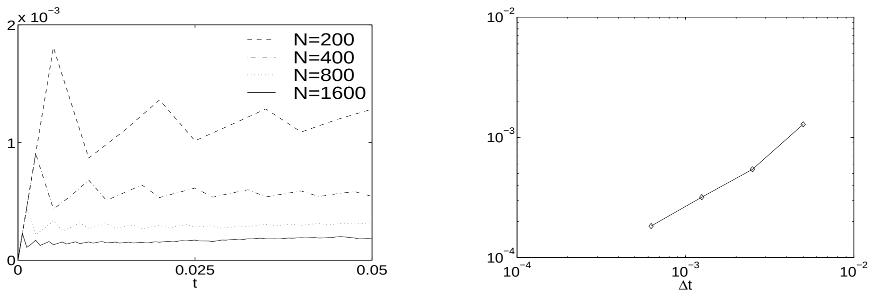


Fig. 6.2. (a) $|\mathbb{E}g(z(n\Delta t)) - \mathbb{E}g(Z^n)|$ error curves from [MP2] with $f \equiv 0$ using method (2.5), (2.6) with $N\Delta t = 1$ and $\theta = \alpha = 0$. (b) Log–log plot for the convergence rate of error at $t = 0.05$ as a function of Δt; the approximate slope is 0.9196.

deviations are negligible in comparison with the quantity $|t - \mathbb{E}g(Z^n)|$ which we wish to estimate.

For our experiment we examined weak convergence up to time $t = 0.05$ with $\theta = 0, \alpha = 0$, and $N = 200, 400, 800$, and 1600. We observed that $|\mathbb{E}g(z(n\Delta t) - \mathbb{E}g(Z^n)|$ at $t = 0.05$ converged at approximate rate of $\mathcal{O}(\Delta t^{0.9196})$, an improvement over the theoretical rate of $\mathcal{O}(\Delta t^{2/3})$. These results are depicted in Figure 6.2.

Finally we repeated this experiment using a nonzero forcing function: $f(z) = z - z^3$. We observed a convergence rate of $\mathcal{O}(\Delta t^{0.9313})$, suggesting that the theory can be extended to incorporate nonzero f.

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Appendix A

Our aim in this Appendix is to prove the estimate (2.30). The starting point is the following decomposition:

$$\int_0^\infty e^{-k^2t^2/2\pi}(1+k)^{-\beta}\min\left(1,\frac{k^2}{\pi N}\right)dk$$
$$= \int_0^{\sqrt{\pi N}} \frac{e^{-k^2t^2/2\pi}}{(1+k)^\beta}\,\frac{k^2}{\pi N}\,dk + \int_{\sqrt{\pi N}}^\infty \frac{e^{-k^2t^2/2\pi}}{(1+k)^\beta}\,dk \equiv I + II. \quad \text{(A.1)}$$

We begin by estimating term I for $t > 0$:

$$I \;=\; \frac{t^{-3}}{\pi N}\int_0^{\sqrt{\pi N}} \frac{e^{-k^2t^2/2\pi}}{(1+kt/t)^\beta}(kt)^2\,d(kt)$$

$$= \frac{t^{\beta-3}}{\pi N}\int_0^{t\sqrt{\pi N}} \frac{e^{-u^2/2\pi}}{(t+u)^\beta} u^2\,du. \tag{A.2}$$

(1a) First, suppose that $0 < t\sqrt{\pi N} \leq 1$. Then, assuming $\beta \neq 3$:

$$\begin{aligned} I &\leq \frac{t^{\beta-3}}{\pi N}\int_0^{t\sqrt{\pi N}} \left(\frac{u}{t+u}\right)^2 \frac{du}{(t+u)^{\beta-2}} \\ &\leq \frac{t^{\beta-3}}{\pi N}\left.\frac{(t+u)^{3-\beta}}{3-\beta}\right|_0^{t\sqrt{\pi N}}, \\ &= \frac{t^{\beta-3}}{\pi N}\frac{t^{3-\beta}}{3-\beta}[(1+\sqrt{\pi N})^{3-\beta}-1] \\ &= \frac{C}{N}[(1+\sqrt{\pi N})^{3-\beta}-1] \\ &\leq \begin{cases} CN^{-1} & \text{when } \beta > 3, \\ CN^{(1-\beta)/2} & \text{when } 1 < \beta < 3, \end{cases} \end{aligned}$$

where $C = C(\beta)$ is a positive constant. Similarly, when $\beta = 3$:

$$\begin{aligned} I &\leq \frac{1}{\pi N}\int_0^{t\sqrt{\pi N}} \frac{du}{t+u} = \frac{1}{\pi N}\log(t+u)\Big|_0^{t\sqrt{\pi N}} \\ &= \frac{1}{\pi N}(\log(t+t\sqrt{\pi N})-\log t) \\ &= \frac{1}{\pi N}\log(1+\sqrt{\pi N}) \leq CN^{-1}\log(1+N), \end{aligned}$$

where C is a positive constant. To summarize the situation, for $0 < t\sqrt{\pi N} \leq 1$ we have that

$$I \leq \begin{cases} CN^{(1-\beta)/2}, & 1 < \beta < 3, \\ CN^{-1}\log(1+N), & \beta = 3, \\ CN^{-1}, & \beta > 3, \end{cases} \tag{A.3}$$

where $C = C(\beta)$ is a positive constant.

(1b) Now suppose that $t\sqrt{\pi N} \geq 1$. Then,

$$\left(\frac{1}{t}\right)^{3-\beta} \leq \left(\sqrt{\pi N}\right)^{3-\beta}, \qquad 1 < \beta < 3. \tag{A.4}$$

We shall make use of this below. First, since $(t+u)^{-\beta}u^2 \leq (t+u)^{2-\beta}$ for $0 \leq u \leq 1$, and $(t+u)^{-\beta} \leq 1$ for $u \geq 1$, we have from (A.2) that

$$\begin{aligned} I &\leq \frac{t^{\beta-3}}{\pi N}\left(\int_0^1 \frac{e^{-u^2/2\pi}}{(t+u)^\beta}u^2\,du + \int_1^\infty \frac{e^{-u^2/2\pi}}{(t+u)^\beta}u^2 du\right) \\ &\leq \frac{Ct^{\beta-3}}{N}\left(\int_0^1 \frac{du}{(t+u)^{\beta-2}} + 1\right) \end{aligned}$$

$$= \begin{cases} \dfrac{C}{N}\left(\dfrac{(1+1/t)^{3-\beta}-1}{3-\beta}+1\right); & \beta \neq 3, \\ \dfrac{C}{N}(\log(1+\dfrac{1}{t})+1); & \beta = 3. \end{cases}$$

Finally, using (A.4) this implies that, for $t\sqrt{\pi N} \geq 1$:

$$I \leq \begin{cases} CN^{(1-\beta)/2}, & 1 < \beta < 3, \\ CN^{-1}\log(1+N), & \beta = 3, \\ CN^{-1}, & \beta > 3. \end{cases} \tag{A.5}$$

From (A.3) and (A.5) we deduce that

$$I \leq \begin{cases} CN^{(1-\beta)/2}, & 1 < \beta < 3, \\ CN^{-1}\log(1+N), & \beta = 3, \\ CN^{-1}, & \beta > 3. \end{cases} \tag{A.6}$$

for all $t > 0$, where $C = C(\beta)$ is a positive constant.

Now we consider term II in (A.1):

$$\begin{aligned} II &= \int_{\sqrt{\pi N}}^{\infty} \frac{e^{-k^2t^2/2\pi}}{(1+k)^\beta}\,dk \\ &= \frac{1}{t}\int_{\sqrt{\pi N}}^{\infty} \frac{e^{-(kt)^2/2\pi}}{(1+kt/t)^\beta}\,d(kt) = t^{\beta-1}\int_{t\sqrt{\pi N}}^{\infty} \frac{e^{-u^2/2\pi}}{(t+u)^\beta}\,du. \end{aligned}$$

(2a) Suppose that $0 < t\sqrt{\pi N} \leq 1$:

$$\begin{aligned} II &\leq t^{\beta-1}\left\{\int_{t\sqrt{\pi N}}^{1} \frac{e^{-u^2/2\pi}}{(t+u)^\beta}\,du + \int_1^\infty \frac{e^{-u^2/2\pi}}{(t+u)^\beta}\,du\right\} \\ &\leq t^{\beta-1}\left\{\int_{t\sqrt{\pi N}}^{1} \frac{1}{(t+u)^\beta}\,du + \int_1^\infty e^{-u^2/2\pi}\,du\right\} \\ &\leq Ct^{\beta-1}\left\{\left.\frac{(t+u)^{1-\beta}}{1-\beta}\right|_{t\sqrt{\pi N}}^{1} + 1\right\} \\ &= Ct^{\beta-1}\left\{\frac{(1+t)^{1-\beta} - t^{1-\beta}(1+\sqrt{\pi N})^{1-\beta}}{1-\beta} + 1\right\} \\ &\leq C(|t^{\beta-1}(1+t)^{1-\beta} - (1+\sqrt{\pi N})^{1-\beta}| + t^{\beta-1}) \\ &\leq C(N^{(1-\beta)/2} + t^{\beta-1}) \\ &\leq CN^{(1-\beta)/2}, \end{aligned}$$

where in the transition to the last line we made use of the fact that $t\sqrt{\pi N} \leq 1$. Here $C = C(\beta)$ is a positive constant.

(2b) Now suppose that $t\sqrt{\pi N} \geq 1$. Then,

$$\begin{aligned} II &\leq t^{\beta-1} \int_{t\sqrt{\pi N}}^{\infty} \frac{e^{-u^2/2\pi}}{(t+u)^{\beta}}\, du \\ &\leq t^{\beta-1} e^{-t^2 N/2} \int_{t\sqrt{\pi N}}^{\infty} \frac{du}{(t+u)^{\beta}} \\ &= t^{\beta-1} e^{-t^2 N/2} \frac{(t + t\sqrt{\pi N})^{1-\beta}}{\beta - 1} \\ &= e^{-t^2 N/2} \frac{(1 + \sqrt{\pi N})^{1-\beta}}{\beta - 1} \\ &\leq \frac{e^{-1/2\pi}}{\beta - 1} N^{(1-\beta)/2} \left(\sqrt{\pi} + \frac{1}{\sqrt{N}} \right)^{1-\beta} \\ &\leq C N^{(1-\beta)/2}, \end{aligned}$$

where $C = C(\beta)$ is a positive constant. Thus, to summarize,

$$II \leq C N^{(1-\beta)/2}, \qquad \beta > 1, \tag{A.7}$$

with $C = C(\beta)$ a positive constant. Finally, substituting the bounds (A.6) and (A.7) into (A.1) we arrive at the estimate (2.30).

Appendix B

Proof of Proposition 2.5. Clearly,

$$\begin{aligned} |\bar{p}_{\mathrm{N}}(z,t) - p(z,t)| &= \frac{1}{2\pi} \left| \int_{-\infty}^{\infty} e^{ik(z_0 - z)} [e^{-\frac{1}{2}k^2 t} - \psi_{\mathrm{N}}(k,t)]\, dk \right| \\ &\leq \int_{-\infty}^{\infty} |e^{-\frac{1}{2}k^2 t} - \psi_{\mathrm{N}}(k,t)|\, dk. \end{aligned} \tag{B.1}$$

We substitute (2.26) into (B.1) to conclude that

$$\begin{aligned} |\bar{p}_{\mathrm{N}}(z,t) - p(z,t)| &\leq \int_{-\infty}^{\infty} e^{-k^2 t^2/2\pi} [1 - e^{-k^2/\pi N}]\, dk \\ &= \frac{1}{t} \int_{-\infty}^{\infty} \exp\left\{ -\frac{(kt)^2}{2\pi} \right\} d(kt) \\ &\quad - \frac{1}{\sqrt{t^2 + 2/N}} \int_{-\infty}^{\infty} \exp\left\{ -\frac{(k\sqrt{t^2 + 2/N}\,)^2}{2\pi} \right\} \\ &\quad \times d\left(k\sqrt{t^2 + \frac{2}{N}} \right) \\ &= C_0 \left[\frac{1}{t} - \frac{1}{\sqrt{t^2 + 2/N}} \right], \end{aligned} \tag{B.2}$$

where we put

$$C_0 = \int_{-\infty}^{\infty} \exp\left\{-\frac{s^2}{2\pi}\right\} ds.$$

Next, we note the elementary inequality

$$1 - \frac{1}{(1+2y)^{1/2}} \leq \min(1, y), \qquad y \geq 0. \tag{B.3}$$

Choosing $y = 1/(Nt^2)$ in (B.3) we deduce that

$$1 - \frac{1}{(1+2/Nt^2)^{1/2}} \leq \min\left(1, \frac{1}{Nt^2}\right).$$

Consequently,

$$|\bar{p}_{\mathrm{N}}(z,t) - p(z,t)| \leq \frac{C_0}{t} \min\left(1, \frac{1}{Nt^2}\right), \tag{B.4}$$

After multiplying (B.4) by t^α, $\alpha > 0$, and integrating with respect to t between 0 and T, we obtain

$$\begin{aligned}
&\int_0^T t^\alpha |\bar{p}_{\mathrm{N}}(z,t) - p(z,t)|\, dt \\
&\qquad = \int_0^{1/\sqrt{N}} t^\alpha |\bar{p}_{\mathrm{N}}(z,t) - p(z,t)|\, dt + \int_{1/\sqrt{N}}^T t^\alpha |\bar{p}_{\mathrm{N}}(z,t) - p(z,t)|\, dt \\
&\qquad \leq C_0 \int_0^{1/\sqrt{N}} t^{\alpha-1}\, dt + \frac{C_0}{N} \int_{1/\sqrt{N}}^T t^{\alpha-3}\, dt \equiv I + II.
\end{aligned} \tag{B.5}$$

Elementary calculations show that

$$I = \frac{1}{\alpha} N^{-\alpha/2}, \qquad \alpha > 0, \tag{B.6}$$

and

$$II = C \begin{cases} \dfrac{1}{N} \dfrac{1}{\alpha - 2} \left(1 - \left(\dfrac{1}{\sqrt{N}}\right)^{\alpha-2}\right) & \text{for } \alpha \neq 2, \\[2ex] \dfrac{1}{2N} \log N & \text{for } \alpha = 2. \end{cases} \tag{B.7}$$

It follows from (B.7) that

$$II \leq \begin{cases} CN^{-\alpha/2} & \text{for } 0 < \alpha < 2, \\ CN^{-1} \log(1+N) & \text{for } \alpha = 2, \\ CN^{-1} & \text{for } \alpha > 2, \end{cases} \tag{B.8}$$

where $C = C(\alpha, T)$ is a positive constant. Finally, inserting (B.6) and (B.8) into (B.5), we obtain (2.31).

Next we derive a similar bound where instead of the L_∞-norm we have the L^2-norm under the integral sign. By Parseval's identity and (2.26):

$$
\begin{aligned}
\|\bar{p}_{\mathrm{N}}(\cdot,t)-p(\cdot,t)\|^2_{L^2(R)} &\le C\int_{-\infty}^{\infty}[e^{-\frac{1}{2}k^2t}-\psi_{\mathrm{N}}(k,t)]^2\,dk\\
&\le C\int_{-\infty}^{\infty}e^{-(1/\pi)k^2t^2}[1-2e^{-k^2/\pi N}+e^{-2k^2/\pi N}]\,dk\\
&\le C\left[\int_{-\infty}^{\infty}e^{-k^2t^2/\pi}\,dk-2\int_{-\infty}^{\infty}e^{-(k^2/\pi)(t^2+N^{-1})}\,dk\right.\\
&\qquad\left.+\int_{-\infty}^{\infty}e^{-(k^2/\pi)(t^2+2N^{-1})}\,dk\right]\\
&\le C\left[\frac{1}{t}-\frac{2}{(t^2+1/N)^{1/2}}+\frac{1}{(t^2+2/N)^{1/2}}\right].
\end{aligned}
$$

Now,

$$1-2(1+y)^{-1/2}+(1+2y)^{-1/2}\le C_2\min(1,y^2),$$

where C_2 is a positive constant. Taking

$$y=\frac{1}{Nt^2}$$

in this inequality, we deduce that

$$\|\bar{p}_{\mathrm{N}}(\cdot,t)-p(\cdot,t)\|_{L^2(R)}\le\frac{C}{\sqrt{t}}\min\left(1,\frac{1}{Nt^2}\right),$$

where C is a positive constant. Thus

$$\int_0^1 t^{\alpha}\|\bar{p}_{\mathrm{N}}(\cdot,t)-p(\cdot,t)\|_{L^2(R)}\,dt\le C\left[\int_0^{1/\sqrt{N}}t^{\alpha-\frac{1}{2}}dt+\int_{1/\sqrt{N}}^{1}\frac{t^{\alpha-\frac{5}{2}}}{N}\,dt\right].$$

Consequently, we obtain (2.32).

Appendix C

We wish to evaluate

$$S:=\Delta t\sum_{m=0}^{M-1}\left|\sum_{j=1}^{N}\beta_j[v_m^{(j)}-w_m^{(j)}]\right|^2,$$

where

$$\begin{pmatrix}v_n^{(j)}\\ w_n^{(j)}\end{pmatrix}=\begin{pmatrix}\sin(\varphi_j n)\\ \sin(jn\Delta t)\end{pmatrix}\qquad\text{or}\qquad\begin{pmatrix}\cos(\varphi_j n)\\ \cos(jn\Delta t)\end{pmatrix}.$$

In the two applications of this result

$$|\beta_j| \leq \frac{C}{j}.$$

Now

$$S = \sum_{j,k=1}^{N} \beta_j \beta_k [S_1^{j,k} - 2S_2^{j,k} + S_3^{j,k}],$$

where

$$S_1^{j,k} = \langle v^{(j)}, v^{(k)} \rangle_M, \qquad S_2^{j,k} = \langle v^{(j)}, w^{(k)} \rangle_M, \qquad S_3^{j,k} = \langle w^{(j)}, w^{(k)} \rangle_M.$$

Here $M\Delta t = \pi$. But, for example,

$$\begin{aligned} S_1^{j,k} &= \Delta t \sum_{n=0}^{M-1} v_n^{(j)} v_n^{(k)} \\ &= \frac{\Delta t}{2} \sum_{n=0}^{M-1} \cos[(\varphi_j - \varphi_k)n] \pm \frac{\Delta t}{2} \sum_{n=0}^{M-1} \cos[(\varphi_j + \varphi_k)n] \end{aligned}$$

with $+$ for the cosine case and—for the sine case. Similar expressions are found for the other inner products $S_2^{j,k}$, $S_3^{j,k}$. Using [**8**, 1.342(2)] it follows that

$$\sum_{n=0}^{M-1} \cos(nx) = \frac{\sin[Mx]}{2\tan[x/2]} + \sin^2[Mx/2]. \tag{C.1}$$

Summing two terms of the form (C.1) with $x = x^{\pm}$ and

$$x^{\pm} = \varphi_j \pm \varphi_k, \qquad x^{\pm} = \varphi_j \pm k\Delta t, \qquad x^{\pm} = (j \pm k)\Delta t,$$

gives the three inner products required to compute S.

In all three cases there is $k^* = k^*(j)$ which minimizes x^-. Since $\varphi_j = j\Delta t + \mathcal{O}(j^3 \Delta t^3)$ we have $\kappa > 0$ such that

$$k^*(j) = j \qquad \forall\, j \leq \kappa N^{2/3}.$$

Then, for $l = 1, 2, 3$:

$$S_l^{j,k} = \frac{\pi}{2} + \mathcal{O}(j^2 \Delta t^2) + \mathcal{O}(\Delta t) \quad \forall j \leq \kappa N^{2/3}. \tag{C.2}$$

Otherwise

$$S_l^{j,k^*} \leq C. \tag{C.3}$$

Using $|\tan(y)| \geq |y|/C$ for $|y| \leq y_{\max} < \pi$ we deduce that, for $k \neq k^*(j)$:

$$|S_l^{j,k}| \leq C \left[\Delta t + \Delta t \frac{\min\{1, (j^3 + k^3)\Delta t^2\}}{|x^{\pm}|} \right] \tag{C.4}$$

noting that $x^{\pm}$ depends upon j and k. From the properties of φ_j it follows that

$$\sum_{k=1, k\neq k^*(j)}^{N} \frac{\Delta t}{k|x^{\pm}|} \leq \frac{C}{j \log(N)}. \tag{C.5}$$

Thus if $|\beta_j| \leq C/j$ then, by (C.2)–(C.4),

$$\begin{aligned} S \;\leq\; & \sum_{j=1}^{\kappa N^{2/3}} \frac{C}{j^2}[j^2 \Delta t^2 + \Delta t] \\ & + \sum_{j>\kappa N^{2/3}}^{N} \frac{C}{j^2} \\ & + \sum_{j=1}^{N} \left[\frac{C}{j} \min\{1,\, j^3 \Delta t^2\} \sum_{k=1, k\neq k^*}^{N} \frac{\Delta t}{k|x^{\pm}|} \right]. \end{aligned}$$

Hence by (C.5) we obtain

$$S \leq C \log|\Delta t^{-1}| \Delta t^{2/3}.$$