The Roughness and Smoothness of Numerical Solutions to the Stochastic Heat Equation

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Abstract

The stochastic heat equation is the heat equation driven by white noise. We consider its numerical solutions using the finite difference method. Its true solutions are Hölder continuous with parameter $(\frac{1}{2} - \epsilon)$ in the space variable, and $(\frac{1}{4} - \epsilon)$ in the time variable. We show that the numerical solutions share this property in the sense that they have non-trivial limiting quadratic variation in x and quartic variation in t. These variations are discontinuous functionals on the space of continuous functions, so it is not automatic that the limiting values exist, and not surprising that they depend on the exact numerical schemes that are used; it requires a very careful choice of scheme to get the correct limiting values. In particular, part of the folklore of the subject says that a numerical scheme with excessively long time-steps makes the solution much smoother. We make this precise by showing exactly how the length of the time-steps affects the quadratic and quartic variations.

1 Introduction

In its simplest form—which is all we shall consider here—the stochastic heat equation is just the heat equation driven by additive[1] white noise:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \dot{W},$$

where $\dot{W}$ is a standard space-time white noise. White noise is a distribution, not a function, so this has to be interpreted in the distribution sense. With proper intial and boundary conditions, the associated initial-boundary-value problem has a unique solution. This solution is continuous, but very rough, in fact nowhere differentiable.

There are various representations of the solution, but as no closed form solution exists, one is tempted to solve it numerically.

One general fact has emerged: the simplest numerical schemes do about as well as any: indeed, the optimal rate of convergence is known [1], and the very first scheme one might think of, the forward Euler, already attains it. It suffers from a serious defect: it is unstable unless the time step is less than half the space-step squared. One can get around this by using implicit methods which are stable for any choice of the time step, such as, for instance, some of the "one-step theta" schemes. This family includes the forward Euler ($\theta = 0$), and the backward Euler ($\theta = 1$), both of which are first-order schemes, and the Crank-Nicholson scheme ($\theta = 1/2$), which is second-order. If $\theta \geq 1/2$, these methods are stable with no restriction on the time-step.

Let $h = \Delta x$ be the space step and let $k = \Delta t$ be the time step. Davie and Gaines have shown that for any scheme whatsoever, the size of the error is on the order of—at least—the maximum of $h^{1/2}$ and $k^{1/4}$. The one-step-theta schemes attain that error [1, 2, 9].

This suggests that k should be somewhere on the order of h^2. If k is fixed, decreasing h may not help—and may even hurt—the accuracy.

But the temptation is still there: since the method is stable, why not take a longer time-step and speed up the calculations? Instead of taking $k = O(h^2)$, why not be greedy and take $k = O(h)$, for example?

One of the aims of this paper is to show why not.

It is well-known that a greedy time-step smooths the numerical solution. However, there does not seem to be a large literature on this. See [3]. In the case of the stochastic

[1]This is additive noise in contrast to multiplicative noise, in which there would be a term $f(u)$ mulriplying $\dot{W}$, where f is a sufficiently nice function. We would expect similar results for multiplicative noise: the quadratic and quartic variation of both the solution and its discrete approximations should still exist and be locally-determined, but they would no longer be deterministic in the limit, since the value of u would intervene [4].

heat equation, we can see this effect quite precisely in the sense that the quadratic variations of the sequence of numerical approximations actually determine the "greediness" of the time-stepping scheme (Theorem 5.1); and the effect is visible to the naked eye in simulations: some of the simulations in Section 5.3, for instance, make the numerical solution appear impossibly smooth.

This last point is important: one often uses numerics to simulate the solutions, hoping to discover new and interesting properties. So the relevant questions in the study of numerical SPDEs do not stop with "Does the scheme converge, and, if so, how fast?" (Although that is certainly the first question to ask.) One also wants to know if the numerical approximation actually reflects the properties of the true solution. Does it "look like" the true solution?

The numerical scheme converges uniformly on compacts to the true solution, which implies quite a lot, but it says little about the smoothness or roughness properties of the approximations: that usually requires control of the derivatives. But the solutions are nowhere-differentiable.

For instance, do the simulations have the same smoothness properties as the true solutions? (Given that the solutions have no derivatives, "roughness" might be a better term here.)

In fact, the solution u to the stochastic heat equation is a.s. Hölder continuous: for fixed t, $x \to u(x,t)$ is Hölder continuous with parameter $1/2 - \varepsilon$ for any $\varepsilon > 0$, and for fixed x, $t \to u(x,t)$ is Hölder continuous with parameter $1/4 - \varepsilon$. [7, 8].

Hölder continuity is one way to measure roughness, and we might ask if the simulations have about the same Hölder continuity properties as the true solutions. (We hasten to say that we are not proposing this as the best measure of the roughness of arbitrary functions, but the Hölder continuity properties of the solutions of the stochastic heat equation are so remarkably regular that it seems appropriate in this case.)

The numerical approximations are discrete, so we cannot measure their Hölder continuity directly, but we can measure their higher-order variations. These give us a handle on the smoothness/roughness question, and provide a good measure of the Hölder parameters. Indeed, the true solutions have non-trivial higher order variations: $x \mapsto u(x,t)$ has non-trivial quadratic variation, and $t \mapsto u(x,t)$ has non-trivial quartic variation. (See Theorem 8.2[2].) We can measure the same variations of the discrete approximations: if $Q_n^{(2)}(t)$ is the quadratic variation of the nth approximation at time t, and if $Q_n^{(4)}(x;t)$ is its quartic variation on $(0,t)$ for fixed x, then both have deterministic limits as $n \to \infty$ and the limits depend on the parameters θ, and $c = \Delta t/(\Delta x)^2$.

[2]The fact that they have quadratic variation in x and quartic variation in t is another instance of the rule of thumb that solutions of the heat equation are roughly twice as smooth in x as in t, or, inversely, twice as rough in t as in x

We show the following:

- The limiting quadratic variation $Q^{(2)}(t)$ is deterministic, and its value is independent of t for $t > 0$;
- If c is held constant, $Q^{(2)}(t)$ decreases as θ increases;
- if $\theta = 1/2$, then $Q^{(2)}(t)$ is independent of c;
- if $\theta > 1/2$ is held constant, then $Q^{(2)}(t)$ decreases in c, and tends to zero as c tends to infinity;
- This decrease in quadratic variation corresponds to a smoothing in the space coordinate; c can increase without bound, and this smoothing can be quite evident, as is shown by Figures 2–5.
- The limiting quartic variation $Q^{(4)}(x,t)$ is deterministic, and is independent of x for rational $0 < x < 1$. It depends on both θ and c. It tends to zero as c tends to zero, but otherwise its behavior is not as simple as that of the quadratic variation.
- If $0 \le \theta \le 1/2$, $Q^{(4)}(x,t)$ increases with c;
- if $\theta > 1/2$, $Q^{(4)}(x,t)$ increases to a maximum, then decreases to a strictly positive limit as c increases.
- This behavior is independent of the initial conditions.

The last point is shown in §8

The quadratic and quartic variations converge to a function of θ and c, but, as the true values are unique, evidently most schemes do not produce the correct limit. This is not surprising: the higher-order variations are highly discontinuous functionals on the space of continuous functions. There is no a priori reason to expect that they even converge, much less that they converge to the correct values. We might ask if there is any scheme which does give the correct limiting values. There is exactly one. Interestingly enough, it is a second-order method, one of the Crank-Nicholson schemes. (See §5.2.)

2 The stochastic heat equation

A standard white noise on $\boldsymbol{R}^2$ is a random L^2-valued measure W on the Borel sets $\mathcal{B}$ of $\boldsymbol{R}^2$ such that for each $A \in \mathcal{B}$ of finite Lebesgue measure, $W(A)$ is a Gaussian random variable of mean zero and variance equal to the Lebesgue measure of A, and such that if $A \cap B = \emptyset$, $W(A)$ and $W(B)$ are independent.

We can also think of it as a random Schwartz distribution, which we shall denote $\dot W$: $\{\dot W(\varphi),\ \varphi$ is a test function$\}$ is a Gaussian process with mean zero and covariance function $E\{\dot W(\varphi)\,\dot W(\psi)\} = \int \varphi(z)\,\psi(z)\,dz$. The connection between the two is that $\dot W(\phi) = \int \phi(z)\,W(dz)$.

Consider the initial-boundary-value problem on $(0,1)\times[0,\infty)$:

$$\begin{cases} u_t(x,t) = u_{xx}(x,t) + \dot W(x,t) \\ u(x,0) = u_0(x) \quad \text{if} \quad 0 < x < 1 \\ u(0,t) = u(1,t) = 0 \quad \text{if} \quad t \geq 0\,. \end{cases} \tag{1}$$

The initial condition $u_0(x)$ may be random. We assume that it is independent of the white noise, that $x \mapsto u_0(x)$ is continuous, and that $E\{u_0(x)^2\}$ is bounded on $0 \leq x \leq 1$.

The problem (1) is defined rigorously in [8], and it is shown that there is a unique Hölder-continuous solution u, such that $x \mapsto u(x,t)$ is Hölder $(1/2-\varepsilon)$ a.s. for each $t > 0$, and $t \mapsto u(x,t)$ is a.s Hölder $(1/4-\varepsilon)$ for each $0 < x < 1$.

3 Finite difference schemes

Let $0 \leq \theta \leq 1$, and take $h = \Delta x = 1/(n+1)$, $k = \Delta t$. Let $x_j = jh$, $t_m = mk$. Let $R_{j,m}$ be the rectangle $(x_j, x_{j+1}) \times (t_m, t_{m+1})$, and put $W_{j,m} = W(R_{j,m})$. Notice that the $W_{j,m}$ are i.i.d. $N(0,hk)$ random variables.

The one-step-theta finite difference scheme is:

$$\begin{cases} \dfrac{u_j^{m+1} - u_j^m}{k} = \theta\,\dfrac{u_{j+1}^{m+1} - 2u_j^{m+1} + u_{j-1}^{m+1}}{h^2} + (1-\theta)\,\dfrac{u_{j+1}^m - 2u_j^m + u_{j-1}^m}{h^2} + \dfrac{W_{j,m}}{hk} \\ u_0^m = u_{n+1}^m = 0, \quad m = 0,1,2,\ldots \\ u_j^0 = u_0(x_j) \quad j = 1,2,\ldots,n-1. \end{cases} \tag{2}$$

where $j = 1,2,\ldots,n$, $m = 1,2,\ldots$. Note that the $W_{j,m}$ are i.i.d. $N(0,hk)$ random variables.

If $\theta = 0$, this is the forward Euler scheme, if $\theta = 1$, it is the backward Euler, both of which are first-order schemes, and if $\theta = 1/2$ it is the Crank-Nicholson scheme, which is second order. The scheme is stable if $\theta \geq 1/2$; for $\theta < 1/2$, it is conditionally stable, requiring a condition on the length of the time step. Given the proper relations between the space and time steps, the scheme converges in probability to the true solution as $n \to \infty$, and there are subsequences n_r along which it converges a.s. uniformly on compact sets [1, 2, 5, 9].

4 Higher-order Variations

Let $u(x,t)$ be the solution of (1) and let (u_j^m) be the numerical approximation (2). It is known [7] [8] that $x \mapsto u(x,t)$ is Hölder continuous of order $1/2-\varepsilon$ for any $\varepsilon > 0$, and $t \mapsto u(x,t)$ is Hölder continuous of order $1/4-\varepsilon$ for any $\varepsilon > 0$. Moreover, if $t > 0$ is fixed, $x \mapsto u(x,t)$ has a non-trivial quadratic variation $\hat{Q}^{(2)}(t)$, and if $0 < x < 1$ is fixed, $t \mapsto u(x,t)$ has a non-trivial quartic variation $\hat{Q}^{(4)}(x,t)$. Put $x_i = ih$ and $t_j = jk$. Then set

$$\hat{Q}_n^{(2)}(t) = \sum_{i=0}^{n} \big(u(x_{i+1},t) - u(x_i,t)\big)^2 \tag{3}$$

$$\hat{Q}_n^{(4)}(x,t) = \sum_{j=0}^{[t/k]-1} \big(u(x,t_{j+1}) - u(x,t_j)\big)^4 . \tag{4}$$

Then the **quadratic** and **quartic variations** of u are given respectively by

$$\hat{Q}^{(2)}(t) = \lim_{n\to\infty} \hat{Q}_n^{(2)}(t) \tag{5}$$

$$\hat{Q}^{(4)}(x,t) = \lim_{n\to\infty} \hat{Q}_n^{(4)}(x,t) . \tag{6}$$

Both limits are in probability; if we take the subsequence $n_k = 2^k$, the limits exist a.s. (See Section 7.)

Both $\hat{Q}^{(2)}(t)$ and $\hat{Q}^{(4)}(x,t)$ turn out to be deterministic. We can define both variations for the discrete numerical approximation u_j^m. For a fixed n, h, and k, and $t > 0$, and $x_i = i/(n+1)$, let $[t]$ be the greatest integer in t, and define

$$Q_n^{(2)}(t) = \sum_{i=0}^{n} \big(u_{i+1}^{[t/k]} - u_i^{[t/k]}\big)^2 \tag{7}$$

$$Q_n^{(4)}(x_i,t) = \sum_{m=0}^{[t/k]-1} \big(u_i^{m+1} - u_i^m\big)^4 . \tag{8}$$

Then define the limiting quadratic and quartic variations (if they exist) by, respectively,

$$Q^{(2)}(t) = \lim_{n\to\infty} Q_n^{(2)}(t) \tag{9}$$

$$Q^{(4)}(x,t;\delta) = \lim_{n\to\infty} \big(Q_n^{(4)}(x,t) - Q_n^{(4)}(x,\delta)\big) \tag{10}$$

$$Q^{(4)}(x,t) = \lim_{\delta\to 0} Q_n^{(4)}(x,t,\delta) . \tag{11}$$

The reason for the two-stage definition of the quartic variation is that in certain schemes, the numerical approximations fluctuate excessively near $t = 0$. This side-steps that problem.

Some remarks are in order. The PDE is linear, so the solution can be written as $u + v$, where u is a solution of the inhomogeneous PDE with zero initial conditions, and v solves the homogeneous equation with the given, non-zero initial condition. That is, u solves

$$\begin{cases} u_t = u_{xx} + \dot{W} \\ u(\cdot, 0) = 0 \\ u(0, \cdot) = u(1, \cdot) = 0\,, \end{cases} \tag{12}$$

while v solves

$$\begin{cases} v_t = v_{xx} \\ v(\cdot, 0) = u_0(\cdot) \\ v(0, \cdot) = v(1, \cdot) = 0\,. \end{cases} \tag{13}$$

We can do exactly the same for the numerical solution, writing it $u_j^m + v_j^m$, where u solves the inhomogeneous difference equation with zero initial conditions, and v solves the homogeneous difference equation with the given initial conditions.

The solution v of the homogeneous boundary-value problem is infinitely differentiable, so it has zero quadratic and quartic variations. Thus, it does not change the quadratic and quartic variations of the solution. Consequently, the quadratic and quartic variations of the solution of (1) do not depend on the initial conditions: u and $u + v$ have the same quadratic and quartic variations. The same is also true of the limiting variations of the numerical solutions: they do not depend on the initial values.

Indeed, if we let $Q_n^p(u)$ be defined by either (7) (if $p = 2$) or (8) (if $p = 4$) then by Minkowski's inequality,

$$\left|Q_n^{(p)}(u+v)^{1/p} - Q_n^{(p)}(u)^{1/p}\right|^p \leq Q_n^{(p)}(v).$$

But by Theorem 8.2, this goes to zero, so the limiting p-variation is indeed independent of the initial condition.

This means that we can choose the initial values as we please, and in particular, we can choose them to make the solutions of both (1) and (2) into stationary processes. This significantly simplifies the calculations.

5 The Basic Results

We know that for the most efficient computation, k should be more-or-less comparable to h^2, so let

$$c = \frac{k}{h^2}\,.$$

The ratio c may vary as $n \to \infty$. However, it cannot vary arbitrarily: some restrictions are necessary to guarantee stability: if $\theta < 1/2$, c can be at most $1/(2-4\theta)$. Even if $\theta \geq 1/2$, further restrictions may be necessary to guarantee that the scheme converges to the true solution of the stochastic heat equation. Shardlow [5] proves convergence for the finite difference scheme when $c(1-\theta) < 1/4$.For the finite element method, it was shown in [9] Theorem 2.1 that if $\theta = 1/2$, the scheme converges if $k^2/h^3 \longrightarrow 0$, and if $1/2 < \theta < 1$, it converges if $k/h \longrightarrow 0$. Counter-examples in §6 of the same paper show that these conditions are close to necessary. It is an open question whether or not similar conditions are necessary in the finite difference method we use here, but we conjecture that they are.

The following conditions on c are sufficient to guarantee that the scheme is stable and that the quadratic and quartic variations converge[3].

Hypothesis[4] (C)

(i) $c > 0$;

(ii) if $0 \leq \theta < 1/2$, *there is an* $\epsilon_\theta > 0$ *such that if* $c_\theta \stackrel{\text{def}}{=} \frac{1}{2-4\theta} - \varepsilon_\theta$, *then* $c \leq c_\theta$;

(iii) if $\theta = 1/2$, $c \leq \sqrt{n}$;

(iv) if $1/2 < \theta \leq 1$, $c \leq n$.

Hypothesis (C) will be in force for the remainder of the paper.

We are interested in the limiting values of the variations in a one-step theta scheme as the number n of space steps goes to infinity. Let $h_n = 1/(n+1)$ be the space step, k_n be the time step, and let $c_n = k_n/h_n^2$. Let $Q_n^{(2)}(t)$ and $Q_n^{(4)}(y,t)$ be the quadratic variation in x and their quartic variation in t respectively.

Theorem 5.1 *Fix* $0 \leq \theta \leq 1$ *and* $t > 0$. *Let* (c_n) *be a sequence satisfying Hypothesis (C). Suppose that* $c_n \to c_\infty$ *for an extended real* $c_\infty \in [0,\infty]$. *Then the following limit exists in probability, and exists almost surely along the subsequence* $n_i = 2^i$:

$$\lim_{n\to\infty} Q_n^{(2)}(t) = \frac{1}{2\sqrt{1+2c_\infty(2\theta-1)}}\,. \tag{14}$$

[3]The question of whether these conditions also assure that the numerical approximations themselves converge to the true solution is, as we said, open

[4]There are no hypotheses A and B; this is just named for the coefficient.

Remark 5.2 *1. The right-hand side of (14) should be interpreted as the limit as c increases to c_∞. In particular, if $c_\infty = \infty$, it equals 1/2 if $\theta = 1/2$, and zero if $\theta > 1/2$.*

2. The limit is deterministic and, as long as t is strictly positive, independent of t. This is perhaps not surprising once one realizes that the limit is independent of the initial values, and that it is possible to choose the initial values to make the solution a stationary process.

3. In the special cases where θ is 0, 1/2, and 1, we have

$$\lim_{n\to\infty} Q_n^{(2)}(t) = \begin{cases} \dfrac{1}{2\sqrt{1-2c_\infty}} & \text{if } \theta = 0 \\ \dfrac{1}{2} & \text{if } \theta = \dfrac{1}{2} \\ \dfrac{1}{2\sqrt{1+2c_\infty}} & \text{if } \theta = 1\,. \end{cases}$$

In particular, for the Crank-Nicholson scheme, the limiting quadratic variation is independent of c.

4. If $\theta < 1/2$, c_∞ is bounded. If $\theta \geq 1/2$, c_∞ can take any value in $[0,\infty]$ inclusive, and the limiting quadratic variation is a decreasing function of c_∞. It is also decreasing in θ, which illustrates the fact that larger values of θ tend to smooth the solution.

5. One can see from the simulations (see Figures 2–5 below) that decreasing the quadratic variation does actually indicate a smoothing of the solution.

Let us consider the quartic variation in t for a fixed y. Notice that to measure the quartic variation at y, y must be a lattice point, that is, it must be one of the points h, $2h$, $3h$, …, nh, where $h = 1/(n+1)$. For any rational y, there will be infinitely many n for which this is true, and we can only take the limit along those n. So the limit of the $Q_n^{(4)}(y)$ is necessarily along a subsequence of n. One could interpolate, or use a finite element scheme as in [9][5], but we will only consider limits for fixed rational y.

Theorem 5.3 *Fix $0 \leq \theta \leq 1$ and a rational $y \in (0,1)$. Let (c_n) be a sequence satisfying Hypothesis (C), and suppose $c_n \to c_\infty$ for some extended real $c_\infty \in [0,\infty]$. We also suppose that $c_n/\sqrt{n} \to 0$ if $\theta = 1/2$, and that $c_n/n^{3/2} \to 0$ if $\theta > 1/2$. Then the following limits exist in probability, and exist almost surely along any subsequence (n_i) for which $n_i \geq 2^i$ for all i and y is a lattice point for each n_i:*

$$\lim_{N\to\infty}\lim_{n\to\infty}\big(Q_n^{(4)}(y,t) - Q_n^{(4)}(y,1/N)\big) = 3c_\infty t\Big(\frac{1-2\theta}{\sqrt{1+2c_\infty(2\theta-1)}} + \frac{2\theta}{\sqrt{1+4c_\infty\theta}}\Big)^2. \tag{15}$$

[5]Given the unusual form of the error term in Theorem 7.5 this might be interesting

Note: 1. *If $\theta \geq 1/2$, c_∞ can be infinite. In that case, the right-hand side of (15) should be interpreted as the limit as $c \to \infty$, namely $3t\big(\sqrt{\theta} - \sqrt{\theta - 1/2}\big)^2$.*

2. *We repeat: y is fixed and the above limits are over n for which y is a lattice point, i.e. for which there is an integer m such that $y = m/(n+1)$.*

Remark 5.4 **1.** *The value of the limiting quartic variation is deterministic, and independent of y as long as y is rational and $0 < y < 1$. (The solution is identically zero on the boundaries, so that $Q^{(4)}(y,t) \equiv 0$ if $y = 0$ or 1.)*

2. *In the special cases $\theta = 0$, 1/2, and 1,*

$$Q^{(4)}(y,t) = \begin{cases} \dfrac{3tc_\infty}{1 - 2c_\infty} & \text{if} \quad \theta = 0 \\ \dfrac{3tc_\infty}{1 + 2c_\infty} & \text{if} \quad \theta = \dfrac{1}{2} \\ 3tc_\infty\Big(\dfrac{2}{\sqrt{1+4c_\infty}} - \dfrac{1}{\sqrt{1+2c_\infty}}\Big)^2 & \text{if} \quad \theta = 1\,. \end{cases}$$

3. *The behavior of the limiting quartic variation is not as simple as it is for the quadratic variation. It is not necessarily monotone in c, and it is bounded away from zero. If $\theta = 0$ or 1/2, it is increasing in c, while if $\theta > 1/2$, $Q^{(4)}(y,t)$ first increases to a maximum value, and then decreases to a strictly positive limit. So long time steps smooth the solution in x, but they may not smooth it very much in t.*

5.1 Proofs of Theorems 5.1 and 5.3

The proofs of both theorems are straightforward moment arguments: they show that the expectation of the variation converges, and that its variance goes to zero. It is a simple exercise to show that if X_n is a sequence of random variables whose expectations tend to a limit L and whose variances tend to zero, that $X_n \to L$ in the mean square and therefore in probability. The real work is done in Theorems 7.1 and 7.5 below. All we need to do here is to use those results to check that the expectations tend to the correct limiting values and that the variances tend to zero.

The constant c_θ is defined in Hypothesis (C) for $\theta < 1/2$. For $\theta \geq 1/2$, define $c_\theta = \infty$.

Proof. (Of Theorem 5.1) Define $L(\theta, c)$ by $L(\theta, \infty) = 0$ and, for $c < c_\infty$, let

$$L(\theta, c) = \frac{1}{2\sqrt{1 + 2c(2\theta - 1)}}\,.$$

Then L is bounded and continuous in c for $0 \leq c \leq c_\theta$. By Proposition 7.1 $|E\{Q^{(2)}(t)\} - L(\theta, c_n)| \leq 1/2n$, so $|E\{Q^{(2)}(t)\} - L(\theta, c_\infty)| \leq 1/2n + |L(\theta, c_n) - L(\theta, c_\infty)|$. But this goes to zero as $n \to \infty$ by the continuity of L.

Next, by (33), Var $\big(Q^{(2)}(t)\big) \le K(\theta)/n$ for some constant $K(\theta)$. So the variance tends to zero, the expectation tends to $L(\theta, c_\infty)$, and therefore $Q^{(2)}(t) \to L(\theta, c_\infty)$ in probability. If we take the limit along the subsequences $n = 2^k$, the variances are summable, and an application of the Borel-Cantelli lemma shows that the quadratic variation converges almost surely. ♣

Proof. (Of Theorem 5.3.) Define $L(\theta, c, t)$ for $0 \le c < c_\theta$ by

$$L(\theta, c, t) \stackrel{\text{def}}{=} 3ct\Big(\frac{1-2\theta}{\sqrt{1+2c(2\theta-1)}} + \frac{2\theta}{\sqrt{1+4c\theta}}\Big)^2,$$

and let $L(\theta, c_\theta, t) = \lim_{c\uparrow c_\theta} L(\theta, c, t)$. Then L is a bounded continuous function of c in $0 \le c \le c_\theta$.

Let $y = q/p$ in lowest terms, i.e. q and p are relatively prime. Note that the quartic variation $Q_n^{(4)}(y, t)$ is only defined when y is a lattice point, i.e. a multiple of $1/(n+1)$, which means in turn that $n+1$ is a multiple of p, say $n+1 = kp$. Thus the limit is over $n = kp-1$ as $k \to \infty$. By Theorem 7.5 (37), for fixed y and t, $|E\{Q^{(4)}(y,t) - L(\theta, c_n, t)\}|$ is bounded by Kp/n for some constant K. (K depends only on θ, not on c, t, or n.) In terms of k, the bound is $K(n+1)/kn \sim K/k$. Thus as $n = np-1$ and $k \to \infty$, $E\{Q_n^{(4)}(y,t)\} \to L(\theta, c_\infty, t)$ as $n \to \infty$.

By Theorem 7.5 (38), the variance of $Q_n^{(4)}$ is bounded either by Kc_n^3/n^2 (if $\theta \ne 1/2$) or by $Kc_n^3/n^{3/2}$ (if $\theta = 1/2$.) Thus the variance goes to zero, and we conclude that $Q^{(4)}(y,t) \to L(\theta, c_\infty, t)$ in the mean square, and hence in probability. ♣

Remark 5.5 **1.** *Notice that the limiting quartic variation in (15) vanishes at $y = 0$ and $y = 1$ (because the solution does) and is a non-zero constant in between, so that it is discontinuous in y. Evidently the convergence is not uniform in y. Thus, any extension of Theorem 5.3 which allows y to vary with n would be delicate.*

To see why it is delicate, even away from $y = 0$ and $y = 1$, suppose again that $y = q/p$ in lowest terms. We showed in the above proof that the variance of the quartic variation tends to zero and its expectation differs from the function L by at most Kp/n. For a fixed y, $Kp/n \to 0$ as n tends to infinity, and this implies the desired convergence. If y is allowed to vary with n, however, something else can happen. Take, for example, $y = 1/2$, and $y_n = 1/2 + 1/(n+1)$. These are lattice points for odd n. If $y_n = q/p$ in lowest terms, then $p = n+1$, so for y_n, $Kp/n \sim K$. Thus the error term does not go to zero, and we cannot conclude that $E\{Q_n^{(4)}(y_n, c, t)\} \to L(\theta, c, t)$. Consequently, it is no longer clear that $Q_n^{(4)}(y_n, c, t)$ converges to $L(\theta, c, t)$, and, in fact, it is not even clear that it converges.

2. *One can also give an almost-everywhere convergence theorem, but it requires further restrictions on the convergence of the c_n. However, if c_∞ is finite, there is no problem:*

the quartic variation actually converges a.e. This follows since the variance of the nth term is then bounded by $K/n^{3/2}$, which is summable.

5.2 The True Values

It was shown in [7] that parabolic equations driven by white noise have non-trivial quadratic variation in space and non-trivial quartic variation in time[6]. That paper looked at the stochastic cable equation with reflecting boundary conditions, which differs from the heat equation by the addition of a non-zero drift term. Pospisil and Tribe [4] have computed the values of the variations for more general parabolic spde's, and for the initial-boundary-value problem (1) they get values of $Q^{(2)}(t) = 1/2$ for the quadratic variation at any $t > 0$, and $Q^{(4)}(x;t) = 3t/\pi$ for the quartic variation on $(0, t)$ for any $t > 0$ and $0 < x < 1$. These agree with the values computed in [7]. Indeed, the higher-order variations are purely local phenomena, and are unaffected by either drift terms, boundary conditions, or initial conditions.

The proof in [7] of the existence of the quadratic variation is rather different from that in [4], and one of its auxiliary results, when applied to the stochastic heat equation (1), leads to an interesting consequence: if $u(x, 0)$ is given the stationary distribution (so that $u(\cdot\,, t), t \geq 0\}$ is a stationary process) then for each $t_0 > 0$, if we set $B_s = \sqrt{2}\,u(s, t_0)$, then $\{B_s, s \geq 0\}$ is a standard Brownian bridge. Since the Brownian bridge has the same quadratic variation as Brownian motion, this immediately confirms that the quadratic variation is 1/2.

This leads to the question, "Do the one-step-theta numerical schemes give the correct limiting quadratic and quartic variations? This is answered by Theorems 5.1 and 5.3: there is exactly one which does. It is, perhaps surprisingly[7], a Crank-Nicholson scheme: $\theta = 1/2$ and $c = 1/(\pi - 2)$.

In fact, the Crank-Nicholson is the only scheme to get even the quadratic variation right. However, if we let $c \to 0$ in the schemes for $\theta \neq 1/2$, then the limiting quadratic variation will be correct, but the limiting quartic variation will be zero. There are other schemes which get the quartic variation right, such as, for example, $\theta = 0$ and $c = 1/(\pi + 2)$.

One final point is worth repeating: the quadratic and quartic variations of the limiting process have well-defined, deterministic values. The numerical schemes also have well-defined deterministic quadratic and quartic variations, and these variations converge... but, with the exception of the critical Crank-Nicholson scheme, they converge to the wrong values!

---

[6] Though the existence of a quadratic variation was surely known earlier.

[7] At least, it surprised us. We expected the Crank-Nicholson scheme to misbehave, for it is reputed to exaggerate any singular behavior of the solutions... and we are dealing with very rough solutions indeed.

5.3 Numerical Simulations

The following are pictures of simulations of numerical solutions to the stochastic heat equation. All simulations have 1000 space steps (n = 999) and 100 time steps. They were made using Matlab.

Remark 5.6 *The number of space steps and the number of time steps in these simulations are both fixed, but the length of the time steps changes. Thus t_0, the length of time covered by the simulation, changes from simulation to simulation. This is not a problem. The underlying process is stationary, so that the behavior of $x \mapsto u(t,x)$ is statistically the same at each time t, and in particular, its quadratic variation is the same at each time. So one time will do as well as another for comparing the smoothness of the underlying process and its numerical approximations. However, it does make a difference to the actual values: $x \mapsto u(t,x)$ is* not *the same at different values of t. Now the simulations were all made with the same seed, so the initial values and, up to rescaling, the noise increments $w_{i,j}$ are also the same in each. There is an interesting consequence: the different simulations of $x \mapsto u(x,t_0)$ involve different times t_0. Yet the graphs look as if they all describe the same time. We leave it to the reader to explain why.*

Figures 1 and 2 show the critical Crank-Nicholson scheme ($\theta = .5$, $c = 1/(\pi - 2)$) Figures 3 to 7 are for $\theta = .51$ and the backward Euler ($\theta = 1$) scheme; they show the smoothing effect as the ratio $c = \Delta x/(\Delta t)^2$ is increased. The solution starts with the stationary initial distribution, so the solutions themselves are stationary in time.

The critical Crank-Nicholson scheme, with $c = 1/(\pi - 2)$, has the correct limiting quadratic and quartic variation, so that the first two figures should give a fairly accurate picture of a typical sample path in time (Figure 1) and in space (Figure 2). (See §5.2.)

The sample paths are Hölder (1/4) as a function of time, and Hölder (1/2) as a function of space. One can see that the first is noticeably rougher than the second, as it should be. Figure 1 is the graph of a simulation of $t \mapsto u(.5,t)$. The simulation has quartic variation $.9546 t_0$, while the quartic variation of the true solution is $.9549 t_0$. Figure 2 is the graph of a simulation of $x \mapsto u(x,t_0)$. It has quadratic variation $Q_n^{(2)}(t_0) = .4732$, while the quadratic variation of the true solution is $\hat{Q}^{(2)}(t_0) = .50$

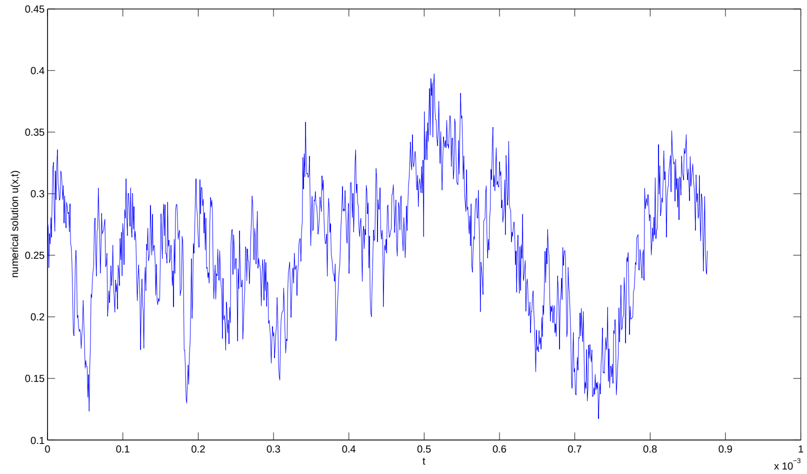

Figure 1: The solution as a function of time: $t \mapsto u(.5,t)$ for $0 \le t \le t_0$, as seen by the critical Crank-Nicholson scheme with $c = \frac{1}{\pi-2}$. The observed quartic variation is $.9546t_0$, and the expected quartic variation and true quartic variation are both $.9549\, t_0$.

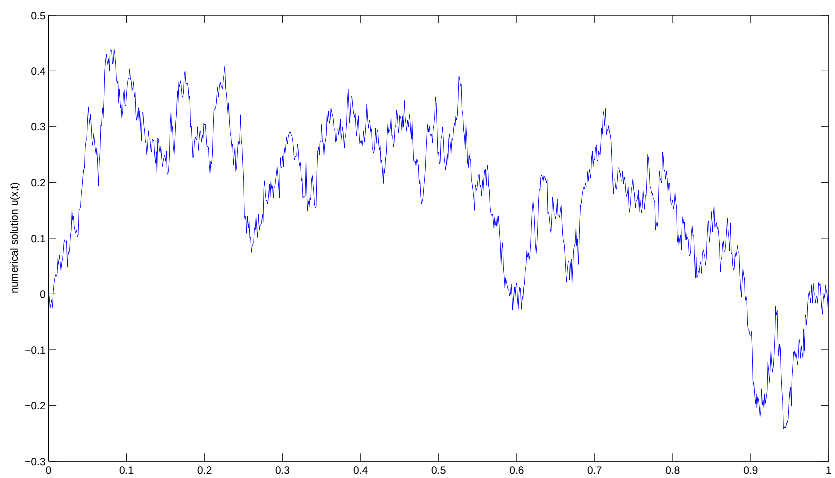

Figure 2: The solution as a function of space: $x \mapsto u(x,t_0)$ for $0 \le x \le 1$, as seen by the critical Crank-Nicholson scheme with $c = \frac{1}{\pi-2}$. The observed quadratic variation is .4732, while the expected quadratic variation and true quadratic variation are both .50.

Figures 3 – 7 show the smoothing effects of increasingly long time steps on $x \mapsto u(x, t_0)$. The number of space steps is fixed at $n = 999$, and there are 100 time steps. The initial values and the "noise" are the same for each graph. The ratio $c = \Delta t/(\Delta x)^2$ increases: $c = 1/(\pi - 2) \sim .876$, $c = 10$, $c = 100$, $c = 1000$, and $c = 10,000$ in Figures 3–7, respectively[8]. This is illustrated for $\theta = .51$ and the backward Euler ($\theta = 1$) schemes. Since the number of time steps is fixed, t_0 varies with c. However, it is the same for both graphs in each figure, so that they are different approximations to the same sample path. Notice that as c increases, the change from $\theta = .51$ to $\theta = 1$ smooths over ever-larger-scale features.

The observed quadratic variation $Q_n^{(2)}(t_0)$ decreases when c increases and when θ increases, going from .5107 ($\theta = .51$, $c = 1/(\pi - 2)$ to .0039 ($\theta = 1$, $c = 10,000$.) (The "true" value is .50.) The progressive smoothing is evident to the naked eye.

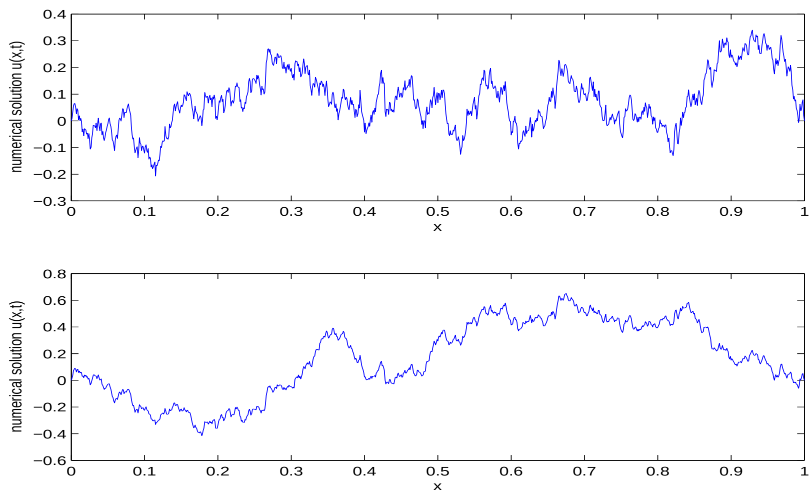

Figure 3: $u(x, t_0)$, for $0 \leq x \leq 1$, as seen by the $\theta = .51$ (top) and $\theta = 1$ (bottom) schemes with 1000 space steps, $t_0 = 8.7597 \times 10^{-5}$, and $c = \frac{1}{\pi - 2}$. The observed and expected quadratic variations for $\theta = .51$ are .5107 and .4915 respectively, and the observed and expected quadratic variations for $\theta = 1$ are .3093 and .3014 respectively, while the true quadratic variation is .50.

[8]The reader will notice that the simulation with $\theta = .51$ and $c = 10,000$ does not satisfy Hypothesis (C); however, it does show that the smoothing effect continues, even when the size of the time step is increased beyond reasonable limits.

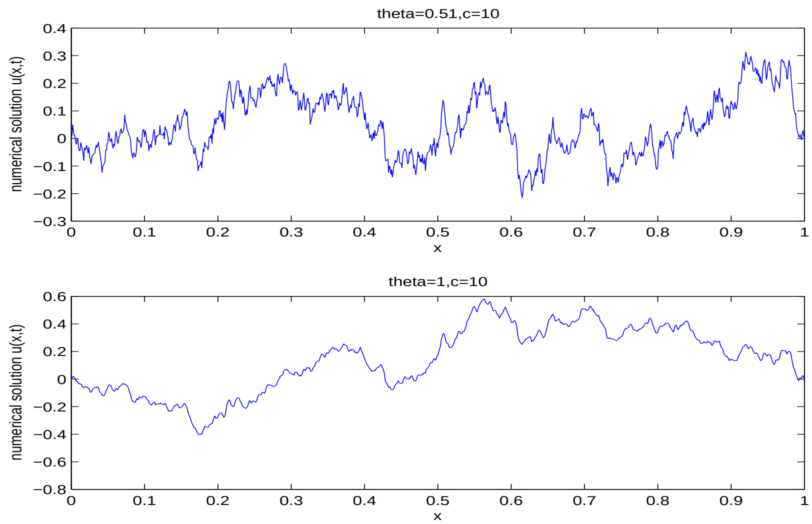

Figure 4: Same as Figure 3, but with $c = 10$ and $t_0 = .001$, for $\theta = .51$ (top) and $\theta = 1$ (bottom). The observed and expected quadratic variations for $\theta = .51$ are .4565 and .4226 resp. and for $\theta = 1$ they are .1109 and .1091 resp. The true quadratic variation is .50.

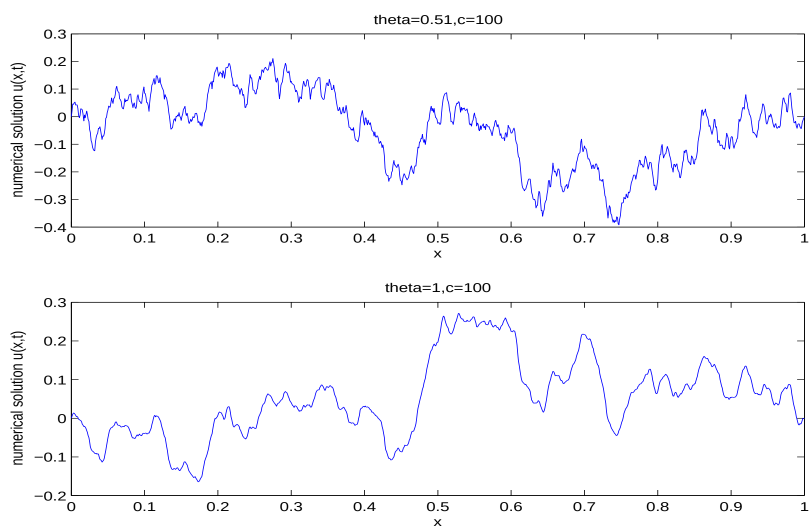

Figure 5: Same as Figure 3, but with $c = 100$ and $t_0 = .01$. For $\theta = .51$ (top) the observed and expected quadratic variations are .2198 and .2236 resp., and for $\theta = 1$ they are .0290 and .0353 resp. The true quadratic variation is .50.

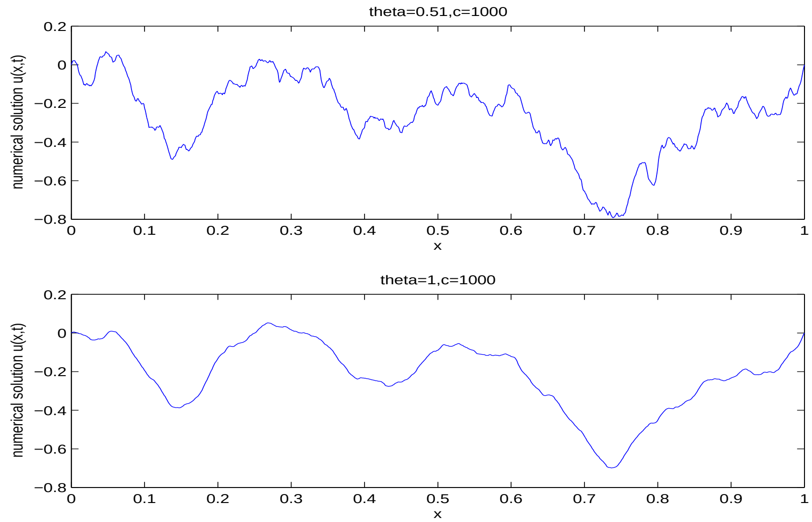

Figure 6: Same as Figure 3, but with $c = 1000$ and $t_0 = .1$. For $\theta = .51$ (top) the observed and expected quadratic variations are .0819 and .07809 resp., and for $\theta = 1$ they are .0136 and .0112 resp. The true quadratic variation is .50.

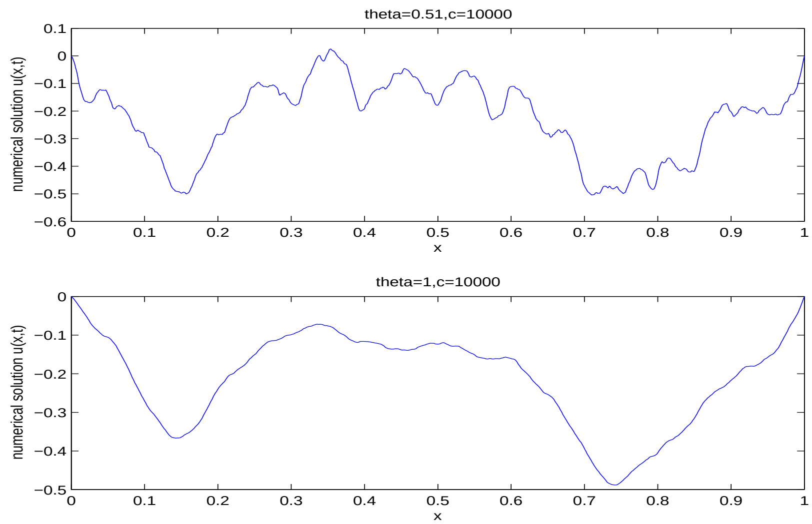

Figure 7: Same as Figure 3, but with $c = 10,000$ and $t_0 = 1$. For $\theta = .51$ (top) the observed and expected quadratic variations are .0259 and .02497 resp., and for $\theta = 1$ they are .0039 and .0035 resp. The true quadratic variation is .50.

6 Eigenfunction Representations

Let (u_j^m) be the solution of (2), and let U^m be the vector

$$U^m = (u_1^m, u_2^m, \ldots, u_n^m)\,.$$

Similarly, let

$$W^m = (W_{1,m}, W_{2,m}, \ldots, W_{n,m})\,,$$

where $W_{j,m} = W\big((jh,(j+1)h)\times(mk,(m+1)k)\big)$. The $W_{j,m}$ are independent $N(0,hk)$ random variables.

Let $\mathcal{A}$ be the tridiagonal $n\times n$ matrix with twos in the main diagonal, and minus ones in the diagonals above and below:

$$\mathcal{A} = \begin{pmatrix} 2 & -1 & & \ldots & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \ldots & & -1 & 2 \end{pmatrix}_{n\times n.}$$

Multiply (2) on both sides by k and write it in vector form:

$$U^{m+1} - U^m = (\theta-1)c\mathcal{A}\,U^m - c\theta\mathcal{A}\,U^{m+1} + \frac{1}{h}W^m\,.$$

Solve for U^{m+1}:

$$U^{m+1} = \big(I + c\theta\mathcal{A}\big)^{-1}\big(I + c(\theta-1)\,\mathcal{A}\big)U^m + \frac{1}{h}\big(I + c\theta\mathcal{A}\big)^{-1}W^m\,. \tag{16}$$

The eigenvalues λ_j and eigenvectors ξ_j of $\mathcal{A}$ are [10], [11]:

$$\lambda_j = 4\sin^2\frac{j\pi}{2(n+1)}\,; \tag{17}$$

$$\xi_j = \sqrt{\frac{2}{n+1}}\Big(\sin\frac{j\pi}{n+1}, \sin\frac{2j\pi}{n+1}, \ldots, \sin\frac{nj\pi}{n+1}\Big)\,. \tag{18}$$

The eigenvectors form a complete orthonormal system, so that, putting $t_m = mk$, U^m and W^m can be expressed in the form

$$U^m = \sum_{j=1}^{n} A_j(t_m)\xi_j \tag{19}$$

$$W^m = \sum_{j=1}^{n} w_{j,m}\xi_j \,, \tag{20}$$

where $w_{j,m} = \langle W^m, \xi_j\rangle \stackrel{\text{def}}{=} \sum_{i=1}^n W_{i,m}\xi_j(i)$, and $A_j(t_m) = \langle U^m, \xi_j\rangle$. It is easily seen from the ortho-normality of the ξ_j that the $w_{j,m}$ are independent $N(0, hk)$ random variables.

Plug (19) into (16) to get a recurrence relation for the A_j:

$$\sum_{j=1}^{n} A_j(t_{m+1})\xi_j = \sum_{j=1}^{n} A_j(t_m)\big(I + c\theta\mathcal{A}\big)^{-1}\big(I + (\theta-1)c\mathcal{A}\big)\xi_j + \frac{1}{h}\sum_{j=1}^{n} w_{j,m}\big(I + c\theta\mathcal{A}\big)^{-1}\xi_j \,.$$

The ξ_j are eigenvectors of $\mathcal{A}$, and also of I, and therefore they are eigenvectors of all the matrices in the above equation, so that in terms of the λ_j:

$$\sum_{j=1}^{n} A_j(t_{m+1})\xi_j = \sum_{j=1}^{n} \frac{1 + (\theta-1)c\lambda_j}{1 + c\theta\lambda_j} A_j(t_m)\xi_j + \frac{1}{h}\sum_{j=1}^{n} \frac{w_{j,m}}{1 + c\theta\lambda_j}\xi_j \,.$$

The ξ_j are linearly independent, so the equation must hold for each $j = 1, 2, \dots$ and $m = 0, 1, 2, \dots$:

$$A_j(t_{m+1}) = \frac{1 + (\theta-1)c\lambda_j}{1 + c\theta\lambda_j} A_j(t_m) + \frac{w_{j,m}}{h(1 + c\theta\lambda_j)} \,. \tag{21}$$

Let

$$\alpha_j \stackrel{\text{def}}{=} \frac{1 + (\theta-1)c\lambda_j}{1 + c\theta\lambda_j} = 1 - \frac{c\lambda_j}{1 + c\theta\lambda_j} \,,$$
$$\beta_j \stackrel{\text{def}}{=} \frac{1}{h(1 + c\theta\lambda_j)} \,.$$

Then (21) becomes

$$A_j(t_{m+1}) = \alpha_j A_j(t_m) + \beta_j w_{j,m} \,, \quad m = 0, 1, 2, \dots \tag{22}$$

The processes $\{A_j(t_m), m = 0, 1, 2, \dots\}$ are discrete versions of the Ornstein-Uhlenbeck process.

Note that we must have $|\alpha_j| \leq 1$ for all j in order that the scheme be stable. This is equivalent to asking that $c\lambda_j/(1+c\theta\lambda_j) \leq 2$. This increases in λ and $0 < \lambda_j < 4$ for all j, so it holds if $4c/(1+4\theta c) \leq 2$ or $(2-4\theta)c \leq 1$. This is true for $\theta \geq 1/2$, and it is also true for $\theta < 1/2$ by Hypothesis (C). In fact $|\alpha_j| < 1$ for all j.

We can write the A_j explicitly in terms of the white noise. Indeed, $A_j(t_1) = \alpha_j A_j(0) + \beta_j w_{j,0}$, $A_j(t_2) = \alpha_j A_j(t_1) + \beta_j w_{j,1} = \alpha_j^2 A_j(t_0) + \beta_j\big(\alpha_j w_{j,0} + w_{j,1}\big)$ and, by induction,

$$A_j(t_m) = \alpha_j^m A_j(0) + \beta_j \sum_{i=0}^{m-1} \alpha_j^{m-i-1} w_{j,i}\,. \tag{23}$$

From this we see that if the $A_j(0)$ are independent and independent of the white noise, then the processes $\{A_j(t_m),\ m = 0,1,2\ldots\}$ are independent, and, for each A_j:

$$E\{A_j(t_m)\} = \alpha_j^m E\{A_j(0)\} \tag{24}$$

$$\begin{aligned}\mathrm{Var}\,\{A_j(t_m)\} &= \alpha_j^{2m}\mathrm{Var}\,\{A_j(0)\} + \beta_j^2 \sum_{i=0}^{m-1} \alpha_j^{2m-2i-2}\mathrm{Var}\,\{w_{j,i}\} \\ &= \alpha_j^{2m}\mathrm{Var}\,\{A_j(0)\} + \beta_j^2 hk \frac{1-\alpha_j^{2m}}{1-\alpha_j^2}\,,\end{aligned} \tag{25}$$

since the $w_{j,k}$ are independent $N(0,hk)$ random variables, independent of $A_j(0)$. The same logic leads to the covariance of the A_j:

$$\mathrm{Cov}\,\big(A_j(t_m), A_j(t_{m+p})\big) = \alpha_j^{2m+p}\mathrm{Var}\,\{A_j(0)\} + hk\beta_j^2\alpha_j^p \frac{1-\alpha_j^{2m}}{1-\alpha_j^2}\,. \tag{26}$$

Notice that the expectation, variance and covariance all tend to limits as $m \longrightarrow \infty$. Since the A_j are Gaussian processes, this implies that they tend to stationarity, and, moreover, if the initial values $A_j(0)$ have the stationary distribution, the $\{A_j(t_m),\ m = 0,1,2,\ldots\}$ are stationary independent Gaussian processes. Thus we have:

Proposition 6.1 *If the $A_j(0)$, $j = 1,\ldots,n$ are independent $N(0,\sigma_j^2)$ random variables, independent of $\dot W$, then the processes $\{A_j(t_m),\ m = 0,1,2,\ldots\}$ are independent stationary Gaussian processes with mean zero, variance $\sigma_j^2 = E\{A_j^2(t_0)\}$ and covariance function $\Gamma_j(p) = E\{A_j(t_m)A_j(t_{m+p})\}$, where*

$$\sigma_j^2 = \frac{h}{(2+(2\theta-1)c\lambda_j)\lambda_j} \tag{27}$$

$$\Gamma_j(p) = \sigma_j^2\alpha_j^p,\ p = 0,1,2,\ldots\,. \tag{28}$$

We will need some bounds on the absolute values of the α_j. Now α_j depends on n, c, and θ, so consider the function

$$\alpha(\theta, c, x) \stackrel{\text{def}}{=} \frac{1-(1-\theta)cx}{1+\theta cx}\,.$$

When there is no danger of ambiguity, we will write $\alpha(x)$ instead of $\alpha(\theta, c, x)$ below. Note that $\alpha_j = \alpha(\lambda_j)$. Moreover, $\alpha(0) = 1$ and for $x \geq 0$ and $c \geq 0$, α is strictly decreasing and convex in both x and c. To see this, just compute the derivatives of α. For $x \geq 0$ the first derivative of α is negative—so it is decreasing—and the second positive—so it is convex. This is true for both x and c because they appear symmetrically.

Let us also define a strictly positive function $\delta(\theta, n)$ by

$$\delta(\theta,n) = \begin{cases} 2(1-2\theta)\varepsilon_\theta & \text{if} \quad 0 \leq \theta < \dfrac{1}{2} \\ \dfrac{2}{1+2\sqrt{n}} & \text{if} \quad \theta = \dfrac{1}{2} \\ \dfrac{2\theta-1}{2\theta} & \text{if} \quad \dfrac{1}{2} < \theta \leq 1\,. \end{cases} \tag{29}$$

Here is a bound on the function $|\alpha(x)|$.

Lemma 6.2 *Assume Hypothesis (C), with the given ε_θ. Then*

$$|\alpha(x)| \leq e^{-\gamma(x)} \quad on \quad 0 \leq x \leq 4\,,$$

where

$$\gamma(x) = \min\Big(\frac{cx}{2}, \delta(\theta, n)\Big)\,.$$

Proof. We know that $-1 < \alpha_j < 1$. To bound $|\alpha|$, we will bound α away from both 1 and -1. Write $1-\alpha(x) = \frac{cx}{1+\theta cx}$. This is greater than $cx/2$ for small x. Indeed, since α is convex, the inequality is true until the first time that $\alpha(x) = cx/2$, that is, on $0 \leq x \leq 1/c\theta$. (If $\theta = 0$, it is true for all x.) Since α is decreasing, $x > 1/c\theta \Longrightarrow 1-\alpha(x) \geq 1/2\theta$. Thus

$$1-\alpha(x) \geq \min\Big(\frac{cx}{2}, \frac{1}{2\theta}\Big) \quad \text{for } x \geq 0\,. \tag{30}$$

In order to bound α away from -1, note that $1+\alpha(x) = \frac{2+(2\theta-1)cx}{1+\theta cx}$. If $\theta = 1/2$, then Hypothesis (C) requires that $c \leq \sqrt{n}$. As α is decreasing in both c and x, $1+\alpha(x,c) \geq 1+\alpha(4,\sqrt{n}) = 2/(1+2\sqrt{n})$. If $\theta \neq 1/2$, $1+\alpha$ is bounded away from zero. Indeed, if

$0 \le \theta < 1/2$, then c must be less than $c_\theta \equiv (1/(2-4\theta)) - \varepsilon_\theta$. Therefore $1+\alpha(x,c) \ge 1+\alpha(4,c_\theta) \ge 2(1-2\theta)\varepsilon_\theta$. And if $\theta > 1/2$, $1+\alpha(x,c) \ge 1+\lim_{c\to\infty}\alpha(4,c) = (2\theta-1)/\theta$. To summarize:

$$
(31) \qquad 1+\alpha(x) \ge \begin{cases} 2(1-2\theta)\varepsilon_\theta & \text{if } 0 \le \theta < \frac{1}{2} \\ \frac{2}{1+2\sqrt{n}} & \text{if } \theta = \frac{1}{2} \\ 2-\frac{1}{\theta} & \text{if } \frac{1}{2} < \theta \le 1\,. \end{cases}
$$

But now, since $|\alpha(x)| < 1$, $1-|\alpha(x)| \ge \min\big(1-\alpha(x), 1+\alpha(x)\big)$. We claim this is exactly $\gamma(x)$. Indeed, according to (30) and (31), $1-|\alpha|$ is the minimum of three quantities, one of which is $1/2\theta$. But $1/2\theta$ can never be the minimum, for it is greater than or equal to one if $\theta \le 1/2$, while $1-|\alpha|$ is less than one; and if $1/2 < \theta \le 1$, $1/2\theta \ge (2\theta-1)/2\theta$. Thus $1-|\alpha(x)| \ge \gamma(x)$. But this implies that $|\alpha(x)| \le e^{-\gamma(x)}$, as claimed. Indeed, for any x, $1-x \le e^{-x}$, so, if $y = 1-x$, $y \le e^{-(1-y)}$. ♣

Now $\alpha_j = \alpha(\lambda_j)$, $\sin x \ge 2x/\pi$ on $0 \le x \le \pi/2$, and $x \mapsto \gamma(x)$ is increasing, so Lemma 6.2 immediately implies

Corollary 6.3 $\qquad |\alpha_j| \le e^{-\gamma\left(\frac{4j^2}{(n+1)^2}\right)}\,.$

7 The Variations of the Numerical Approximations

Theorem 7.1 *Suppose Hypothesis (C) holds. There are η_1 and η_2 (which depend on c, n, and θ) with $|\eta_i| \le 1$ such that with probability one, for each $t > 0$*

$$
(32) \qquad E\big\{Q_n^{(2)}(t,c,\theta)\big\} = \frac{1}{2\sqrt{1+2c(2\theta-1)}} + \frac{\eta_1}{2(n+1)}\,,
$$

and

$$
(33) \qquad Var\big(Q_n^{(2)}(t,c,\theta)\big) = \frac{3}{2(n+1)}\,\frac{1+(2\theta-1)c}{\big(1+2c(2\theta-1)\big)^{\frac{3}{2}}} + \frac{\eta_2}{2(n+1)^2}\,.
$$

Before proving this, we need three lemmas. The first just records some information about the moments of Gaussian random variables. It follows from the usual calculations with the joint characteristic function. The second lists some trigonometric identities needed for the third lemma, which gives orthogonality relations for the increments of the eigenvectors of $\mathcal{A}$.

Lemma 7.2 *Let X and Y be $N(0,\sigma^2)$ random variables with correlation coefficient ρ. Then $Var(X^2) = 2\sigma^4$, $E\{X^4\} = 3\sigma^4$, $Var(X^4) = 96\sigma^8$, and $Cov(X^4, Y^4) = (72\rho^2 + 24\rho^4)\sigma^8 \le 96\rho^2\sigma^8 = 96\sigma^4 Cov(X,Y)^2 \le 96\sigma^6 Cov(X,Y)$.*

Lemma 7.3 *Let n and r be integers, $-n \le r \le n$. Then*

$$\sum_{p=0}^{n} \cos\frac{(2p+1)r\pi}{2(n+1)} = \begin{cases} n+1 & \text{if } r=0 \\ 0 & \text{if } r \ne 0 \end{cases} \tag{34}$$

$$\sum_{p=0}^{n} \cos^2\frac{(2p+1)r\pi}{2(n+1)} = \begin{cases} n+1 & \text{if } r=0 \\ \dfrac{n+1}{2} & \text{if } r \ne 0\,. \end{cases} \tag{35}$$

Proof. If $r = 0$, every summand in (34) equals 1, so the sum is $n+1$. If $r \ne 0$, write it as the real part of

$$e^{\frac{r\pi i}{2(n+1)}} \sum_{p=0}^{n} e^{\frac{pr\pi i}{n+1}} = e^{\frac{r\pi i}{2(n+1)}} \frac{1-e^{r\pi i}}{1-e^{\frac{r\pi i}{n+1}}}\,,$$

for, as $r < n+1$, $e^{r\pi i} \ne 1$, we can sum the geometric series explicitly. But this is

$$= \frac{1-(-1)^r}{e^{\frac{-r\pi i}{2(n+1)}} - e^{\frac{r\pi i}{2(n+1)}}} = \frac{i}{2}\,\frac{1-(-1)^r}{\sin\frac{r\pi}{2(n+1)}}\,,$$

which is purely imaginary, so its real part is zero.

To see (35), just note that $\cos^2\frac{(2p+1)r\pi}{2(n+1)} = (1/2)(1+\cos(\frac{(2p+1)2r\pi}{2(n+1)}))$. If $2r = 0$, then each term equals 1, and the sum is $n+1$, while if $2r \ne 0$, then by (34) the sum of the cosines vanishes, leaving $\sum_p (1/2) = (n+1)/2$. ♣

Lemma 7.4 *Let $\Delta\xi_j(i) = \xi_j(i+1) - \xi_j(i)$, $i = 0, \ldots, n$, where we define $\xi_j(0) = \xi_j(n+1) = 0$. Let j and k be integers, $1 \le j, k \le n$. Then*

$$\sum_{i=0}^{n} \Delta\xi_j(i)\Delta\xi_k(i) = \begin{cases} \lambda_j & \text{if } j=k \\ 0 & \text{if } j \ne k\,. \end{cases} \tag{36}$$

Proof. Use the identity $\sin x - \sin y = 2\cos((x+y)/2)\sin((x-y)/2)$ to see that

$$\begin{aligned}\Delta\xi_j(i) &= \sqrt{\frac{2}{n+1}}\left(\sin\frac{(i+1)j\pi}{n+1} - \sin\frac{ij\pi}{n+1)}\right)\\ &= 2\sqrt{\frac{2}{n+1}}\sin\frac{j\pi}{2(n+1)}\cos\frac{(2i+1)j\pi}{2(n+1)}\\ &= \sqrt{\frac{2}{n+1}}\sqrt{\lambda_j}\cos\frac{(2i+1)j\pi}{2(n+1)}\,.\end{aligned}$$

Thus

$$\sum_{i=0}^{n}\Delta\xi_j(i)\Delta\xi_k(i) = \frac{2}{n+1}\sqrt{\lambda_j\lambda_k}\sum_{i=0}^{n}\cos\frac{(2i+1)j\pi}{2(n+1)}\cos\frac{(2i+1)k\pi}{2(n+1)}\,.$$

Set $x = (2i+1)j/(2(n+1))$, $y = (2i+1)k/(2(n+1))$ in the identity $\cos x\,\cos y = (1/2)(\cos(x+y)+\cos(x-y))$ to see that this is

$$= \frac{1}{n+1}\sqrt{\lambda_j\lambda_k}\sum_{i=0}^{n}\left(\cos\frac{(2i+1)(j+k)\pi}{2(n+1)} + \cos\frac{(2i+1)(j-k)\pi}{2(n+1)}\right)\,.$$

By Lemma 7.3, both sums vanish if $j \neq k$. If $j = k$, the first sum vanishes and the second equals $n+1$, proving the lemma. ♣

Proof. (Of Theorem 7.1) Let $t = t_m$ and write $u_{i+1}^m - u_i^m = \sum_{j=1}^n A_j(t)\Delta\xi_j$.

$$\begin{aligned}Q_n^{(2)}(x,c,\theta) &= \sum_{i=0}^{n}\left(\sum_{j=1}^{n}A_j(t)\,\Delta\xi_j(i)\right)^2\\ &= \sum_{i=0}^{n}\sum_{j=1}^{n}\sum_{p=1}^{n}A_j(t)A_p(t)\Delta\xi_j(i)\,\Delta\xi_p(i)\\ &= \sum_{j=1}^{n}\sum_{p=1}^{n}A_j(t)A_p(t)\sum_{i=0}^{n}\Delta\xi_j(i)\,\Delta\xi_p(i)\\ &= \sum_{j=1}^{n}A_j(t)^2\lambda_j\,,\end{aligned}$$

since by Lemma 7.4, the sum over i equals zero if $j \neq p$ and equals λ_j if $j = p$. The A_j are independent $N(0,\sigma_j^2)$ r.v. so

$$
\begin{aligned}
E\{Q_n^{(2)}\} &= \sum_{j=1}^{n} \sigma_j^2 \lambda_j \\
&= \sum_{j=1}^{n} \frac{h}{2+(2\theta-1)c\lambda_j} \\
&= \sum_{j=1}^{n} \frac{h}{2+4(2\theta-1)c\sin^2\left(\frac{j\pi}{2(n+1)}\right)}\,.
\end{aligned}
$$

Now let $f(x) = \frac{1}{2+4(2\theta-1)c\sin^2\frac{\pi x}{2}}$. Note that f is positive, decreasing and the above sum equals $\sum_{j=1}^{n} f(j/(n+1))h$. This can be approximated by the integral $\int_0^1 f(x)\,dx$ with an error bounded by the first term, $f(0)h = h/2 = 1/(2(n+1))$. We will need the integral of f and of f^2. Both can be calculated in closed form, either (the hard way) by substituting $t = \tan(x/2)$ to turn them into integrals of rational functions of t which can be calculated by the usual methods, or (the easy way) by using Maple, Matlab, or Mathematica. Now

$$
\int_0^1 f(x)\,dx = \frac{1}{2\sqrt{1+2c(2\theta-1)}}\,,
$$

and (32) follows from:

$$
\left| E\{Q^{(2)}(x,c,\theta)\} - \frac{1}{2\sqrt{1+2c(2\theta-1)}} \right| \le \frac{1}{2(n+1)}\,.
$$

Note that the term under the square root is strictly positive. This is clear if $\theta \ge 1/2$, and it follows from Hypothesis (C) if $\theta < 1/2$.

To prove (33), note that

$$
\begin{aligned}
\mathrm{Var}\left(Q_n^{(2)}(t)\right) &= \mathrm{Var}\left(\sum_{j=1}^{n} A_j(t)^2\lambda_j\right) \\
&= \sum_{j=1}^{n} \mathrm{Var}\,(A_j(t)^2)\lambda_j^2 \\
&= 2\sum_{j=1}^{n} \sigma^4\lambda_j^2\,,
\end{aligned}
$$

since the A_j are independent and (see Lemma 7.2) the variance of the square of a $N(0,\sigma^2)$ r.v. is $2\sigma^4$. This is

$$= 2h \sum_{j=1}^{n} \frac{h}{\left[2 + 4(2\theta - 1)c \sin^2\left(\frac{j\pi}{2(n+1)}\right)\right]^2} = 2h \sum_{j=1}^{n} f^2\left(\frac{j}{n+1}\right) h\,.$$

As above, the sum can be approximated to within its first term, $hf(0)^2 = h/4$, by an integral. Let the actual error be $\eta_2 h/4$ for some $|\eta_2| \le 1$. Then it is

$$\begin{aligned} &= 2h \left(\int_0^1 f^2(x)\, dx + \eta_2 \frac{h}{4}\right) \\ &= \frac{1}{2(n+1)} \frac{1 + (2\theta - 1)c}{\left(1 + 2(2\theta - 1)c\right)^{\frac{3}{2}}} + \frac{\eta_2}{2(n+1)^2}\,. \end{aligned}$$

This proves the theorem. ♣

Theorem 7.5 *Let $n \ge 1$, $0 \le \theta \le 1$ and let c satisfy Hypothesis (C). Let $y = ih$ be one of the lattice points x_i, with $y = q/p$ in lowest terms. Let t be an integer multiple of k, and let $Q_n^{(4)}(y,t)$ be the quartic variation up to time t at the point y. Then there is a constant $K = K(\theta)$ and an $\eta = \eta(\theta, c, i, n)$, with $|\eta| \le 1$, such that*

$$E\{Q_n^{(4)}(y,t)\} = 3ct\left(\frac{1 - 2\theta}{\sqrt{1 + 2c(2\theta - 1)}} + \frac{2\theta}{\sqrt{1 + 4c\theta)}}\right)^2 + \eta K p h\,; \tag{37}$$

$$Var\left(Q_n^{(4)}(y,t)\right) \le \begin{cases} K(\theta)\dfrac{c^3}{n^2}\left(1 + \eta p h\right) & \text{if } \theta \ne \dfrac{1}{2} \\ K(\theta)\dfrac{c^3}{n^{\frac{3}{2}}}\left(1 + \eta p h\right) & \text{if } \theta = \dfrac{1}{2}\,. \end{cases} \tag{38}$$

Proof. Let $Y_m = u_i^{m+1} - u_i^m = \sum_{j=1}^{n} \Delta A_j(t_m)\xi_j(i)$. Then $Q_n^{(4)}(y,t) = \sum_{m=0}^{t/k-1} Y_m^4$. The A_j are stationary, so the distribution of Y_m is independent of m. It is Gaussian with mean zero, so by Lemma 7.2

$$\begin{aligned} E\{Q_n^{(4)}(y,t)\} &= \sum_{m=0}^{t/k-1} E\{Y_m^4\} \\ &= 3\frac{t}{k}\left(\mathrm{Var}\,(Y_m)\right)^2\,. \end{aligned}$$

Now $\mathrm{Var}\,(\Delta A_j(t_m)) = 2\Gamma_j(0) - 2\Gamma_j(1)$ and if $r \ge 1$, $\mathrm{Cov}\,(\Delta A_j(t_m), A_j(t_{m+r})) = 2\Gamma_j(r) - \Gamma_j(r+1) - \Gamma_j(r-1)$, so that, by Proposition 6.1, for $j = 1, 2, \ldots$

$$\text{(39)} \qquad \mathrm{Var}\left(\Delta A_j(t_m)\right) = 2\sigma_j^2(1-\alpha_j)$$
$$\text{(40)} \qquad \mathrm{Cov}\left(\Delta A_j(t_m), \Delta A_j(t_{m+r})\right) = -\sigma_j^2(1-\alpha_j)^2\alpha_j^{r-1}\,, \quad \text{if } \; r \geq 1\,.$$

$$\begin{aligned}
\mathrm{Var}\,(Y_m) &= \sum_{j=1}^{n} \mathrm{Var}\left(\Delta A_j(t_m)\right)\xi_j^2(i) \\
&= 2\sum_{j=1}^{n} \sigma_j^2(1-\alpha_j)\xi_j^2(i) \\
&= 2ch\sum_{j=1}^{n} \xi_j^2(i)\, \frac{1}{\left(1+4c\theta\sin^2\frac{j\pi}{2(n+1)}\right)\left(2+4c(2\theta-1)\sin^2\frac{j\pi}{2(n+1)}\right)}\,.
\end{aligned}$$

If we define a function g by

$$g(x) \stackrel{\text{def}}{=} \frac{1}{\left(1+4c\theta\sin^2\frac{\pi x}{2}\right)\left(2+4c(2\theta-1)\sin^2\frac{\pi x}{2}\right)}\,,$$

then

$$\text{(41)} \qquad \mathrm{Var}\,(Y_m) = 2ch\sum_{j=1}^{n}\xi_j^2(i)g\left(\frac{j}{n+1}\right)\,.$$

Now y is rational, and $y = q/p$ in lowest terms. Since y also equals $i/(n+1)$, p must divide $n+1$. By taking a larger n if necessary, we will assume that p divides $(n+1)/2$, say $(n+1)/2p = N$ for some integer N. (This is not necessary for the proof. It merely simplifies the notation.)

Recall that $\xi_j^2(i) = 2h\sin^2\frac{ij\pi}{n+1} = 2h\sin^2\frac{jq\pi}{p}$, so $j \mapsto \xi_j(i)$ is periodic with period p: $\xi_{p+\ell}(i) = \xi_\ell(i)$. Let us write $j = mp+\ell$, where $0 \leq m \leq N-1$ and $1 \leq \ell \leq q$. The sum in (41) becomes a double sum over m and ℓ. Since $\xi_{mp+\ell}(i) = \xi_\ell(i)$, we can factor it out of the sum over m to see that this is

$$= 2ch\sum_{\ell=0}^{p}\xi_\ell^2(i)\sum_{m=0}^{N-1} g\left(\frac{mp+\ell}{n+1}\right)\,.$$

Consider the sum over m. Under Hypothesis (C), the denominator of g does not vanish. Moreover, the denominator is a quadratic function of $\sin^2(\pi x/2)$, which itself is increasing on $[0,1]$. Thus g can have at most one local maximum or minimum. We can break up the sum into two parts, such that g is monotone on each. We can approximate the sum by an integral on each interval, and the error in each will be at most the largest term. Let $\mu = \mu(\theta, c)$ be the maximum of $|g|$ on $[0,1]$. Then error in the integral approximation is bounded by 2μ, so we can write

$$\sum_{m=0}^{N-1} g\left(\frac{mp+\ell}{n+1}\right) = \int_0^{N-1} g\left(\frac{xp+\ell}{n+1}\right) dx + 2\eta\mu$$
$$= \frac{n+1}{p}\int_0^{1-\frac{1}{N}} g\left(z + \frac{\ell}{n+1}\right) dz + 2\eta\mu\,.$$

where $|\eta| \le 1$. Now $\ell/(n+1) \le p/(n+1) = 1/2N$, so the integrals of g from 0 to $1/N$ and from $1-1/N$ to 1 contribute at most $(n+1)/p \times \mu/N = 2\mu$, so this is, with perhaps a different η,

$$= \frac{n+1}{p}\int_0^1 g\left(z\right)\, dz + 4\eta\mu\,.$$

Putting this together,

$$\mathrm{Var}\left(Y_m\right) = 2ch\sum_{\ell=1}^{p} \xi_\ell^2(i)\left(\frac{n+1}{p}\int_0^1 g(z)\,dz + 4\eta(\mu+1)\right)\,.$$

But $\xi_\ell^2(i) = 2h\sin^2\frac{i\ell\pi}{2p}$ so $\sum_{\ell=1}^{p}\xi_\ell^2(i) = 2h\sum_{\ell=1}^{p}\sin^2\frac{i\ell\pi}{2p}$. The sum is either $p/2$ or $(p+1)/2$, depending on whether i is even or odd. Just to be concrete, suppose it equals $p/2$. Then this is

$$= ch\Big(2\int_0^1 g(z)\,dz + 8ph(\mu+1)\Big)\,. \tag{42}$$

Now $t/k = t/(ch^2)$ so

$$E\big\{Q_n^{(4)}(y,t)\big\} = 3\frac{t}{ch^2}\mathrm{Var}\left(Y_m\right)^2 = 3ct\Big(2\int_0^1 g(z)\,dz + 8p(\mu+1)h\Big)^2\,.$$

The integral over g can be done explicitly: the substitution $t = \tan(x/2)$ reduces it to an integral of a rational function of t, readily checked by Maple. Then (37) follows from the fact that

$$\int_0^1 g(z)\,dz = \frac{1}{2}\Big(\frac{1-2\theta}{\sqrt{1+2c(2\theta-1)}} + \frac{1}{\sqrt{1+4c\theta}}\Big)\,,$$

coupled with the bound on μ: $\mu = 1/2$ if $\theta \geq 1/2$, and $\mu \leq \max(1/2, 1/8\varepsilon_\theta)$ if $\theta < 1/2$. (This can be seen by noting that if $\theta \geq 1/2$, g is decreasing in x and θ, so that its maximum occurs when these are at their minimum: $\theta = 1/2$ and $x = 0$, giving 1/2. If $0 \leq \theta \leq 1/4$, g is increasing in both x and c. As c is bounded by some c_θ, the maximum must occur when $x = 1$, $c = c_\theta$. If $1/4 < \theta < 1/2$, g decreases in x and c for a time and then (possibly) increases, so its maximum value occurs either at $x = 0$ or when $x = 1$ and $c = c_\theta$. But $g(\theta, 1, c_\theta) \leq 1/8\varepsilon_\theta$, which verifies the claimed error term.)

Now let us consider the variance of $Q_n^{(4)}$.

$$\begin{aligned}
\text{Var}\left(Q_n^{(4)}(t, x_i)\right) &= \text{Var}\Big(\sum_{m=0}^{t/k-1} Y_m^4\Big) \\
&= \sum_{m=0}^{t/k-1}\sum_{r=0}^{t/k-1} \text{Cov}\left(Y_m^4, Y_r^4\right) \\
&\leq 96 \sum_{m=0}^{t/k-1}\sum_{r=0}^{t/k-1} \text{Var}\left(Y_m\right)^3 \text{Cov}\left(Y_m, Y_r\right) \\
&= 96\Big(\sum_{m=0}^{t/k-1} \text{Var}\left(Y_m\right)^4 + 2\sum_{m=0}^{t/k-1} \text{Var}\left(Y_m\right)^3 \sum_{r=1}^{t/k-m-1} \text{Cov}\left(Y_m, Y_{m+r}\right)\Big)
\end{aligned}$$

by Lemma 7.2. Consider the sum over r and sum the geometric series:

$$\begin{aligned}
\sum_{r=1}^{t/k-m-1} \left|\text{Cov}\left(Y_m, Y_{m+r}\right)\right| &= \sum_{r=1}^{t/k-m-1} \sum_{j=1}^{n} \xi_j^2(i)\sigma_j^2(1-\alpha_j)^2|\alpha_j|^{r-1} \\
&\leq \sum_{j=1}^{n} \xi_j^2(i)\sigma_j^2(1-\alpha_j)^2 \frac{1}{1-|\alpha_j|}\,.
\end{aligned}$$

Note that $(1-\alpha_j)/(1-|\alpha_j|) = 1$ if $\alpha_j \geq 0$, and, if $\alpha_j < 0$, $(1-\alpha_j)/(1-|\alpha_j|) = (1+|\alpha_j|)/(1-|\alpha_j|) \leq 2/(1-|\alpha_j|)$. But now, if $\alpha_j < 0$, $1-|\alpha_j| \geq \delta(\theta, n)$, where $\delta(\theta, n)$ is defined in (29).

Thus, in any case,

$$\frac{(1-\alpha_j)^2}{1-|\alpha_j|} \leq (1-\alpha_j)\left(1 + \frac{1}{\delta(\theta, n)}\right),$$

and we have that

$$\sum_{r=1}^{t/k} \left|\mathrm{Cov}\left(Y_m, Y_{m+r}\right)\right| \leq \left(1 + \frac{1}{\delta(\theta,n)}\right) \sum_{j=1}^{n} \xi_j^2(i)\sigma_j^2(1-\alpha_j)$$
$$= \frac{1}{2}\left(1 + \frac{1}{\delta(\theta,n)}\right) \mathrm{Var}\left(Y_m\right).$$

Thus

$$\mathrm{Var}\left(Q_n^{(4)}(t,x_i)\right) \leq 96 \sum_{m=0}^{t/k} \mathrm{Var}\left(Y_m\right)^4 \left(2 + \frac{1}{\delta(\theta,n)}\right).$$

But $\mathrm{Var}\,(Y_m)$ is independent of m, and there are t/k terms in the sum, so this is

$$= 96\frac{t}{k}\mathrm{Var}\left(Y_m\right)^4 \left(2 + \frac{1}{\delta(\theta,n)}\right).$$

If $\theta = 1/2$, then $2 + 1/\delta \leq 4\sqrt{n}$, and if $\theta \neq 1/2$, $2 + 1/\delta$ is bounded, so

$$\theta \neq 1/2 \implies \mathrm{Var}\left(Q_n^{(4)}(t,x_i)\right) \leq K\frac{t}{k}\mathrm{Var}\left(Y_m\right)^4$$
$$\theta = 1/2 \implies \mathrm{Var}\left(Q_n^{(4)}(t,x_i)\right) \leq K\sqrt{n}\frac{t}{k}\mathrm{Var}\left(Y_m\right)^4.$$

Now $\mathrm{Var}\,(Y_m) = chF(\theta)$, where F is defined above. If $\theta \neq 1/2$, this is $KF^4\frac{t}{k}c^4h^4 = O(c^3/n^2)$. If $\theta = 1/2$, it is $KF^4\frac{t}{k}\sqrt{n}c^4h^4 = O(c^3/n^{3/2})$. ♣

8 Higher-order Variations for the Homogeneous Heat Equation

It remains to show that the limiting variations are independent of the initial conditions. As noted in §4, this is equivalent to showing that the limiting variations for the homogeneous equation tend to zero.

The solutions of the homogeneous PDE—that is, with no driving white noise—are infinitely differentiable, so that all their higher-order variations vanish. We might expect that this would also hold for the numerical approximations. This is by-and-large true, but we must be careful. If we take, for example, the Crank-Nicholson method with a large value of the ratio $c = k/h^2$, then for large j, α_j is close to -1. This means that if the initial value u_0 is proportional to the corresponding eigenvector, then at the very first step, the value will be close to $-u_0$, so that the quartic variation of u at the point x is about $16u(x)^4$—and that is after just one step. In a few more steps, it can be quite large indeed. But if $0 < \delta < t$, the limiting quartic variation from time δ to time t does indeed tend to zero as $n \to \infty$. And so does the quadratic variation at t. This section aims to establish this.

Lemma 8.1 *Let $p \geq 0$, $0 \leq \theta \leq 1$, $\delta > 0$, and $t \geq \delta$. Let (c_n) be a sequence of reals satisfying Hypothesis (C). Then*

$$\sup_{t \geq \varepsilon, n \geq 1} \sum_{j=1}^{n} j^p |\alpha_j|^{\frac{tn^2}{c_n}} < \infty \,.$$

Proof. From Corollary 6.2,

$$|\alpha_j| \leq e^{-\gamma\left(\frac{4j^2}{(n+1)^2}\right)} \,. \tag{43}$$

Now $\gamma(x)$ is the minimum of several values which depend on θ and x. Let δ be either $(2-4\theta)\varepsilon_\theta$ or $1 - 1/2\theta$, if θ is less or greater than $1/2$, respectively, and ε_θ comes from Hypothesis (C). Then $\delta > 0$ and $\gamma(x) = \min\big(cx/2, \delta, 2/(1+2\sqrt{n})\big)$. Since $\gamma(x)$ is an increasing function, for any $q \geq 1$,

$$|\alpha_j|^q \leq e^{-\frac{2cj^2 q}{(n+1)^2}} + e^{-q\delta} + e^{-2q/(1+2\sqrt{n})} \,.$$

Thus

$$|\alpha_j|^{t(n+1)^2} \leq e^{-2cj^2 t} + e^{-(n+1)^2 t\delta} + e^{-2tn^{3/2}} \,,$$

and

$$\sum_{j=1}^{n} j^p |\alpha_j|^{t(n+1)^2} \leq \sum_{j=1}^{n} \left(j^p e^{-2cj^2 t} + j^p e^{-(n+1)^2 t\delta} + j^p e^{-2tn^{3/2}} \right) .$$

All three terms are bounded in n. ♣

This brings us to the theorem:

Theorem 8.2 *Let $0 \leq \theta \leq 1$ and $\delta > 0$. Let (c_n) be a sequence of reals satisfying Hypothesis (C). Let $u_0(x)$ be a bounded function on $[0,1]$, say $|u_0(x)| \leq K$ for all x. Let (u_j^m) be the solution of the homogeneous form of (2) (i.e. with $W_{j,m} \equiv 0$) with initial value u_0, $h_n = 1/(n+1)$, and $k_n = c_n h_n^2$. Then for all $t > 0$, $\lim_{n\to\infty} Q_n^{(2)}(t) = 0$, and for all $0 < x < 1$, and $t > \delta$, $\lim_{n\to\infty} Q_n^{(4)}(x;t) - Q_n^{(4)}(x;\delta) = 0$.*

Remark 8.3 (*i*) *We will actually prove more: we show that the quadratic variation in t tends to zero, which implies that all variations of all orders greater than two—including the quartic variation—tend to zero.*

Proof. For each n, let U_0 be the vector $U_0 = \big(u_0(h), u_0(2h), \dots, u_0(nh)\big)$. Write $U_0 = \sum_{j=0}^n a_j(0)\xi_j(i)$, where $a_j(0) = \langle U_0, \xi_j\rangle$. By (23), with $w_{j,m} \equiv 0$,

$$a_j(q) = a_j(0)\alpha_j^q\,. \tag{44}$$

The ξ_j are ortho-normal, so

$$\sum_{j=1}^n a_j^2(0) = \sum_{i=1}^n u_0^2(ih) \le nK^2\,. \tag{45}$$

Then

$$Q_n^{(2)}(t) = \sum_{i=0}^n\Big(\sum_{j=1}^n a_j(0)\alpha_j^{\frac{t}{k}}(\xi_j(i+1)-\xi_j(i))\Big)^2 \tag{46}$$

$$\le \sum_{i=0}^n\sum_{j=1}^n a_j^2(0)\sum_{\ell=1}^n |\alpha_\ell|^{\frac{2t}{k}}(\xi_\ell(i+1)-\xi_\ell(i))^2\,, \tag{47}$$

by Schwartz' inequality. Sum first over i and use Lemma 7.4 to see this is

$$= \sum_{j=1}^n a_j^2(0)\,\sum_{\ell=1}^n |\alpha_\ell|^{\frac{2t}{k}}\lambda_\ell\,.$$

But $\lambda_\ell = 4\sin^2\big(\pi\ell/2(n+1)\big) \le \pi^2\ell^2/(n+1)^2$, and $t/k = (n+1)^2 t/c_n$, so that

$$Q_n^{(2)}(t) \le \frac{\pi^2}{(n+1)^2}nK^2\sum_{j=1}^n j^2|\alpha_j|^{\frac{2(n+1)^2t}{c_n}}\,.$$

The sum is uniformly bounded in n by Lemma 8.1, so this tends to zero as $n\to\infty$, proving the first claim.

The quadratic variation at a point $x = ih$ from time δ to time t is

$$Q_n^{(2)}(x;t) - Q^{(2)}(x;\delta) = \sum_{q=\delta/k}^{t/k}\Big(\sum_{j=1}^n \xi_j(i)(a_j(t_{q+1}) - a_j(t_q))\Big)^2\,.$$

Since $\xi_j(i) \le \sqrt{2}/\sqrt{n+1}$, and $a_j(q) = a_j(0)\alpha_j^q$, this is

$$\leq \sum_{q=\delta/k}^{t/k} \Big(\sum_{j=1}^{n} \frac{\sqrt{2}}{\sqrt{n+1}} \big(a_j(t_q)(\alpha_j - 1) \big) \Big)^2$$

$$\leq \frac{2}{n+1} \sum_{q=\delta/k}^{t/k} \Big(\sum_{j=1}^{n} a_j^2(0) \Big)^2 \sum_{j=1}^{n} \alpha_j^{2q} (1-\alpha_j)^2 \,,$$

by Schwartz' inequality. Now $\alpha(x)$ is convex with $\alpha'(0) = -c_n$, so $\alpha(x) \geq 1 - c_n x$, or $1 - \alpha_j = 1 - \alpha(|\lambda_j|) \leq c_n |\lambda_j| \leq c_n \pi^2 j^2/(n+1)^2 = \pi^2 k j^2$. Use (45) on the sum of the α_j^2 to see that the above is

$$\leq 2K^2 \pi^4 k \sum_{q=\delta/k}^{t/k} k \sum_{j=1}^{n} j^4 \alpha_j^{2q} \,.$$

By Lemma 8.1 the sum over j is uniformly bounded for $q > \delta/k = \delta(n+1)^2 t/c_n$, by M, say, and there are $(t-\delta)/k$ terms between δ/k and t/k, so that

$$Q_n^{(4)}(x;t) - Q_n^{(4)}(x;\delta) \leq 2MK^2\pi^4 k \,.$$

This tends to zero, for $k \to 0$ as $n \to \infty$.

Thus the quadratic variation tends to zero. Therefore every variation of order higher than two—and this includes the quartic variation—also tends to zero.

♣

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