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# A second-order discretization scheme for the CIR process: application to the Heston model

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## Abstract

This paper presents a weak second-order scheme for the Cox-Ingersoll-Ross process, without any restriction on its parameters. At the same time, it presents a general recursive construction method to get weak second-order schemes, extending the ideas of Ninomiya and Victoir [15]. Combining these both results, this allows to propose a rather accurate scheme for the Heston model. Simulation results are given to illustrate this.

*Keywords:* simulation, discretization scheme, squared Bessel process, Cox-Ingersoll-Ross model, Heston model.

## Introduction

In this paper, we are interested in the discretization schemes for the Cox-Ingersoll-Ross process (CIR for short), and more generally in multidimensional diffusion processes that contain this square-root diffusion, such as the Heston model [10]. Initially introduced in 1985 to model the short interest rate [6], the CIR process is now widely used in finance because it presents many interesting qualitative features such as positivity and mean-reversion. Moreover, it belongs to the class of affine models, and some standard expectations are thus analytically or semi-analytically known. We will use in this paper the following parametrization of the CIR processes

$$\begin{cases} X_t^x = x + \int_0^t (a - kX_s^x) ds + \sigma \int_0^t \sqrt{X_s^x} dW_s, t \in [0, T] \\ x \geq 0 \end{cases} \quad (1)$$

with parameters  $(a, k, \sigma) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+$ . Let us recall that if  $x > 0$  and  $2a \geq \sigma^2$  the process  $(X_t, t \geq 0)$  is always positive. We will also exclude the trivial case  $\sigma = 0$  and assume  $\sigma > 0$  in the whole paper.

First, let us say that exact simulation methods exist for the CIR process (see Glasserman [9]) and also for the Heston model (Broadie and Kaya [5]). With respect to discretization schemes, the drawback of these exact simulation methods is the computation time that they require. This is analysed in Alfonsi [1], Broadie and Kaya [5], and Lord, Koekoek and van Dijk [13]. What comes out is that exact methods are competitive when one has to simulate the process just at one time (or few times), for example to compute European options prices with a Monte-Carlo algorithm. On the contrary, they are drastically too slow if one has to simulate along a time-grid, as it is the case to calculate pathwise options prices. This is one of the reasons to investigate discretization schemes for square-root SDEs.

The main difficulty when discretizing the CIR process is located in 0, where the square-root is not Lipschitzian. General schemes such as the Euler scheme or the Milstein scheme are in general not well defined, and one has to modify them or to create ad-hoc schemes. Discretization schemes dedicated to the square-root diffusion processes have thus been studied in the recent years by Deelstra and Delbaen [7], Bossy, Diop and Berkaoui ([8, 4]), Alfonsi [1], Kahl and Schurz [12], Lord, Koekoek and van Dijk [13] and recently Andersen [2]. A possible criteria to chose the scheme may be its capacity to support large values of  $\sigma$  (i.e.  $\sigma^2 \gg 4a$ ). When dealing with the Heston model, it happens to observe indeed large values of  $\sigma$ . Heuristically, the larger is  $\sigma$ , the more the CIR process spends time in the neighbourhood of 0 where the square-root is very sensitive. This is why most of the cited schemes fail to be accurate for large  $\sigma$ . The QE scheme proposed by Andersen is in fact the only one that is really well suited for these large values.

In another direction, Ninomiya and Victoir [15] have proposed recently a general method to get weak second-order discretization schemes for a broad class of multidimensional SDEs. We will present their method in detail in the first part. They apply it to the Heston model (though the regularity assumptions required for their method are not satisfied) and get encouraging results, but only for  $\sigma^2 \leq 4a$  because their scheme may not be defined for  $\sigma^2 > 4a$ .

This paper has two main contributions. The first one is that we construct a weak second-order discretization scheme for the CIR process without any restriction on the parameters. In particular, our scheme supports high values of  $\sigma$ . The second one is a simple extension of the results of Ninomiya and Victoir, which allows to get a more flexible recursive construction of second-order schemes. It is structured as follows. The first part introduces notations and assumptions. In that framework, it presents the analysis of the weak error made by Talay and Tubaro. It is then given a recursive construction of second order schemes for multidimensional SDEs that encompasses the results of Ninomiya and Victoir. The second part is devoted to the construction of a weak second-order discretization scheme for the CIR. The third part puts into practice the general results of the first part to the Heston model, though here also the required assumptions are not truly satisfied. This gives a second-order scheme candidate for the Heston model. Simulations results are gathered in the fourth part for the CIR process, and for the Heston model. European and Asian options prices are in particular computed. The numerical behaviour of these schemes is rather encouraging.

# 1 Second order discretization schemes for SDEs.

## 1.1 Assumptions on the SDE and notations

We consider a  $d_W$ -dimensional standard Brownian motion  $(W_t, t \geq 0)$  and will denote in the sequel  $(\mathcal{F}_t)_{t \geq 0}$  its augmented associated filtration that satisfies the usual conditions. Let  $d \in \mathbb{N}^*$ , and  $\mathbb{D} \subset \mathbb{R}^d$  a domain that we assume for sake of simplicity to be a product of  $d$  intervals. We define for any multi-index  $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ ,  $\partial_\alpha = \partial_1^{\alpha_1} \dots \partial_d^{\alpha_d}$  and  $|\alpha| = \sum_{l=1}^d \alpha_l$ . We introduce the following functional space:

$$\mathcal{C}_{\text{pol}}^\infty(\mathbb{D}) = \{f \in \mathcal{C}^\infty(\mathbb{D}, \mathbb{R}), \forall \alpha \in \mathbb{N}^d, \exists C_\alpha > 0, e_\alpha \in \mathbb{N}^*, \forall x \in \mathbb{D}, |\partial_\alpha f(x)| \leq C_\alpha(1 + \|x\|^{e_\alpha})\}$$

where  $\|\cdot\|$  is a norm on  $\mathbb{R}^d$ . We will say that  $(C_\alpha, e_\alpha)_{\alpha \in \mathbb{N}^d}$  is a good sequence for  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  if one has  $\forall x \in \mathbb{D}, |\partial_\alpha f(x)| \leq C_\alpha(1 + \|x\|^{e_\alpha})$ . We assume that  $b : \mathbb{D} \rightarrow \mathbb{R}^d$  and  $\sigma : \mathbb{D} \rightarrow \mathcal{M}_{d \times d_W}(\mathbb{R})$  are such that for  $1 \leq i, j \leq d$ , the functions  $x \in \mathbb{D} \mapsto b_i(x)$  and  $x \in \mathbb{D} \mapsto (\sigma \sigma^*)_{i,j}(x)$  are in  $\mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$ . For  $x \in \mathbb{D}$ , we introduce the general  $\mathbb{R}^d$ -valued SDE:

$$t \geq 0, X_t^x = x + \int_0^t b(X_s^x) ds + \int_0^t \sigma(X_s^x) dW_s. \quad (2)$$

We assume that for any  $x \in \mathbb{D}$ , there is a unique weak solution defined for  $t \geq 0$ , and therefore  $\mathbb{P}(\forall t \geq 0, X_t^x \in \mathbb{D}) = 1$ . It satisfies then the strong Markov property (Theorem 4.20, p. 322 in [11]). The differential operator associated to the SDE is given by

$$f \in \mathcal{C}^2(\mathbb{D}, \mathbb{R}), Lf(x) = \sum_{i=1}^d b_i(x) \partial_i f(x) + \frac{1}{2} \sum_{i=1}^d \sum_{j=1}^d \sum_{k=1}^{d_W} \sigma_{i,k}(x) \sigma_{j,k}(x) \partial_i \partial_j f(x). \quad (3)$$

Thanks to the regularity assumptions made on  $b$  and  $\sigma$ , if  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$ , then all the iterated functions  $L^k f(x)$  are well defined on  $\mathbb{D}$  and belong to  $\mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  for any  $k \in \mathbb{N}$ .

Now, let us turn to the discretization schemes for the SDE (2). Let us fix a time horizon  $T > 0$ . We will consider in the whole paper the time interval  $[0, T]$  and the regular time discretization  $t_i^n = iT/n$  for  $i = 0, 1, \dots, n$ .

**Definition 1.1.** A family of transition probabilities  $(\hat{p}_x(t)(dz), t > 0, x \in \mathbb{D})$  on  $\mathbb{D}$  is such that  $\hat{p}_x(t)$  is a probability law on  $\mathbb{D}$  for  $t > 0$  and  $x \in \mathbb{D}$ .

A discretization scheme with transition probabilities  $(\hat{p}_x(t)(dz), t > 0, x \in \mathbb{D})$  is a sequence  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  of  $\mathbb{D}$ -valued random variables such that:

- for  $0 \leq i \leq n$ ,  $\hat{X}_{t_i^n}^n$  is  $\mathcal{F}_{t_i}$ -measurable,
- the law of  $\hat{X}_{t_{i+1}^n}^n$  is given by  $\mathbb{E}[f(\hat{X}_{t_{i+1}^n}^n) | \mathcal{F}_{t_i}^n] = \int_{\mathbb{R}^d} f(z) \hat{p}_{\hat{X}_{t_i^n}^n}(T/n)(dz)$  and thus only depends on  $\hat{X}_{t_i^n}^n$  and  $T/n$ .

For convenience, we will denote, for  $t > 0$  and  $x \in \mathbb{D}$ ,  $\hat{X}_t^x$  a random variable distributed according to the probability law  $\hat{p}_x(t)(dz)$ . The law of a discretization scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  is thus entirely determined by its initial value and its transition probabilities. Since the initial value is quite always taken equal to the initial value of the SDE, we will identify with a slight abuse of language the scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  with its transition probabilities  $(\hat{p}_x(t)(dz)$  or  $\hat{X}_t^x$ ).

**Definition 1.2.** Let us denote  $\mathcal{C}_K^\infty(\mathbb{D}, \mathbb{R})$  the set of the  $\mathcal{C}^\infty$  real valued functions with a compact support in  $\mathbb{D}$ . Let  $x \in \mathbb{D}$ . A discretization scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  is a weak  $\nu$ th-order scheme for the SDE  $(X_t^x, t \in [0, T])$  if:

$$\forall f \in \mathcal{C}_K^\infty(\mathbb{D}, \mathbb{R}), \exists K > 0, |\mathbb{E}(f(X_T^x)) - \mathbb{E}(f(\hat{X}_{t_n^n}^n))| \leq K/n^\nu.$$

The quantity  $\mathbb{E}(f(X_T^x)) - \mathbb{E}(f(\hat{X}_{t_n^n}^n))$  is called the weak error associated to  $f$ .

## 1.2 Analysis of the weak error

In this section, we develop in our setting the weak error analysis of Talay and Tubaro [17]. For that purpose, we introduce the following definitions.

**Definition 1.3.** A discretization scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  has uniformly bounded moments if one has

$$\forall q \in \mathbb{N}^*, \kappa(q) = \max_{0 \leq i \leq n} \mathbb{E}[\|\hat{X}_{t_i^n}^n\|^q] < \infty.$$

**Proposition 1.4.** Let us suppose that there is  $\eta > 0$  such that for  $t \in (0, \eta)$ ,

$$\forall q \in \mathbb{N}^*, \exists C_q > 0, \forall x \in \mathbb{D}, \mathbb{E}[\|\hat{X}_t^x\|^q] \leq \|x\|^q(1 + C_q t) + C_q t.$$

Then, the discretization scheme has uniformly bounded moments when  $n > T/\eta$ .

*Proof.* If  $n > T/\eta$ , we have clearly  $\mathbb{E}[\|\hat{X}_{t_{i+1}^n}^n\|^q] \leq (1 + C_q T/n)\mathbb{E}[\|\hat{X}_{t_i^n}^n\|^q] + C_q T/n$  and thus  $\mathbb{E}[\|\hat{X}_{t_i^n}^n\|^q] \leq u_i$  where  $u_0 = (\hat{X}_{t_0^n}^n)^q$  and  $u_{i+1} = (1 + C_q T/n)u_i + C_q T/n$ . Since  $u_i = (1 + C_q T/n)^i u_0 - 1 \leq (\hat{X}_{t_0^n}^n)^q e^{C_q T}$ , we get the desired result.  $\square$

**Definition 1.5.** Let us consider a mapping  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D}) \mapsto Rf$  such that  $Rf : \mathbb{R}_+^* \times \mathbb{D} \rightarrow \mathbb{R}$ . It is a remainder of order  $\nu \in \mathbb{N}$  if for any function  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  with a good sequence  $(C_\alpha, e_\alpha)_{\alpha \in \mathbb{N}^d}$ , there exist positive constants  $C$ ,  $E$ , and  $\eta$  depending only on  $(C_\alpha, e_\alpha)_{\alpha \in \mathbb{N}^d}$  such that

$$\forall t \in (0, \eta), \forall x \in \mathbb{D}, |Rf(t, x)| \leq C t^\nu (1 + \|x\|^E).$$

The upper bound of a remainder is thus assumed to be the same for two functions that have the same good sequence. In the following to get upper bounds, we will say with a slight abuse of language that a constant depends on a good sequence of  $f$  when this constant can be chosen only with a good sequence of  $f$ , independently from  $f$  itself. From the definition, we get the following straightforward properties.

**Proposition 1.6.** *Let  $\nu \in \mathbb{N}$ , and  $R_1$  and  $R_2$  be remainders of order  $\nu$ . Then,  $R_1 + R_2$  and  $\mu R_1$  (with  $\mu \in \mathbb{R}$ ) are remainders of order  $\nu$ . If  $\nu' \leq \nu$ ,  $R_1$  is also a remainder of order  $\nu'$ .*

**Definition 1.7.** *For any scheme  $(\hat{p}_x(t)(dz), t > 0, x \in \mathbb{D})$  we define*

$$\forall f \in \mathcal{C}^\infty, R_{\nu+1}^{\hat{p}(t)} f(x) = \mathbb{E}[f(\hat{X}_t^x)] - \left[ f(x) + \sum_{k=1}^{\nu} \frac{1}{k!} t^k L^k f(x) \right].$$

as soon as  $\mathbb{E}[|f(\hat{X}_t^x)|] < \infty$ .

We will say that  $\hat{p}_x(t)(dz)$  is a potential weak  $\nu$ th-order scheme for the operator  $L$  if  $R_{\nu+1}^{\hat{p}(t)} f(x)$  is defined for  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  and  $t > 0$ , and is a remainder of order  $\nu + 1$ .

Thanks to the previous proposition, a potential weak  $\nu$ th-order scheme  $\hat{X}_t^x$  for the operator  $L$  is also a potential weak  $\nu'$ th-order scheme for the operator  $L$  when  $\nu' \leq \nu$ . In particular taking  $\nu' = 0$ , there are constants  $C, E, \eta > 0$  that depend only on a good sequence of  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  such that

$$\forall t \in (0, \eta), |\mathbb{E}[f(\hat{X}_t^x)]| \leq C(1 + \|x\|^E). \quad (4)$$

One has then the following key result which is a direct consequence of the weak error analysis of Talay and Tubaro [17].

**Theorem 1.8.** *Let us consider a discretization scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  with transition probabilities  $\hat{p}_x(t)(dz)$  starting from  $\hat{X}_{t_0^n}^n = x$ . We assume that*

1. *the scheme has uniformly bounded moments and is a potential weak  $\nu$ th-order discretization scheme for the operator  $L$ .*
2.  *$f : \mathbb{D} \rightarrow \mathbb{R}$  is a function such that  $u(t, x) = \mathbb{E}[f(X_{T-t}^x)]$  is defined on  $[0, T] \times \mathbb{D}$ ,  $\mathcal{C}^\infty$ , solves  $\forall t \in [0, T], \forall x \in \mathbb{D}, \partial_t u(t, x) = -Lu(t, x)$ , and satisfies:*

$$\forall l \in \mathbb{N}, \alpha \in \mathbb{N}^d, \exists C_{l,\alpha}, e_{l,\alpha} > 0, \forall x \in \mathbb{D}, t \in [0, T], |\partial_t^l \partial_\alpha u(t, x)| \leq C_{l,\alpha}(1 + \|x\|^{e_{l,\alpha}}). \quad (5)$$

*Then, there is a positive constant  $K$  such that  $|\mathbb{E}[f(\hat{X}_{t_i^n}^n)] - \mathbb{E}[f(X_{T-t_i}^x)]| \leq K/n^\nu$ .*

Our statement here puts in evidence that the assumption 1 only concerns the discretization scheme while the assumption 2 mainly relies on the test function  $f$  and the diffusion coefficients  $b$  and  $\sigma$ .

*Proof.* Following Talay and Tubaro [17], we write the weak error  $\mathbb{E}[f(\hat{X}_{t_i^n}^n)] - \mathbb{E}[f(X_{T-t_i}^x)]$  as  $\mathbb{E}[f(\hat{X}_{t_i^n}^n)] - \mathbb{E}[f(X_T^x)] = \mathbb{E}[u(T, \hat{X}_{t_i^n}^n) - u(0, \hat{X}_{t_0^n}^n)] = \sum_{i=0}^{n-1} \mathbb{E}[u(t_{i+1}^n, \hat{X}_{t_{i+1}^n}^n) - u(t_i, \hat{X}_{t_i^n}^n)]$ . From the Taylor expansion of  $u$  at the point  $(t_{i+1}^n, \hat{X}_{t_i^n}^n)$  and  $\partial_t u = -Lu$  (assumption 2), we obtain

$$\left| u(t_i^n, \hat{X}_{t_i^n}^n) - \left[ u(t_{i+1}^n, \hat{X}_{t_i^n}^n) + \sum_{k=1}^{\nu} \frac{1}{k!} \left( \frac{T}{n} \right)^k L^k u(t_{i+1}^n, \hat{X}_{t_i^n}^n) \right] \right| \leq \frac{(T/n)^{\nu+1}}{(\nu+1)!} C_{\nu+1,0} (1 + \|\hat{X}_{t_i^n}^n\|^{e_{\nu+1,0}}).$$

On the other hand, we deduce from (5) and assumption 1 that there are positive constants  $C$ ,  $E$ ,  $n_0$  that depend on  $\nu$  and  $(C_{0,\alpha}, e_{0,\alpha})_\alpha$  such that for  $n \geq n_0$ ,

$$u(t_{i+1}^n, \hat{X}_{t_{i+1}}^n) = u(t_{i+1}^n, \hat{X}_{t_i}^n) + \sum_{k=1}^{\nu} \frac{1}{k!} \left(\frac{T}{n}\right)^k L^k u(t_{i+1}^n, \hat{X}_{t_i}^n) + R_{\nu+1}^{\hat{p}(T/n)} u(t_{i+1}^n, \cdot)(\hat{X}_{t_i}^n)$$

with

$$|R_{\nu+1}^{\hat{p}(T/n)} u(t_{i+1}^n, \cdot)(x)| \leq C(T/n)^{\nu+1}(1 + \|x\|^E).$$

Gathering the both expansions, we get  $|\mathbb{E}[u(t_{i+1}, \hat{X}_{t_{i+1}}^n) - u(t_i, \hat{X}_{t_i}^n)]| \leq \frac{K}{n^{\nu+1}}$  with  $K = T^{\nu+1} \left( \frac{C_{\nu+1,0}}{(\nu+1)!} (1 + \kappa(e_{\nu+1,0})) + C(1 + \kappa(E)) \right)$  (denoting for  $E > 0$ ,  $\kappa(E) = \max_{0 \leq i \leq n} \mathbb{E}[\|\hat{X}_{t_i}^n\|^E]$ ) and thus  $|\mathbb{E}(f(X_T^x)) - \mathbb{E}(f(\hat{X}_T^n))| \leq K/n^\nu$ .  $\square$

We give now two propositions that allow to extend easily potential weak  $\nu$ th-order scheme, when a coordinate is simply a function of the time and of the other coordinates.

**Proposition 1.9.** *If  $\hat{X}_t^x$  is a potential weak  $\nu$ th-order scheme for the operator  $L$ , then  $(\hat{X}_t^x, t)$  is a potential weak  $\nu$ th-order scheme for the operator  $L + \partial_t$ .*

*Proof.* Let  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D} \times \mathbb{R}_+)$ . Then, there is a family  $(C_\alpha, e_\alpha)_{\alpha \in \mathbb{N}^d}$  such that

$$\forall x \in \mathbb{D}, \forall t \in [0, 1), |\partial_\alpha f(x, t)| \leq C_\alpha (1 + \|x\|^{e_\alpha}),$$

and therefore there are constants  $C$ ,  $E$ ,  $\eta > 0$ , depending on  $(C_\alpha, e_\alpha)_{\alpha \in \mathbb{N}^d}$  such that

$$\forall t \in (0, \eta), \left| \mathbb{E}[f(\hat{X}_t^x, t)] - \sum_{k=0}^{\nu} \frac{1}{k!} t^k L^k f(x, t) \right| \leq Ct^{\nu+1} (1 + \|x\|^E).$$

The quantity  $\mathbb{E}[f(\hat{X}_t^x, t)] - \sum_{k=0}^{\nu} \frac{1}{k!} t^k L^k f(x, t)$  is thus a remainder of order  $\nu + 1$ . The Taylor's formula applied to  $L^k f(x, t)$  up to order  $\nu - k + 1$  gives:

$$L^k f(x, t) = L^k f(x, 0) + \dots + \frac{t^{\nu-k}}{(\nu-k)!} \partial_t^{\nu-k} L^k f(x, 0) + \int_0^t \frac{(t-s)^{\nu-k}}{(\nu-k)!} \partial_t^{\nu-k+1} L^k f(x, s) ds.$$

It is easy then to check that the integral is a remainder of order  $\nu - k + 1$ , and therefore  $\mathbb{E}[f(\hat{X}_t^x, t)] - \sum_{k=0}^{\nu} \sum_{l=0}^{\nu-k} \frac{1}{k!l!} t^{k+l} L^k \partial_t^l f(x, 0) = \mathbb{E}[f(\hat{X}_t^x, t)] - \sum_{k=0}^{\nu} \frac{1}{k!} t^k (L + \partial_t)^k f(x, 0)$  is a remainder of order  $\nu + 1$ .  $\square$

**Proposition 1.10.** *Let  $h \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$ . We define the operator  $L^h$  for  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D} \times \mathbb{R})$  by  $L^h f(x) = L\tilde{f}(x)$  where  $\tilde{f}(x) = f(x, h(x))$ . If  $\hat{X}_t^x$  is a potential weak  $\nu$ th-order scheme for the operator  $L$ , then  $(\hat{X}_t^x, h(\hat{X}_t^x))$  is a potential weak  $\nu$ th-order scheme for the operator  $L^h$ .*

*Proof.* Let  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D} \times \mathbb{R})$ . Then  $\tilde{f}(x) \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$ , and therefore we get

$$\forall t \in (0, \eta), \left| \mathbb{E}[\tilde{f}(\hat{X}_t^x)] - \left[ \tilde{f}(x) + \sum_{k=1}^{\nu} \frac{1}{k!} t^k L^k \tilde{f}(x) \right] \right| \leq Ct^{\nu+1} (1 + \|x\|^E),$$

for constants  $C$ ,  $E$ ,  $\eta$  that only depend on a good sequence of  $\tilde{f}$ . The function  $h \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  being fixed, these constants only depend also on a good sequence of  $f$ .  $\square$

Now we introduce the following standard assumption when studying the weak error.

**Assumption (A):**  $\mathbb{D} = \mathbb{R}^d$ , and the function  $b$  and  $\sigma$  are  $\mathcal{C}^\infty$  with bounded derivatives.

This assumption is stronger than the one done until now on  $b$  and  $\sigma$ . We will recall it each time it is necessary, otherwise it means that we are under the more general framework described in Section 1.1. It mainly ensures that we have good control on the function  $u$  as it is already mentioned in Talay [16].

**Theorem 1.11.** *We make the assumption (A), and consider  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$ . Then,  $u(t, x) = \mathbb{E}[f(X_{T-t}^x)]$  is  $\mathcal{C}^\infty$ , solves  $\partial_t u = -Lu$  on  $[0, T] \times \mathbb{R}^d$ , and its derivatives satisfy*

$$\forall l \in \mathbb{N}, \alpha \in \mathbb{N}^d, \exists C_{l,\alpha}, e_{l,\alpha} > 0, \forall x \in \mathbb{R}^d, t \in [0, T], |\partial_t^l \partial_\alpha u(t, x)| \leq C_{l,\alpha}(1 + \|x\|^{e_{l,\alpha}}). \quad (6)$$

One deduces then easily from Theorems 1.11 and 1.8 the following result.

**Corollary 1.12.** *We make the assumption (A). Let us consider a discretization scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  with transition probabilities  $\hat{p}_x(t)(dz)$  starting from  $\hat{X}_{t_0^n}^n = x$ . If the scheme has uniformly bounded moments and is a potential weak  $\nu$ th-order discretization scheme for the operator  $L$ , then it is a scheme of order  $\nu$ , and one has moreover*

$$\forall f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}^d), \exists K > 0, |\mathbb{E}[f(\hat{X}_{t_n^n}^n)] - \mathbb{E}[f(X_T^x)]| \leq K/n^\nu.$$

**Remark 1.13.** *Let us make the assumption (A). Then, using a Taylor expansion and Theorem 1.11, we get that the exact scheme  $(\hat{X}_t^x = X_t^x)$  is a potential weak order scheme of order  $\nu$ , for any  $\nu \in \mathbb{N}$ .*

### 1.3 Composition of discretization schemes

In this section, we will introduce the notion of composition of discretization schemes via their transition probabilities. We consider two operators  $L_1$  and  $L_2$  associated to SDEs that satisfy the assumptions described in Section 1.1 for the same domain  $\mathbb{D}$ .

**Definition 1.14.** *Let us consider two transition probabilities  $\hat{p}_x^1(t)(dz)$  and  $\hat{p}_x^2(t)(dz)$ . Then we define the composition  $\hat{p}^2(t_2) \circ \hat{p}_x^1(t_1)(dz)$  simply as*

$$\hat{p}^2(t_2) \circ \hat{p}_x^1(t_1)(dz) = \int_{\mathbb{R}^d} \hat{p}_y^1(t_2)(dz) \hat{p}_x^1(t_1)(dy).$$

*This amounts to first use the scheme 1 with a time step  $t_1$  and then the scheme 2 with a time step  $t_2$  with independent samples. We name  $\hat{X}_{t_2, t_1}^{2 \circ 1, x} = \hat{X}_{t_2}^{2, \hat{X}_{t_1}^{1, x}}$  a random variable with the law  $\hat{p}^2(t_2) \circ \hat{p}_x^1(t_1)(dz)$ .*

*More generally, if one has  $m$  transition probabilities  $\hat{p}_x^1, \dots, \hat{p}_x^m$ , we define  $\hat{p}^m(t_m) \circ \dots \circ \hat{p}_x^1(t_1)(dz)$  as the composition of  $\hat{p}^{m-1}(t_{m-1}) \circ \dots \circ \hat{p}_x^1(t_1)(dz)$  and then  $\hat{p}_x^m(t_m)$ .*



**Proposition 1.15.** *Let us assume that  $\hat{p}_x^1(t)(dz)$  and  $\hat{p}_x^2(t)(dz)$  are potential weak  $\nu$ th-order discretization schemes for the operators  $L_1$  and  $L_2$ . Then, for  $\lambda_1, \lambda_2 > 0$ ,  $\hat{p}^2(\lambda_2 t) \circ \hat{p}_x^1(\lambda_1 t)(dz)$  is such that for  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$ :*

$$\mathbb{E}[f(\hat{X}_{\lambda_2 t, \lambda_1 t}^{2 \circ 1})] = \sum_{l_1 + l_2 \leq \nu} \frac{\lambda_1^{l_1} \lambda_2^{l_2}}{l_1! l_2!} t^{l_1 + l_2} L_2^{l_2} L_1^{l_1} f(x) + R^{\hat{p}^2(\lambda_2 t) \circ \hat{p}^1(\lambda_1 t)} f(x)$$

where  $R^{\hat{p}^2(\lambda_2 t) \circ \hat{p}^1(\lambda_1 t)} f(x)$  is a remainder of order  $\nu + 1$

*Proof.* One has  $\mathbb{E}[f(\hat{X}_{\lambda_2 t, \lambda_1 t}^{2 \circ 1}) | \hat{X}_{\lambda_1 t}^{1, x}] = f(\hat{X}_{\lambda_1 t}^{1, x}) + \sum_{k=1}^{\nu} \frac{1}{k!} \lambda_2^k t^k L_2^k f(\hat{X}_{\lambda_1 t}^{1, x}) + R_{\nu+1}^{\hat{p}^2(\lambda_2 t)} f(x)$  and then

$$\mathbb{E}[f(\hat{X}_{\lambda_2 t, \lambda_1 t}^{2 \circ 1})] = \sum_{l_1 + l_2 \leq \nu} \frac{\lambda_1^{l_1} \lambda_2^{l_2}}{l_1! l_2!} t^{l_1 + l_2} L_2^{l_2} L_1^{l_1} f(x) + R^{\hat{p}^2(\lambda_2 t) \circ \hat{p}^1(\lambda_1 t)} f(x)$$

where  $R^{\hat{p}^2(\lambda_2 t) \circ \hat{p}^1(\lambda_1 t)} f(x) = \mathbb{E}[R_{\nu+1}^{\hat{p}^2(\lambda_2 t)} f(\hat{X}_{\lambda_1 t}^{1, x})] + \sum_{k=1}^{\nu} \frac{1}{k!} \lambda_2^k t^k R_{\nu+1-k}^{\hat{p}^1(\lambda_1 t)} L^k f(x)$ .

Since  $R_{\nu+1-k}^{\hat{p}^1(\lambda_1 t)} L^k f(x)$  is a remainder of order  $\nu + 1 - k$ , it is easy to get that the sum is a remainder of order  $\nu + 1$  using Proposition 1.6. We have also  $|R_{\nu+1}^{\hat{p}^2(\lambda_2 t)} f(\hat{X}_{\lambda_1 t}^{1, x})| \leq C_2 \lambda_2^{\nu+1} t^{\nu+1} (1 + \|\hat{X}_{\lambda_1 t}^{1, x}\|^{E_2})$  for some constants  $C_2 > 0$  and  $E_2 \in 2\mathbb{N}$  that only depend on a good sequence  $(C_\alpha, e_\alpha)$  of  $f$ . Defining  $\Phi(x) = 1 + x_1^{E_2} + \dots + x_d^{E_2}$ , we have  $\Phi \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{D})$  and  $|R_{\nu+1}^{\hat{p}^2(\lambda_2 t)} f(\hat{X}_{\lambda_1 t}^{1, x})| \leq C'_2 \lambda_2^{\nu+1} t^{\nu+1} \Phi(\hat{X}_{\lambda_1 t}^{1, x})$  and therefore we get

$$|\mathbb{E}[R_{\nu+1}^{\hat{p}^2(\lambda_2 t)} f(\hat{X}_{\lambda_1 t}^{1, x})]| \leq C'_2 \lambda_2^{\nu+1} t^{\nu+1} \mathbb{E}[\Phi(\hat{X}_{\lambda_1 t}^{1, x})] \stackrel{\text{Ineq. (4)}}{\leq} C'_2 \lambda_2^{\nu+1} t^{\nu+1} C_\Phi (1 + \|x\|^{E_\Phi})$$

for some positive constants  $C_\Phi, E_\Phi$  that only depend on  $\Phi$ . Since  $\Phi$  just depends on  $E_2$ , these constants depend on a good sequence of  $f$ . Therefore,  $R^{\hat{p}^2(\lambda_2 t) \circ \hat{p}^1(\lambda_1 t)} f(x)$  is a remainder of order  $\nu + 1$ .  $\square$

Thanks to that proposition, one can think a potential scheme of order  $\nu$  as an operator  $I + tL + \dots + \frac{t^\nu}{\nu!} L^\nu + \text{rem}$  on  $f$  where  $\text{rem}$  is a remainder of order  $\nu + 1$ . The composition of two schemes is simply the composition of their operators. We deduce also the following result.

**Corollary 1.16.** *Let us assume that  $\hat{p}_x^1(t)(dz)$  and  $\hat{p}_x^2(t)(dz)$  are potential weak  $\nu$ th-order discretization scheme for the operators  $L_1$  and  $L_2$ . If  $L_1 L_2 = L_2 L_1$ , then  $\hat{p}^2(t) \circ \hat{p}_x^1(t)(dz)$  is a potential weak  $\nu$ th-order discretization scheme for  $L_1 + L_2$ .*

## 1.4 The Ninomiya-Victoir discretization scheme revisited

In this section, we extend to our framework the idea of the Ninomiya-Victoir scheme. We consider  $m$  operators  $L_1, \dots, L_m$  associated to SDEs that satisfy the assumptions made in the Section 1.1 for the same domain  $\mathbb{D}$ .

**Theorem 1.17.** *Let us consider  $\hat{p}_x^1, \dots, \hat{p}_x^m$   $m$  potential second order discretization schemes for the operators  $L_1, \dots, L_m$ . Then, the transition probabilities*

$$\hat{p}^m(t/2) \circ \dots \circ \hat{p}^2(t/2) \circ \hat{p}^1(t) \circ \hat{p}^2(t/2) \circ \dots \circ \hat{p}_x^m(t/2) \quad (7)$$

$$\frac{1}{2} (\hat{p}^m(t) \circ \dots \circ \hat{p}^2(t) \circ \hat{p}_x^1(t) + \hat{p}^1(t) \circ \hat{p}^2(t) \circ \dots \circ \hat{p}_x^m(t)) \quad (8)$$

are potential second order discretization schemes for the operator  $\Sigma L = L_1 + L_2 + \dots + L_m$ .

*Proof.* Thanks to Proposition 1.15, the following expansions are justified. The first scheme gives:  $(I + \frac{t}{2}L_m + \frac{t^2}{8}L_m^2 + rem) \times \dots \times (I + \frac{t}{2}L_2 + \frac{t^2}{8}L_2^2 + rem)(I + tL_1 + \frac{t^2}{2}L_1^2 + rem)(I + \frac{t}{2}L_2 + \frac{t^2}{8}L_2^2 + rem) \times \dots \times (I + \frac{t}{2}L_2 + \frac{t^2}{8}L_m^2 + rem) = I + t\Sigma L + \frac{t^2}{2}\Sigma L^2 + rem$  where  $rem$  denotes a remainder of order 3. In the same manner,  $(I + tL_1 + \frac{t^2}{2}L_1^2 + rem) \times \dots \times (I + tL_m + \frac{t^2}{2}L_m^2 + rem) = I + tL + \frac{t^2}{2}(\sum_{j=1}^m L_j^2 + 2\sum_{j < k} L_j L_k) + rem$  and therefore the second scheme is also a potential second order discretization scheme for  $\Sigma L$ .  $\square$

Let us discuss now which of the two schemes is the more efficient for computational purposes. The first one requires a priori  $2m - 1$  samples for each step while the second one only  $m + 1$  ( $m$  for the schemes themselves and 1 to draw an independent Bernoulli random variable of parameter  $1/2$ ). Since  $2m - 1 \geq m + 1$  for  $m \geq 2$ , the second one is therefore a priori more efficient. There is however an exception when one of the scheme is deterministic. For example, let us assume that  $\hat{p}_x^2(t)$  is a Dirac mass measure. Then,  $\hat{p}^2(t/2) \circ \hat{p}^1(t) \circ \hat{p}_x^2(t/2)$  requires only one sample while the scheme  $\frac{1}{2}(\hat{p}^2(t) \circ \hat{p}_x^1(t) + \hat{p}^1(t) \circ \hat{p}_x^2(t))$  needs two samples.

**Theorem 1.18.** (*Ninomiya-Victoir*) *We make the assumption (A). One can write the operator  $L$  defined in (3) as  $L = V_0 + \frac{1}{2} \sum_{k=1}^{d_W} V_k^2$  with*

$$\begin{aligned} V_0 f(x) &= \sum_{i=1}^d b_i(x) \partial_i f(x) - \frac{1}{2} \sum_{i,j=1}^d \sum_{k=1}^{d_W} \partial_j \sigma_{i,k} \sigma_{j,k} \partial_i f(x) \\ V_k f(x) &= \sum_{i=1}^d \sigma_{i,k}(x) \partial_i f \text{ for } k = 1, \dots, d_W. \end{aligned}$$

Let us define  $v_k$  as  $V_k f(x) =: v_k(x) \cdot \nabla f$  for  $k = 0, \dots, d_W$  and denote, for  $t \in \mathbb{R}$ ,  $X_k(t, x)$  the solution of  $\frac{dX_k(t, x)}{dt} = v_k(X_k(t, x))$  starting from  $X_k(0, x) = x$ . Let  $\hat{p}_x^0(t)(dz)$  be the law of  $X_0(t, x)$  and for  $k = 1, \dots, d_W$ ,  $\hat{p}_x^k(t)(dz)$  the law of  $X_k(\sqrt{t}N, x)$  where  $N \sim \mathcal{N}(0, 1)$ . Then for any  $\nu \in \mathbb{N}^*$ ,  $\hat{p}_x^0(t)(dz)$  is a potential  $\nu$ th-order scheme for  $V_0$  and  $\hat{p}_x^k(t)(dz)$  is a potential  $\nu$ th-order scheme for  $\frac{1}{2}V_k^2$ . Moreover,

$$\frac{1}{2} (\hat{p}^0(t/2) \circ \hat{p}^m(t) \circ \dots \circ \hat{p}^1(t) \circ \hat{p}_x^0(t/2) + \hat{p}^0(t/2) \circ \hat{p}^1(t) \circ \dots \circ \hat{p}^m(t) \circ \hat{p}_x^0(t/2)) \quad (9)$$

is a potential second order scheme for  $L$ .

*Proof.* We just have to check that  $\hat{p}_x^0(t)(dz)$  and  $\hat{p}_x^k(t)(dz)$  ( $k > 0$ ) are respectively potential  $\nu$ th-order schemes for  $V_0$  and  $\frac{1}{2}V_k^2$ . The result is then a straightforward consequence of Theorem 1.17.

First, let us remark that assumption **(A)** implies that there is a positive constant  $K$  such that  $\|v_k(x)\| \leq K(1 + \|x\|)$  for  $k = 0, \dots, d_W$ . It is well known then that the solutions to the ODEs  $X_k(t, x)$  are well defined on  $\mathbb{R}$ , and satisfy thanks to the Gronwall lemma

$$\exists c, c' > 0, \forall t \in \mathbb{R}, k = 0, \dots, d_W, \|X_k(t, x)\| \leq ce^{c'|t|}(\|x\| + 1).$$

Now let us consider  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}^d)$ . We have for  $l \in \mathbb{N}$ :

$$f(X_k(t, x)) = f(x) + tV_k f(x) + \dots + \frac{t^l}{l!} V_k^l f(x) + \int_0^t \frac{(t-s)^l}{l!} V_k^{l+1} f(X_k(s, x)) ds. \quad (10)$$

It is easy to check that  $V_k^{l+1} f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}^d)$  and that there are positive constants  $C, E > 0$  that depend on a good sequence of  $f$  such that  $\|V_k^{l+1} f(x)\| \leq C(1 + \|x\|^E)$  for  $k = 0, \dots, d_W$  and  $l \in \{\nu, 2\nu + 1\}$ .

Now, let us consider the case  $k = 0$  and take  $l = \nu$  and  $t \in (0, 1)$ . One can bound  $|\int_0^t \frac{(t-s)^\nu}{\nu!} V_0^{\nu+1} f(X_0(s, x)) ds| \leq \frac{t^{\nu+1}}{\nu!} C(1 + (ce^{c'}(\|x\| + 1))^E) \leq C' t^{\nu+1} (1 + \|x\|^E)$  for a constant  $C' > 0$  that depends on a good sequence of  $f$ , and therefore  $\hat{p}_x^0(t)(dz)$  is a potential  $\nu$ th-order scheme for  $V_0$ .

Let us take now  $k \in \{1, \dots, d_W\}$  and  $l = 2\nu + 1$ . We get from (10) (recall  $\mathbb{E}[N^{2\nu}] = \frac{(2\nu)!}{2^\nu \nu!}$ ):

$$\begin{aligned} \mathbb{E}[f(X_k(\sqrt{t}N, x))] &= f(x) + \frac{t}{2} V_k^2 f(x) + \dots + \frac{t^\nu}{\nu!} \left(\frac{1}{2} V_k^2\right)^\nu f(x) \\ &\quad + \mathbb{E} \left[ \int_0^{\sqrt{t}N} \frac{(\sqrt{t}N - s)^{2\nu+1}}{(2\nu+1)!} V_k^{2\nu+2} f(X_k(s, x)) ds \right]. \end{aligned}$$

We have  $|\int_0^{\sqrt{t}N} \frac{(\sqrt{t}N - s)^{2\nu+1}}{(2\nu+1)!} V_k^{2\nu+2} f(X_k(s, x)) ds| \leq \frac{t^{\nu+1}}{(2\nu+1)!} |N|^{2\nu+2} C(1 + ce^{c'\sqrt{t}|N|}(\|x\| + 1)^E)$  and remark that for  $t \in (0, 1)$ ,  $\mathbb{E}[|N|^{2\nu+2} C(1 + ce^{c'\sqrt{t}|N|}(\|x\| + 1)^E)] \leq C''(1 + \|x\|^E)$  for a constant  $C''$  that depends on  $f$  only through a good sequence. Therefore,  $\hat{p}_x^k(t)(dz)$  is a potential  $\nu$ th-order scheme for  $\frac{1}{2}V_k^2$ .  $\square$

**Remark 1.19.** *The Ninomiya-Victoir scheme writes for the CIR process (and for  $k \neq 0$ ):*

$$\hat{X}_t^x = e^{-\frac{kt}{2}} \left( \sqrt{(a - \sigma^2/4) \frac{1 - e^{-\frac{kt}{2}}}{k} + e^{-\frac{kt}{2}} x + \frac{\sigma}{2} W_t} \right)^2 + (a - \sigma^2/4) \frac{1 - e^{-\frac{kt}{2}}}{k}, \quad (11)$$

and is not defined as soon as  $\sigma^2 > 4a$  for small values of  $x \geq 0$  since the term in the square-root is then negative.

Now, we would like to give a rather general way to split in two the operator  $L$ . Of course, a recursive application of this method allow to split  $L$  as the sum of many operators. Let us

consider  $I \subset \{1, \dots, d_W\}$  and denote  $W_t^I$  the  $\mathbb{R}^{d_W}$ -valued process such that  $(W_t^I)_i = (W_t)_i$  if  $i \in I$ , and  $(W_t^I)_i = 0$  if  $i \notin I$ . Let us assume that  $b^I(x)$  and  $b^{I^c}(x)$  are such that  $b^I(x) + b^{I^c}(x) = b(x)$ . Then, it is easy to see that  $L = L^I + L^{I^c}$  where  $L^I$  (resp.  $L^{I^c}$ ) is the operator associated to the SDE:

$$dX_t^I = b^I(X_t^I)dt + \sigma(X_t^I)dW_t^I \text{ (resp. } dX_t^{I^c} = b^{I^c}(X_t^{I^c})dt + \sigma(X_t^{I^c})dW_t^{I^c}).$$

The splitting of  $L$  proposed by Ninomiya and Victoir is easily obtained if one writes the SDE of  $(X_t, t \geq 0)$  with the Stratonovitch integral. The operator  $V_0$  is associated to the ODE  $dX_t^\emptyset = v_0(X_t^\emptyset)dt$  and for  $k = 1, \dots, d_W$ ,  $\frac{1}{2}V_k^2$  is associated to  $dX_t^{\{k\}} = \sigma(X_t^{\{k\}}) \star dW_t^{\{k\}} = v_k(X_t^{\{k\}}) \star d(W_t)_k$  where  $\star$  denotes the Stratonovitch integral. This splitting has the main advantage to reduce the problem to the resolution of ODEs instead of SDEs. The laws of  $X_0(t, x)$  and  $X_k(\sqrt{t}N, x)$  give exact schemes for their associated SDEs. If one has exact or very accurate methods to integrate the ordinary differential equations (such as Runge-Kutta method), one can get easily a weak second order scheme. Typically, the numerical integration should be accurate up to  $t^3$  for  $X_0(t, x)$  and up to order  $t^6$  for  $X_k(t, x)$  to have an remainder of order 3 and thus a potential second order scheme.

## 2 A second order scheme for the CIR process.

In this section, we focus on the discretization scheme for the CIR process (1) and have thus  $d_W = 1$  and  $\mathbb{D} = \mathbb{R}_+$ . It satisfies the assumptions of Section 1.1, and we introduce its operator

$$f \in \mathcal{C}^2(\mathbb{R}, \mathbb{R}), L_{\text{CIR}}f(x) = (a - kx)\partial_x f(x) + \frac{1}{2}\sigma^2 x \partial_x^2 f(x)$$

that is well defined not only for functions defined on  $\mathbb{R}_+$ , but also on  $\mathbb{R}$ . The main result of this section is the construction of a second order scheme for the CIR process without any restrictions on the CIR parameters  $(a, k, \sigma) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+^*$ . The main difficulty, not surprisingly, is located in the neighbourhood of 0 where the square-root is not enough regular to satisfy assumption **(A)**. Our solution consists in keeping the nonnegativity of the discretization scheme, taking different schemes whether the discretization is in a neighbourhood of 0 or not.

### 2.1 A second order scheme away from a neighbourhood of 0.

In this section, we are looking for a discretization scheme that writes  $\hat{X}_t^x = \varphi(x, t, W_t)$ . In order to have a second order discretization scheme, we look for a function  $\varphi$  such that the remainder

$$f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}), x \geq 0, R_{f \circ \varphi}(t, x) = \mathbb{E}[f(\varphi(x, t, W_t))] - \left( f(x) + tL_{\text{CIR}}f(x) + \frac{t^2}{2}L_{\text{CIR}}^2f(x) \right) \quad (12)$$

is of order 3 on  $\mathbb{R}_+$ , i.e. it exists positive constants  $C$ ,  $E$  and  $\eta$  depending on a good sequence of  $f$  such that

$$\forall t \in (0, \eta), \forall x \geq 0, |R_{f \circ \varphi}(t, x)| \leq Ct^3(1 + |x|^E).$$

Let  $f \in C_{\text{pol}}^\infty(\mathbb{R})$ . We assume that  $\varphi$  is smooth enough for what follows and define  $g(x, t, w) = f(\varphi(x, t, w))$ . Using a Taylor expansion first on  $t$

$$g(x, t, w) = g(x, 0, w) + t\partial_t g(x, 0, w) + \frac{t^2}{2}\partial_t^2 g(x, 0, w) + \int_0^t \frac{(t-u)^2}{2}\partial_t^3 g(x, u, w)du$$

and then on  $w$ , one gets:

$$g(x, t, w) = \sum_{l+2l' < 6} \frac{w^l t^{l'}}{l!l'!} \partial_t^{l'} \partial_w^l g(x, 0, 0) + \tilde{R}_g(x, t, w) \quad (13)$$

where

$$\begin{aligned} \tilde{R}_g(x, t, w) &= \int_0^t \frac{(t-u)^2}{2} \partial_t^3 g(x, u, w) du + \frac{t^2}{2} \int_0^w (w-z) \partial_t^2 \partial_w^2 g(x, 0, z) dz \\ &\quad + t \int_0^w \frac{(w-z)^3}{3!} \partial_t \partial_w^4 g(x, 0, z) dz + \int_0^w \frac{(w-z)^5}{5!} \partial_w^6 g(x, 0, z) dz. \end{aligned} \quad (14)$$

Therefore, one deduces:

$$\begin{aligned} \mathbb{E}[g(x, t, W_t)] &= f(x) + t \left[ \partial_t g(x, 0, 0) + \frac{1}{2} \partial_w^2 g(x, 0, 0) \right] \\ &\quad + \frac{t^2}{2} \left[ \partial_t^2 g(x, 0, 0) + \partial_t \partial_w^2 g(x, 0, 0) + \frac{1}{4} \partial_w^4 g(x, 0, 0) \right] + \mathbb{E}[\tilde{R}_g(x, t, W_t)]. \end{aligned} \quad (15)$$

Simple calculations lead then to

$$\begin{aligned} \partial_t g &= \partial_t \varphi f'(\varphi) \\ \partial_t^2 g &= \partial_t^2 \varphi f'(\varphi) + (\partial_t \varphi)^2 f''(\varphi) \\ \partial_w^2 g &= \partial_w^2 \varphi f'(\varphi) + (\partial_w \varphi)^2 f''(\varphi) \\ \partial_t \partial_w^2 g &= \partial_t \partial_w^2 \varphi f'(\varphi) + [\partial_w^2 \varphi \partial_t \varphi + 2\partial_w \varphi \partial_t \partial_w \varphi] f''(\varphi) + (\partial_w \varphi)^2 \partial_t \varphi f^{(3)}(\varphi) \\ \partial_w^4 g &= \partial_w^4 \varphi f'(\varphi) + [4\partial_w^3 \varphi \partial_w \varphi + 3(\partial_w^2 \varphi)^2] f''(\varphi) + 6\partial_w^2 \varphi (\partial_w \varphi)^2 f^{(3)}(\varphi) + (\partial_w \varphi)^4 f^{(4)}(\varphi). \end{aligned}$$

We suppose from now that  $\varphi(x, t, w) = \sum_{l+2l' \leq 4} \frac{\varphi_{l,l'}(x)}{l!l'!} w^l t^{l'}$ , so that

$$\partial_w^l \partial_t^{l'} \varphi(x, 0, 0) = \begin{cases} \varphi_{l,l'}(x) & \text{if } l + 2l' \leq 4 \\ 0 & \text{if } l + 2l' > 4. \end{cases}$$

If one wants to cancel the term of order 0 in (12), one has to take  $\varphi_{0,0}(x) = x$ , and for the term of order 1, it implies

$$\varphi_{0,1}(x) + \frac{1}{2}\varphi_{2,0}(x) = a - kx \text{ and } \varphi_{1,0}(x)^2 = \sigma^2 x. \quad (16)$$

Now, we want also to cancel the term of order 2 in (12) and thus calculate

$$\begin{aligned} L_{\text{CIR}}^2 f(x) &= -k(a - kx)f'(x) + [(a - kx)(a - kx + \frac{\sigma^2}{2}) - k\sigma^2 x]f''(x) \\ &\quad + [\frac{1}{2}\sigma^4 x + (a - kx)\sigma^2 x]f^{(3)}(x) + \frac{1}{4}\sigma^4 x^2 f^{(4)}(x). \end{aligned} \quad (17)$$

Since  $\partial_t^2 g(x, 0, 0) + \partial_t \partial_w^2 g(x, 0, 0) + \frac{1}{4}\partial_w^4 g(x, 0, 0) = [\varphi_{0,2}(x) + \varphi_{2,1}(x) + \frac{1}{4}\varphi_{4,0}(x)]f'(x) + [\varphi_{0,1}(x)^2 + \varphi_{2,0}(x)\varphi_{0,1}(x) + 2\varphi_{1,0}(x)\varphi_{1,1}(x) + \varphi_{3,0}(x)\varphi_{1,0}(x) + \frac{3}{4}\varphi_{2,0}(x)^2]f''(x) + [\varphi_{1,0}(x)^2\varphi_{0,1}(x) + \frac{3}{2}\varphi_{1,0}(x)^2\varphi_{2,0}(x)]f^{(3)}(x) + \frac{1}{4}\varphi_{1,0}(x)^4 f^{(4)}(x)$ , we get the following conditions:

$$\begin{aligned} \frac{1}{4}\sigma^4 x^2 &= \frac{1}{4}\varphi_{1,0}(x)^4 \\ \frac{1}{2}\sigma^4 x + (a - kx)\sigma^2 x &= \varphi_{1,0}(x)^2(\varphi_{0,1}(x) + \frac{3}{2}\varphi_{2,0}(x)) \\ (a - kx)(a - kx + \frac{\sigma^2}{2}) - k\sigma^2 x &= \varphi_{0,1}(x)^2 + \varphi_{2,0}(x)\varphi_{0,1}(x) \\ &\quad + 2\varphi_{1,0}(x)\varphi_{1,1}(x) + \varphi_{3,0}(x)\varphi_{1,0}(x) + \frac{3}{4}\varphi_{2,0}(x)^2 \\ -k(a - kx) &= \varphi_{0,2}(x) + \varphi_{2,1}(x) + \frac{1}{4}\varphi_{4,0}(x). \end{aligned} \quad (18)$$

Condition (18) is implied by (16), and using (16), the other ones write:

$$\frac{1}{2}\sigma^2 = \varphi_{2,0}(x) \quad (19)$$

$$\frac{\sigma(a - 3kx - \sigma^2/4)}{2\sqrt{x}} = 2\varphi_{1,1}(x) + \varphi_{3,0}(x) \quad (20)$$

$$-k(a - kx) = \varphi_{0,2}(x) + \varphi_{2,1}(x) + \frac{1}{4}\varphi_{4,0}(x). \quad (21)$$

If the coefficients  $\varphi_{l,\nu}(x)$  satisfy the above conditions, one has then to control  $\mathbb{E}[R_g(x, t, W_t)]$ . The difficulty here is that the coefficients of the scheme (namely  $\varphi_{1,1}(x)$  and  $\varphi_{3,0}(x)$ ) may explode when  $x$  is in the neighbourhood of 0 as soon as  $\sigma^2 \neq 4a$ . It is thus not clear how to control the remainder (12) uniformly in  $x \in \mathbb{R}_+$  and we exclude a neighbourhood of 0. The following proposition gathers all the preceding calculations (observe that they rely only on the five first moments of the Gaussian variable), and precises this point.

**Proposition 2.1.** *Let us assume that the coefficients are such that*

- $\varphi_{0,0}(x) = x$ ,  $\varphi_{1,0}(x) = \sigma\sqrt{x}$ ,  $\varphi_{2,0}(x) = \frac{\sigma^2}{2}$ ,  $\varphi_{0,1}(x) = a - kx - \frac{\sigma^2}{4}$ ,
- $\varphi_{3,0}(x) = \beta_{3,0} \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}}$  and  $\varphi_{1,1}(x) = \beta_{1,1} \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}}$  with  $\beta_{3,0} + 2\beta_{1,1} = 1$ ,
- $\varphi_{0,2}(x) = -\beta_{0,2}k(a - kx)$ ,  $\varphi_{2,1}(x) = -\beta_{2,1}k(a - kx)$ ,  $\varphi_{4,0}(x) = -\beta_{4,0}k(a - kx)$  with  $\beta_{0,2} + \beta_{2,1} + \beta_{4,0}/4 = 1$ ,

so that all the above conditions are satisfied. Let  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R})$  and  $g = f \circ \varphi$ . Let  $Y$  be a random variable with finite moments of any order such that  $\mathbb{E}[Y^q] = \mathbb{E}[N^q]$  for  $q \leq 5$  with  $N \sim \mathcal{N}(0, 1)$ , and define  $R_g^Y(t, x) = \mathbb{E}[f(\varphi(x, t, \sqrt{t}Y))] - \left( f(x) + tL_{\text{CIR}}f(x) + \frac{t^2}{2}L_{\text{CIR}}^2f(x) \right)$ . Then, we have  $R_g^Y(t, x) = \mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y))$ .

Let us assume  $\sigma^2 \neq 4a$ . Then for any  $\mathbf{K} > 0$ , it exists positive constants  $C$ ,  $E$  and  $\eta$  that depend on a good sequence of  $f$  such that

$$\forall t \in (0, \eta), \forall x \geq \mathbf{K}t, |\mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y))| \leq Ct^3(1 + |x|^E) \quad (22)$$

if and only if  $\varphi_{1,1}(x) = -\frac{1}{6}\varphi_{3,0}(x)$  (i.e.  $\beta_{1,1} = -1/4$  and  $\beta_{3,0} = 3/2$ ).

If  $\sigma^2 = 4a$  property (22) is satisfied without further restriction on  $\beta_{1,1}$  and  $\beta_{3,0}$ .

*Proof.* The fact that  $R_g^Y(t, x) = \mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y))$  is a consequence of the previous calculations. Let us denote  $p_Y(dy)$  the probability measure of  $Y$ . From (14), we get with a change of variable:

$$\mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y)) = \int_{\mathbb{R}} p_Y(dy) \left[ \int_0^t \frac{(t-u)^2}{2} \partial_t^3 g(x, u, \sqrt{t}y) du + \frac{t^3}{2} \int_0^y (y-z) \partial_t^2 \partial_w^2 g(x, 0, \sqrt{t}z) dz + t^3 \int_0^y \frac{(y-z)^3}{3!} \partial_t \partial_w^4 g(x, 0, \sqrt{t}z) dz + t^3 \int_0^y \frac{(y-z)^5}{5!} \partial_w^6 g(x, 0, \sqrt{t}z) dz \right].$$

One has then to calculate the following derivatives:

$$\begin{aligned} \partial_t^3 g &= 3\partial_t \varphi \partial_t^2 \varphi f''(\varphi) + (\partial_t \varphi)^3 f^{(3)}(\varphi) \\ \partial_t^2 \partial_w^2 g &= [2\partial_t \partial_w^2 \varphi \partial_t \varphi + \partial_w^2 \varphi \partial_t^2 \varphi + \boxed{2(\partial_t \partial_w \varphi)^2}] f''(\varphi) \\ &\quad + [(\partial_t \varphi)^2 \partial_w^2 \varphi + \underline{4\partial_t \partial_w \varphi \partial_w \varphi \partial_t \varphi} + (\partial_w \varphi)^2 \partial_t^2 \varphi] f^{(3)}(\varphi) + (\partial_w \varphi \partial_t \varphi)^2 f^{(4)}(\varphi) \\ \partial_t \partial_w^4 g &= [\boxed{4\partial_w^3 \varphi \partial_t \partial_w \varphi} + 6\partial_w^2 \varphi \partial_t \partial_w^2 \varphi + \partial_w^4 \varphi \partial_t \varphi] f''(\varphi) \\ &\quad + [\underline{4\partial_w^3 \varphi \partial_w \varphi \partial_t \varphi} + 3(\partial_w^2 \varphi)^2 \partial_t \varphi + 6\partial_t \partial_w^2 \varphi (\partial_w \varphi)^2] f^{(3)}(\varphi) \\ &\quad + [6\partial_w^2 \varphi (\partial_w \varphi)^2 \partial_t \varphi + 4(\partial_w \varphi)^3 \partial_t \partial_w \varphi] f^{(4)}(\varphi) + (\partial_w \varphi)^4 \partial_t \varphi f^{(5)}(\varphi) \\ \partial_w^6 g &= [15\partial_w^4 \varphi \partial_w^2 \varphi + \boxed{10(\partial_w^3 \varphi)^2}] f''(\varphi) + 15[\underline{4\partial_w^3 \varphi \partial_w^2 \varphi \partial_w \varphi} + \partial_w^4 \varphi (\partial_w \varphi)^2 + (\partial_w^2 \varphi)^3] f^{(3)}(\varphi) \\ &\quad + [20\partial_w^3 \varphi (\partial_w \varphi)^3 + 45(\partial_w^2 \varphi \partial_w \varphi)^2] f^{(4)}(\varphi) + 15\partial_w^2 \varphi (\partial_w \varphi)^4 f^{(5)}(\varphi) + (\partial_w \varphi)^6 f^{(6)}(\varphi). \end{aligned}$$

The quantity  $\sqrt{t/x}$  being bounded on  $x \geq \mathbf{K}t$ , a careful examination allows to get that  $\partial_w^i \partial_t^j \varphi(t, u, \sqrt{t}z)$  satisfies the following property for  $(i, j) \notin \{(1, 1), (3, 0)\}$ :

$$\exists C, e, \eta > 0, \forall t \in (0, \eta), \forall u \in [0, t], \forall x \geq \mathbf{K}t, |\psi(t, u, \sqrt{t}z)| \leq C(1 + x^e + |z|^e). \quad (23)$$

On the contrary,  $\partial_t \partial_w \varphi(t, 0, \sqrt{t}z) = \beta_{1,1} \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} + \beta_{2,1}k(kx - a)\sqrt{t}z$  and  $\partial_w^3 \varphi = \beta_{3,0} \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} + \beta_{4,0}k(kx - a)\sqrt{t}z$  do not satisfy this property, because of the exploding term  $\frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}}$ . We have underlined or boxed each quantity that contains this

exploding term. The property (23) is clearly stable by addition and multiplication: if  $\psi_1$  and  $\psi_2$  satisfy (23),  $\psi_1 + \psi_2$  and  $\psi_1\psi_2$  satisfy also (23). It is also stable by composition of a derivative of  $f$  since  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R})$ . Last, let us observe that the underlined terms  $\partial_t \partial_w \varphi \partial_w \varphi$  or  $\partial_w^3 \varphi \partial_w \varphi$  can however be controlled in the same manner. Indeed, the term  $\frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} \partial_w \varphi(x, 0, \sqrt{tz})$  also satisfies (23) since it is proportional to  $\frac{\sigma(a-3kx-\sigma^2/4)}{2} (\sigma + \frac{\sigma^2}{2} \sqrt{t/x} z + \frac{\sigma(a-3kx-\sigma^2/4)}{2} \frac{t}{x} (\frac{\beta_{3,0}}{2} + \beta_{1,1}) z^2 - (\frac{\beta_{4,0}}{6} + \beta_{2,1}) k(a-kx) \sqrt{t/x} t z^3)$ . Therefore, we will control the underlined terms in the same manner as the others. In the same manner, expanding the boxed terms (for example  $\partial_t \partial_w \varphi(t, 0, \sqrt{tz})^2$ ) they are equal to an exploding term (here  $\beta_{1,1}^2 \left( \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} \right)^2$ ) plus a term that satisfies (23) (here  $2\beta_{1,1}\beta_{2,1} \frac{\sigma(a-3kx-\sigma^2/4)}{2} \sqrt{t/x} z + (\beta_{2,1} k(kx-a) \sqrt{tz})^2$ ).

Thus, we split the remainder as the sum  $\mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y)) = R_1(t, x) + R_2(t, x)$  where  $R_1(t, x)$  corresponds to the integration of all the terms that can be bounded as in (23) and  $R_2(t, x)$  contains all the exploding terms in the boxed terms:

$$R_2(t, x) = \left( \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} \right)^2 \int_{\mathbb{R}} p_Y(dy) \left[ \beta_{1,1}^2 t^3 \int_0^y (y-z) f''(\varphi(x, 0, \sqrt{tz})) dz \right. \\ \left. + 4\beta_{1,1}\beta_{3,0} t^3 \int_0^y \frac{(y-z)^3}{3!} f''(\varphi(x, 0, \sqrt{tz})) dz + 10\beta_{3,0}^2 t^3 \int_0^y \frac{(y-z)^5}{5!} f''(\varphi(x, 0, \sqrt{tz})) dz \right].$$

Let us denote  $(C_i, e_i)_{i \in \mathbb{N}}$  a good sequence of  $f$ . We can control  $R_1$  using property (23) and there are constants  $C, E, \eta$  that only depend on  $(C_i, e_i)_{0 \leq i \leq 6}$  such that for  $t \in (0, \eta)$  and  $x \geq \mathbf{K}t$ ,

$$|R_1(t, x)| \leq t^3 \int_{\mathbb{R}} p_Y(dy) \left[ C(1 + |x|^E + |y|^E) + \int_0^{|y|} [|y| + \frac{|y|^3}{3!} + \frac{|y|^5}{5!}] C(1 + |x|^E + |y|^E) dz \right].$$

Since  $Y$  has finite moments of any order,  $|R_1(t, x)| \leq C' t^3 (1 + |X|^{E'})$  for some positive constants  $C', E'$  that depend on  $f$  only through  $(C_i, e_i)_{0 \leq i \leq 6}$ . An integration by parts on  $R_2$  gives:  $R_2(t, x)/t^3 = \left( \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} \right)^2 \left[ \frac{1}{2} (\beta_{1,1} + \beta_{3,0}/6)^2 f''(x) + \int_{\mathbb{R}} p_Y(dy) \int_0^y [\beta_{1,1}^2 \frac{(y-z)^2}{2} + 4\beta_{1,1}\beta_{3,0} \frac{(y-z)^4}{4!} + 10\beta_{3,0}^2 \frac{(y-z)^6}{6!}] f^{(3)}(\varphi(x, 0, \sqrt{tz})) \frac{d}{dz} \varphi(x, 0, \sqrt{tz}) dz \right]$  with

$$\frac{d}{dz} \varphi(x, 0, \sqrt{tz}) = \sigma \sqrt{tx} + \frac{\sigma^2}{2} tz + \frac{\beta_{3,0} \sigma(a-3kx-\sigma^2/4)}{2} \frac{\sqrt{t/x} z^2 t}{2} - \frac{\beta_{4,0}}{6} k(a-kx) z^3 t^2.$$

We observe that  $\left( \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} \right)^2 \frac{d}{dz} \varphi(x, 0, \sqrt{tz})$  satisfies property (23) since  $t/x \leq 1/\mathbf{K}$ . One can thus bound the integral as for  $R_1$  and therefore

$$\mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y)) = \frac{t^3}{2} \left( \frac{\sigma(a-3kx-\sigma^2/4)}{2\sqrt{x}} \right)^2 (\beta_{1,1} + \beta_{3,0}/6)^2 f''(x) + R_3(t, x)$$

with  $\forall t \in (0, \eta), x \geq \mathbf{K}t, |R_3(t, x)| \leq Ct^3 (1 + |x|^E)$  for some constants depending on  $(C_i, e_i)_{0 \leq i \leq 6}$ . Now, it is easy to see that  $\mathbb{E}(\tilde{R}_g(t, x, \sqrt{t}Y))$  satisfies the property (22) if and only if  $\beta_{1,1} + \beta_{3,0}/6 = 0$  when  $\sigma^2 \neq 4a$ , and even without that restriction when  $\sigma^2 = 4a$ .  $\square$



We see incidentally in that proof that if  $\beta_{1,1} + \beta_{3,0}/6 \neq 0$ , the remainder is only in general of order 2. In the sequel we will arbitrarily take  $\beta_{0,2} = 1$  and  $\beta_{2,1} = \beta_{4,0} = 0$  so that:

$$\varphi(x, t, w) = x + \sigma\sqrt{x}w + \frac{\sigma^2}{4}w^2 + (a - kx - \frac{\sigma^2}{4})t + \frac{\sigma(a - 3kx - \sigma^2/4)}{8\sqrt{x}}w(w^2 - t) - \frac{k}{2}(a - kx)t^2. \quad (24)$$

**Remark 2.2.** *It is interesting to make the distinction between the conditions that give here a potential second-order scheme. On the one hand we have conditions (16), (18), (19), (20), (21). These conditions have been obtained algebraically, identifying the first order term to  $L_{\text{CIR}}f(x)$  and the second order term to  $L_{\text{CIR}}^2f(x)$ . They are not specific to the CIR diffusion and could be derived from the same way for general multidimensional diffusion with generator  $L$  defined as in (3). The general results proved in the first part such as Theorems 1.17 and 1.18 are recursive constructions of second order schemes for a large class of coefficients  $b(\cdot)$  and  $\sigma(\cdot)$ . Formally, they can thus be thought as constructions that satisfy automatically these algebraic conditions. On the other hand we have the condition  $\varphi_{1,1}(x) = -\frac{1}{6}\varphi_{3,0}(x)$  that is very specific to the CIR diffusion and comes from a tailored analysis of the remainder. It could have not been guaranteed by the general constructions introduced in the first part.*

To illustrate this, we make a rough Taylor expansion up to order 2 in  $t$  and 4 in  $W_t$  of the Ninomiya-Victoir scheme (11) obtained with Theorem 1.18:

$$\hat{X}_t^x \approx x + \sigma\sqrt{x}W_t + \frac{\sigma^2}{4}W_t^2 + (a - kx - \frac{\sigma^2}{4})t + \frac{\sigma(a - 3kx - \sigma^2/4)}{4\sqrt{x}}tW_t + \frac{k}{2}(kx - a + \frac{\sigma^2}{4})t^2 - \frac{\sigma^2}{8}tW_t^2.$$

This expansion satisfies conditions (16), (18), (19), (20), (21), not  $\varphi_{1,1}(x) = -\frac{1}{6}\varphi_{3,0}(x)$ .

Now, let us point that the scheme  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}N)$  can take in a general manner negative values for each  $x \geq 0$ . We want to avoid that for technical reasons (this point will be discussed in Section 2.4), and this is why we will consider instead the scheme  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}Y)$ , where  $Y$  is a bounded variable that matches the five first moments of the normal variable. The following lemma gives a sufficient condition on  $\mathbf{K}$  to stay nonnegative, while the second lemma will be useful later to control the moments.

**Lemma 2.3.** *Let us assume that  $Y$  is a bounded random variable such that  $\mathbb{P}(|Y| \leq A) = 1$ .*

*If  $A \leq 3$  and  $\mathbf{K} > (\frac{\sigma A}{2} + \sqrt{|\frac{\sigma^2}{4} - a|})^2$ , then*

$$\exists \eta > 0, \forall t \in (0, \eta), \forall x \geq \mathbf{K}t, \varphi(x, t, \sqrt{t}Y) \geq 0, \text{ a.s.}$$

**Lemma 2.4.** *Let us assume that  $Y$  is a bounded r.v. such that  $\mathbb{E}[Y] = 0$ . Let  $q \in \mathbb{N}^*$ . Then, there is a positive constant  $C_q$  such that*

$$\forall 0 < t \leq 1, \forall x \geq \mathbf{K}t, \mathbb{E}[\varphi(x, t, \sqrt{t}Y)^q] \leq x^q(1 + C_q t) + C_q t.$$

The proof of these results is left in Appendix A. Contrary to Lemma 2.3 where the boundedness of the random variable  $Y$  plays a crucial role in order to stay in the nonnegative values, the boundedness assumption of  $Y$  can probably be weakened in Lemma 2.4. However, it allows to give a short proof, and this result would be useful in this paper only in Theorem 2.8 for which we assume anyway the boundedness of  $Y$  to avoid to explore negative values.

**Example 2.5.** *A suitable bounded variable that fits the five first moments is  $Y$  such that  $\mathbb{P}(Y = \sqrt{3}) = \frac{1}{6}$ ,  $\mathbb{P}(Y = -\sqrt{3}) = \frac{1}{6}$ , and  $\mathbb{P}(Y = 0) = 2/3$ . For this example, we can take  $\mathbf{K} = \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a|$  to have  $\varphi(x, t, \sqrt{t}Y) \geq 0$  for  $t$  small enough.*

## 2.2 A potential second order scheme in a neighbourhood of 0.

Now we turn to the simulation of the CIR in the neighbourhood of 0, namely  $x \in [0, \mathbf{K}]$  with  $\mathbf{K} > 0$ . In that region, as soon as  $\sigma^2 > 4a$ , it does not seem possible to find a first-order scheme that writes  $\hat{X}_t^x = \varphi(x, t, W_t)$  that ensures nonnegativity (or more generally  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}Y)$  with  $Y$  matching the two first moments of a Normal variable). Since we want to preserve nonnegativity (see Section 2.4), we have to consider a different type of scheme.

We decide here to take here a discrete random variable that matches the two first moments. Namely, we are looking for  $\hat{X}_t^x$  that takes two possible values  $0 \leq x_-(t, x) < x_+(t, x)$  with respective probabilities  $1 - \pi(t, x)$  and  $\pi(t, x)$  such that

$$\begin{cases} \pi(t, x)x_+(t, x) + (1 - \pi(t, x))x_-(t, x) = \tilde{u}_1(t, x) \\ \pi(t, x)x_+(t, x)^2 + (1 - \pi(t, x))x_-(t, x)^2 = \tilde{u}_2(t, x) \end{cases} \quad \text{where } \tilde{u}_q(t, x) = E((X_t^x)^q) \text{ for } q \in \mathbb{N}. \quad (25)$$

Some calculations give:

$$\tilde{u}_1(t, x) = xe^{-kt} + a\frac{1 - e^{-kt}}{k} \quad \text{and} \quad \tilde{u}_2(t, x) = \tilde{u}_1(t, x)^2 + \sigma^2\left[\frac{a}{2k^2}(1 - e^{-kt})^2 + xe^{-kt}\frac{1 - e^{-kt}}{k}\right]. \quad (26)$$

The singularity in  $k = 0$  is not a real one: these functions can be extended by continuity for  $k = 0$  and their values in  $k = 0$  are indeed the two first moments. Let us define  $\gamma_{\pm}(t, x) = \frac{x_{\pm}(t, x)}{\tilde{u}_1(t, x)}$ . The equations to solve write

$$\begin{cases} \pi(t, x)\gamma_+(t, x) + (1 - \pi(t, x))\gamma_-(t, x) = 1 \\ \pi(t, x)\gamma_+(t, x)^2 + (1 - \pi(t, x))\gamma_-(t, x)^2 = \frac{\tilde{u}_2(t, x)}{\tilde{u}_1(t, x)^2}. \end{cases} \quad (27)$$

We arbitrarily take  $\gamma_+(t, x) = 1/(2\pi(t, x))$  and  $\gamma_-(t, x) = 1/(2(1 - \pi(t, x)))$  which ensures the first equation and the positivity of the random variable when  $\pi(t, x) \in (0, 1)$ . One has thus from the last equation

$$\pi^2(t, x) - \pi(t, x) + \tilde{u}_1(t, x)^2/(4\tilde{u}_2(t, x)) = 0.$$

The discriminant is  $\Delta(t, x) = 1 - \tilde{u}_1(t, x)^2/\tilde{u}_2(t, x) \in [0, 1]$ , and since we want  $\gamma_+ > \gamma_-$ , we take

$$\pi(t, x) = \frac{1 - \sqrt{\Delta(t, x)}}{2}. \quad (28)$$

We have thus  $0 \leq \pi(t, x) \leq 1/2$ . Besides, we have  $\tilde{u}_2(t, x)/\tilde{u}_1(t, x)^2 \leq 1 + \sigma^2/a$  because  $\tilde{u}_1(t, x)^2 \geq \max(a^2(\frac{1-e^{-kt}}{k})^2, 2a\frac{1-e^{-kt}}{k}xe^{-kt})$ . Therefore,  $\Delta(t, x) \geq 1 - 1/(1 + \sigma^2/a)$  and we get

$$0 < \pi_{\min} = \frac{1 - \sqrt{1 - 1/(1 + \sigma^2/a)}}{2} \leq \pi(t, x) \leq 1/2. \quad (29)$$

Let us observe now that on  $0 \leq x \leq \mathbf{K}t$  and  $t \leq 1$ , there is a constant  $C > 0$  that depends on  $\mathbf{K}$ ,  $a$  and  $k$  such that  $\tilde{u}_1(t, x) \leq Ct$ . Therefore

$$\forall x \in [0, \mathbf{K}t], \forall t \in (0, 1), \forall q \in \mathbb{N}, \mathbb{E}[(\hat{X}_t^x)^q] \leq (C/\pi_{\min})^{qt^q}. \quad (30)$$

**Proposition 2.6.** *The scheme defined here is a potential second order scheme on  $0 \leq x \leq \mathbf{K}t$ : for any  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}_+)$ , there are positive constants  $C$  and  $\eta$  that depend on a good sequence of  $f$  s.t.*

$$\exists C, \eta > 0, \forall t \in (0, \eta), \forall x \in [0, \mathbf{K}t], |\mathbb{E}[f(\hat{X}_t^x)] - f(x) - tL_{\text{CIR}}f(x) - \frac{t^2}{2}L_{\text{CIR}}^2f(x)| \leq Ct^3.$$

*Proof.* Let us consider a function  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}_+)$ . First, let us observe that the exact scheme is a potential second order scheme, i.e. it exists positive constants  $C, E, \eta$  depending on a good sequence of  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}_+)$  s.t.

$$\forall x \geq 0, \forall t \in (0, \eta), |\mathbb{E}[f(\hat{X}_t^x)] - f(x) - tL_{\text{CIR}}f(x) - \frac{t^2}{2}L_{\text{CIR}}^2f(x)| \leq Ct^3(1 + x^E).$$

This is a consequence of a result in [1] restated here in Proposition 2.7. It is therefore sufficient to check that one has  $\forall x \in [0, \mathbf{K}t], |\mathbb{E}(f(\hat{X}_t^x)) - \mathbb{E}(f(X_t^x))| \leq Ct^3$  for a constant  $C$  that depends on a good sequence of  $f$ . We make a Taylor expansion of  $f$  up to order 3:

$$x \geq 0, f(x) = f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + \int_0^x \frac{(x-y)^2}{2}f^{(3)}(y)dy.$$

Since  $\hat{X}_t^x$  matches the two first moments and  $f^{(3)}(y) \leq C_3(1 + |y|^q)$ , we get  $|\mathbb{E}(f(\hat{X}_t^x)) - \mathbb{E}(f(X_t^x))| \leq C_3\mathbb{E}[(\hat{X}_t^x)^3 + (\hat{X}_t^x)^{q+3} + (X_t^x)^3 + (X_t^x)^{q+3}]$ . We have shown in (30) that  $\mathbb{E}[(\hat{X}_t^x)^q] \leq (C/\pi_{\min})^{qt^q}$  for  $q \in \mathbb{N}$  and  $t \in (0, 1)$ . We have  $\frac{d\tilde{u}_q(t, x)}{dt} = [aq + \frac{1}{2}q(q-1)\sigma^2]\tilde{u}_{q-1}(t, x) - kq\tilde{u}_q(t, x)$ , we can prove by induction using the Gronwall lemma that  $\exists K_q > 0, \forall 0 \leq x \leq \mathbf{K}t, \mathbb{E}[(X_t^x)^q] \leq K_q t^q$ . Therefore, there is a constant  $K > 0$ , such that  $\forall t \leq 1, \mathbb{E}[(\hat{X}_t^x)^3 + (\hat{X}_t^x)^{q+3} + (X_t^x)^3 + (X_t^x)^{q+3}] \leq Kt^3$ . We finally get  $\forall t \in (0, 1), |\mathbb{E}[f(\hat{X}_t^x)] - f(x) - tL_{\text{CIR}}f(x) - \frac{t^2}{2}L_{\text{CIR}}^2f(x)| \leq C_3Kt^3$ . Last, observe that  $C_3K$  depends on  $f$  only through  $C_3$  and  $q$  and thus depends on a good sequence of  $f$ .  $\square$

### 2.3 The second order scheme

Now, we are in position to get a second order scheme for the CIR process, gathering the results of the two previous sections. First we have to state a result that is analogous to Theorem 1.11 for the CIR diffusion. This is a consequence of a result stated in [1].

**Proposition 2.7.** *Let us assume that  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}_+)$ . Then,  $u(t, x) = \mathbb{E}[f(X_{T-t}^x)]$  is  $\mathcal{C}^\infty$ , solves  $\partial_t u(t, x) = -L_{\text{CIR}}u(t, x)$  on  $(t, x) \in [0, T] \times \mathbb{R}_+$  and its derivatives satisfy*

$$\forall l, \alpha \in \mathbb{N}, \exists C_{l,\alpha}, e_{l,\alpha} > 0, \forall x \in \mathbb{R}_+, t \in [0, T], |\partial_t^l \partial_\alpha u(t, x)| \leq C_{l,\alpha}(1 + x^{e_{l,\alpha}}). \quad (31)$$

We define our scheme as follows. Let us consider  $Y$  a bounded variable ( $|Y| \leq A$ ) that matches the five first moments of the Gaussian variable,  $\mathbf{K} > (\frac{\sigma A}{2} + \sqrt{|\frac{\sigma^2}{4} - a|})^2$  and define for  $x \geq \mathbf{K}t$ ,  $p_x(t)(dz)$  as the probability law of  $\varphi(x, t, \sqrt{t}Y)$  where  $\varphi$  is defined by (24). Typically  $Y$  and  $\mathbf{K}$  can be chosen as in Example 2.5. For  $x \in [0, \mathbf{K}t)$ , we define  $p_x(t)(dz) = \pi(t, x)\delta_{\frac{\tilde{u}_1(t,x)}{2\pi(t,x)}}(dz) + (1 - \pi(t, x))\delta_{\frac{\tilde{u}_1(t,x)}{2(1-\pi(t,x))}}$ , where  $\pi(t, x)$  is defined by (28).

**Theorem 2.8.** *There is a positive constant  $\eta > 0$  such that for  $T/n < \eta$ , the scheme  $(\hat{X}_{t_i^n}^n, 0 \leq i \leq n)$  with the transition probabilities above and starting from  $\hat{X}_{t_0^n}^n = x$  is well-defined and nonnegative. One has,*

$$\forall f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}_+), \exists K > 0, \forall n \geq T/\eta, |\mathbb{E}[f(\hat{X}_{t_n^n}^n)] - \mathbb{E}[f(X_T^x)]| \leq K/n^2$$

and this is therefore a weak second order scheme.

*Proof.* The fact that the scheme is well defined for  $n$  large enough is a consequence of Lemma 2.3. The uniform boundedness of the moments is ensured by Proposition 1.4, Lemma 2.4 and (30), while the fact that it is a potential scheme of order 2 is guaranteed by Propositions 2.1 and 2.6. The point 1 of Theorem 1.8 is thus satisfied, and point 2 is ensured thanks to Proposition 2.7. We can then apply Theorem 1.8.  $\square$

Last, we want to mention here that even if the boundedness of  $Y$  plays an important role in the proof, numerically if one takes  $\varphi(x, t, \sqrt{t}N)^+$  instead of  $\varphi(x, t, \sqrt{t}Y)$  with the constant  $\mathbf{K} = \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a|$  of Example 2.5, we obtain a weak convergence that is qualitatively quadratic. We will see that later in Section 4.1.

### 2.4 Stay or not to stay nonnegative.

In this section, we want to explain briefly our choice for the scheme and especially why we want it to be nonnegative. The decision to let or not the discretization to be negative amounts to decide to take  $\mathbb{D} = \mathbb{R}_+$  or  $\mathbb{D} = \mathbb{R}$  for the CIR domain. Since  $\mathbb{D} = \mathbb{R}$  is not the natural domain of the CIR process, one has therefore to define a discretization scheme for negative values. This roughly amounts to extend the process  $(X_t^x, t \geq 0)$  for  $x < 0$ , typically as a SDE, and find a scheme for the whole process with  $\mathbb{D} = \mathbb{R}$ . This approach has already been considered in the literature. For example, Deelstra and Delbaen [7] (resp.

Lord and al. [13]) choose  $dX_t^x = (a - kX_t^x)dt$  (resp.  $dX_t^x = adt$ ) on  $\{X_t^x < 0\}$  which boils down to extend  $L_{\text{CIR}}$  by  $L_{\text{CIR}}f(x) = (a - kx)f'(x)$  (resp.  $L_{\text{CIR}}f(x) = af'(x)$ ) on  $x < 0$ . Let us first say that it is possible in general to find potential second order schemes for these SDEs: one can take for example the second order scheme proposed here for  $x \geq 0$  and a second order scheme for  $x < 0$ . The difficult point is not that one. The real problem is to find a diffusion in the negative values such that the function  $u(t, x) = \mathbb{E}[f(X_{T-t}^x)]$  is regular enough. With the choice made in [7] or [13], one can show that  $u$  is  $\mathcal{C}^1$ , piecewise  $\mathcal{C}^\infty$  if  $f \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R})$ . This is not enough to make work the proof of Theorem 1.8 with  $\nu = 2$ . Ideally, to have  $u \in \mathcal{C}^\infty$ , one should take  $L_{\text{CIR}}f(x) = (a - kx)f'(x) + \frac{1}{2}\sigma^2x f''(x)$  also for  $x < 0$  to get spatially continuous iterated operators  $L_{\text{CIR}}^k f(x)$  in  $x = 0$ . Unfortunately, this cannot be represented directly by a SDE since the diffusion coefficient is negative. Thus, to get round these difficulties, we have preferred here to construct a scheme that stays in the nonnegative values.

### 3 Application to the Heston model

In this part we are going to apply the ideas developed in the first part to the Heston model [10], since we have now at our disposal a second-order scheme for the CIR process. More precisely, we want to discretize the following SDE:

$$\begin{cases} X_t^1 = X_0^1 + \int_0^t (a - kX_s^1)ds + \sigma \int_0^t \sqrt{X_s^1}dW_s \\ X_t^2 = \int_0^t X_s^1 ds \\ X_t^3 = X_0^3 + \int_0^t rX_s^3 ds + \int_0^t \sqrt{X_s^1}X_s^3(\rho dW_s + \sqrt{1 - \rho^2}dZ_s) \\ X_t^4 = \int_0^t X_s^3 ds \end{cases} \quad (32)$$

with  $X_0^1 \geq 0$ ,  $X_0^3 > 0$ ,  $r \in \mathbb{R}$ ,  $\rho \in [-1, 1]$  and  $(a, k, \sigma) \in \mathbb{R}_+^* \times \mathbb{R} \times \mathbb{R}_+^*$ . The processes  $X^1$  and  $X^3$  are respectively the volatility process and the stock process, and  $X^2$  and  $X^4$  their respective integrals. From a financial point of view, it is common to assume moreover  $r > 0$ ,  $k > 0$  and  $\rho \leq 0$ , but these assumptions are not required for what follows.

The first remark to make is that there is no hope that the theory developed in the first part works for the Heston model. Indeed, all that theory is thought to work when one has a discretization scheme with uniformly bounded moments. Since the discretization scheme is supposed to stick rather closely to the SDE, this roughly amounts to assume that the SDE has uniformly bounded moments, which holds when the drift  $b(x)$  and the volatility function  $\sigma(x)$  have a sublinear growth. In the Heston model the diffusion coefficient  $\sigma(x)$  has not a sublinear growth, and it is proved indeed that the moments explode in a finite time (see Andersen and Piterbarg [3] for details). Therefore, the framework developed in this paper is not well suited to get a rigorous estimate of the weak error within the Heston model.

There are however reasons to think that it is not meaningless to apply the results stated in the first part to the Heston model. For example, in the second part, the conditions on the scheme to be of second-order (namely (16), (18), (19), (20) and (21)) have been

established before that we have controlled the remainder, and they have thus nothing to do with the hypothesis on  $f$  to control the remainder. As it is mentioned in Remark 2.2, these conditions are purely algebraic. They are not specific to the CIR case but can be extended to general diffusion processes. The constructions of the first part suggested by Theorem 1.17, Theorem 1.18, Propositions 1.10 and 1.9, and Corollary 1.16 can be thus thought formally as an automatic way to get these conditions satisfied. Of course, as for the CIR, these conditions are probably necessary but not sufficient to get indeed a second order scheme for the Heston model. Nonetheless, these conditions allow to cancel many biased terms of order 1 and improve really the convergence as it will be observed in the simulation part.

Therefore, we will apply in the sequel in a non rigorous manner the results proved in that paper to get what we will call “a second order scheme candidate”. This is to make the difference with the rigorous definition of a potential second order scheme. Let us first write the associated operator to (32):

$$\begin{aligned} Lf(x) = & (a - kx_1)\partial_1 f(x) + \frac{1}{2}\sigma^2 x_1 \partial_1^2 f(x) + x_1 \partial_2 f(x) \\ & + r x_3 \partial_3 f(x) + \frac{1}{2}x_1 x_3^2 \partial_3^2 f(x) + \rho x_1 x_3 \partial_1 \partial_3 f(x) + x_3 \partial_4 f(x). \end{aligned} \quad (33)$$

We split  $L = L^W + L^Z$  in the two operators  $L^W$  and  $L^Z$  that are associated to the following respective SDEs:

$$\left\{ \begin{array}{l} dX_t^1 = (a - kX_t^1)dt + \sigma\sqrt{X_t^1}dW_t \\ dX_t^2 = X_t^1 dt \\ dX_t^3 = (r - \frac{1}{2}(1 - \rho^2)X_t^1)X_t^3 dt + \rho\sqrt{X_t^1}X_t^3 dW_t \\ dX_t^4 = X_t^3 dt \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} dX_t^1 = 0 \\ dX_t^2 = 0 \\ dX_t^3 = \sqrt{(1 - \rho^2)X_t^1}X_t^3 \star dZ_t \\ dX_t^4 = 0. \end{array} \right. \quad (34)$$

Here,  $\star$  denotes the Stratonovitch integral. We have  $L^W f(x) = (a - kx_1)\partial_1 f(x) + \frac{1}{2}\sigma^2 x_1 \partial_1^2 f(x) + x_1 \partial_2 f(x) + (r - \frac{1}{2}(1 - \rho^2)x_1)x_3 \partial_3 f(x) + \rho x_1 x_3 \partial_1 \partial_3 f(x) + x_3 \partial_4 f(x)$  and  $L^Z f(x) = \frac{1}{2}(1 - \rho^2)x_1 x_3 \partial_3^2 f(x) + \frac{1}{2}x_1 x_3^2 \partial_3^2 f(x)$ . From Theorem 1.17, it is sufficient to have a second order scheme candidate for  $L^W$  and  $L^Z$ .

*A second order scheme candidate for  $L^Z$ .*

The solution to  $(x^1(t), x^2(t), x^3(t), x^4(t))' = (0, 0, \sqrt{(1 - \rho^2)x^1(t)}x^3(t), 0)$  is simply given by  $(x^1(0), x^2(0), x^3(0) \exp(\sqrt{(1 - \rho^2)x^1(0)t}), x^4(0))$ . Using Theorem 1.18, we thus consider  $\widehat{XZ}_t^x = (x_1, x_2, x_3 \exp(\sqrt{(1 - \rho^2)x_1}Z_t), x_4)$ .

*A second order scheme candidate for  $L^W$ .*

From Theorem 2.8, we have a potential second order scheme for the CIR process, i.e. for  $(a - kx_1)\partial_1 f(x) + \frac{1}{2}\sigma^2 x_1 \partial_1^2 f(x)$ . We denote by  $\widehat{X1}_t^x$  such a scheme. The solution of  $(x^1(t), x^2(t), x^3(t), x^4(t))' = (0, x_1(t), 0, 0)$  is  $(x^1(0), x^2(0) + x^1(0)t, x^3(0), x^4(0))$ , and from Theorem 1.18,  $\widehat{X}_t^x = (x_1, x_2 + x_1 t, x_3, x_4)$  is a potential second order scheme for  $x_1 \partial_2 f(x)$ . Therefore, from Theorem 1.17 (here it is fully rigorous),  $\widehat{X2}_t^x = (\widehat{X1}_t^{(x_1, x_2 + x_1 t/2, x_3, x_4)}, x_2 +$

$(x_1 + \widehat{X}_1^x)^{(x_1, x_2 + x_1 t/2, x_3, x_4)} t/2, x_3, x_4)$  is a potential second order scheme for  $(a - kx_1)\partial_1 f(x) + \frac{1}{2}\sigma^2 x_1 \partial_1^2 f(x) + x_1 \partial_2 f(x)$ .

Now let us observe that we can rewrite the SDE on  $X^3$  as

$$dX_t^3 = X_t^3 \left[ \left( r - \frac{\rho}{\sigma} a + \left[ \frac{\rho}{\sigma} k - \frac{1}{2}(1 - \rho^2) \right] X_t^1 \right) dt + \frac{\rho}{\sigma} dX_t^1 \right]$$

and therefore  $X_t^3 = X_0^3 \exp \left[ \left( r - \frac{\rho}{\sigma} a \right) t + \left[ \frac{\rho}{\sigma} k - \frac{1}{2} \right] (X_t^2 - X_0^2) + \frac{\rho}{\sigma} (X_t^1 - X_0^1) \right]$ . We thus define,  $\widehat{X}_3^x = ((\widehat{X}_2^x)_1, (\widehat{X}_2^x)_2, x_3 \exp \left[ \left( r - \frac{\rho}{\sigma} a \right) t + \left[ \frac{\rho}{\sigma} k - \frac{1}{2} \right] ((\widehat{X}_2^x)_2 - x_2) + \frac{\rho}{\sigma} ((\widehat{X}_2^x)_1 - x_1) \right], x_4)$  following Proposition 1.9 and 1.10. This is a second order scheme candidate for  $(a - kx_1)\partial_1 f(x) + \frac{1}{2}\sigma^2 x_1 \partial_1^2 f(x) + x_1 \partial_2 f(x) + (r - \frac{1}{2}(1 - \rho^2)x_1)x_3 \partial_3 f(x) + \rho x_1 x_3 \partial_1 \partial_3 f(x)$ . Last, since  $(x^1(0), x^2(0), x^3(0), x^4(0) + x^3(0)t)$  is a potential second order scheme for  $x_3 \partial_4$ , we define according to Theorem 1.17  $\widehat{XW}_t^x = \widehat{X}_3^{(x_1, x_2, x_3, x_4 + x_3 t/2)} + (0, 0, 0, (\widehat{X}_3^{(x_1, x_2, x_3, x_4 + x_3 t/2)})_4 t/2)$  which is a second order scheme candidate for  $L^W$ .

Now, if  $B$  denotes an independent Bernoulli variable of parameter  $1/2$ , the scheme  $\widehat{X}_t^x = B \widehat{XW}_t^x + (1 - B) \widehat{XZ}_t^x$  is a second order scheme candidate for  $L$ .

**Remark 3.1.** *Let us mention that it is fully possible to derive a second-order scheme candidate without writing the second SDE with Stratonovitch integral if one splits  $L = \widetilde{L}^W + \widetilde{L}^Z$  where  $\widetilde{L}^W$  and  $\widetilde{L}^Z$  are the operators respectively associated to*

$$\begin{cases} dX_t^1 = (a - kX_t^1)dt + \sigma \sqrt{X_t^1} dW_t \\ dX_t^2 = X_t^1 dt \\ dX_t^3 = rX_t^3 dt + \rho \sqrt{X_t^1} X_t^3 dW_t \\ dX_t^4 = X_t^3 dt \end{cases} \quad \text{and} \quad \begin{cases} dX_t^1 = 0 \\ dX_t^2 = 0 \\ dX_t^3 = \sqrt{(1 - \rho^2)X_t^1} X_t^3 dZ_t \\ dX_t^4 = 0. \end{cases}$$

*Indeed, in that particular case, we are able to integrate exactly the second Itô SDE. However, we believe that it is a good habit to switch to the Stratonovitch when it is possible in order to use numerical ODE (Runge-Kutta) techniques when exact integration is not possible.*

Writing the whole formula for  $\widehat{X}_t^x$  would be rather cumbersome, and we prefer to write here directly the algorithm that compute  $\widehat{X}_t^x$  in function of  $x = (x_1, x_2, x_3, x_4)$ . We set  $\mathbf{K} = \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a|$ ,  $U$  is a uniform variable on  $[0, 1]$ ,  $B$  is a Bernoulli variable of parameter  $1/2$ ,  $N$  and  $N'$  are standard normal variables and  $Y$  is distributed according to Example 2.5. All these variables are independent. The function  $\varphi$  is defined in (24),  $\tilde{u}_1$  and  $\tilde{u}_2$  are defined in (26). The algorithm is written in Table 1. Let us recall here that with our choice of  $\mathbf{K}$  and with the random variable  $Y$ , the discretization for the CIR process remains nonnegative for a time-step small enough. We however put a positive part, so that the scheme is defined for any time-step.

```

function XW (x1, x2, x3, x4):
if (x1 > Kt) Δx1 ← φ(x1, t, √tY)+ - x1 ( or Δx1 ← φ(x1, t, √tN)+ - x1)
else π ←  $\frac{1 - \sqrt{1 - \tilde{u}_1(t, x_1)^2 / \tilde{u}_2(t, x_1)}}{2}$  if (U < π) Δx1 ←  $\frac{\tilde{u}_1(t, x_1)}{2\pi} - x_1$  else Δx1 ←  $\frac{\tilde{u}_1(t, x_1)}{2(1-\pi)} - x_1$ 
x2 ← x2 + (x1 + 0.5Δx1)t
x4 ← x4 + 0.5x3t
x3 ← x3 exp [(r - ρa/σ)t + ρΔx1/σ + (ρk/σ - 0.5)(x1 + 0.5Δx1)t]
x4 ← x4 + 0.5x3t
x1 ← x1 + Δx1
function XZ (x1, x2, x3, x4): x3 ← x3 exp(√(1 - ρ2)x1tN')
function X (x1, x2, x3, x4):
if (B = 1) XZ(x1, x2, x3, x4) XW(x1, x2, x3, x4) else XW(x1, x2, x3, x4) XZ(x1, x2, x3, x4)

```

Table 1: Algorithm for the Heston model.

## 4 Simulation results

### 4.1 Simulations for the CIR process

In this section, we want to illustrate the results of the second part with parameters such that  $\sigma^2 \gg 4a$ , for which few existing discretization schemes are accurate as it has been mentioned in the introduction. We consider here five schemes, and for each of them, we take the scheme described in Section 2.2 for  $0 \leq x \leq \mathbf{K}t$ . The two first schemes are those that we recommend:

1.  $\mathbf{K} = \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a|$ , and  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}Y)^+$  for  $x > \mathbf{K}t$  as in Example 2.5.
2.  $\mathbf{K} = \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a|$ , and  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}N)^+$  for  $x > \mathbf{K}t$  with  $N \sim \mathcal{N}(0, 1)$ .

Their simulations are plotted in solid line in Figure 1. To check the importance of the choice of  $\mathbf{K}$ , we have considered:

3.  $\mathbf{K} = \frac{1}{2} \left( \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a| \right)$ , and  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}N)^+$  for  $x > \mathbf{K}t$ .
4.  $\mathbf{K} = \frac{3}{2} \left( \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a| \right)$ , and  $\hat{X}_t^x = \varphi(x, t, \sqrt{t}N)^+$  for  $x > \mathbf{K}t$ .

Last, to check numerically the importance of the condition  $\varphi_{1,1}(x) = -\frac{1}{6}\varphi_{3,0}(x)$  in Theorem 2.1, we have considered:

5.  $\mathbf{K} = \frac{3}{2}\sigma^2 + 2|\frac{\sigma^2}{4} - a|$ , and  $\hat{X}_t^x = \tilde{\varphi}(x, t, \sqrt{t}N)^+$  where  $\tilde{\varphi}(x, t, w) = x + \sigma\sqrt{x}w + \frac{\sigma^2}{4}w^2 + (a - kx - \frac{\sigma^2}{4})t + \frac{\sigma(a-3kx-\sigma^2/4)}{4\sqrt{x}}w(2t - \frac{w^2}{3}) - \frac{k}{2}(a - kx)t^2$ . Note that  $\tilde{\varphi}$  satisfies all the other conditions (16), (18), (19), (20) and (21).

In Figure 1, we have set  $T = 1$  and plotted for  $n = 5, 7, 10, 14, 20, 30, 50$  the values of  $\mathbb{E}(\exp(-\hat{X}_{\frac{T}{n}}^n))$  in function of the time step  $1/n$ . In these simulations, the precision up to two standard deviations is about  $2.7 \times 10^{-5}$ .

Let us first comment the schemes 1 and 2 in solid line. If the boundedness of  $Y$  was a crucial property to prove that it is a second-order scheme, qualitatively the scheme 2



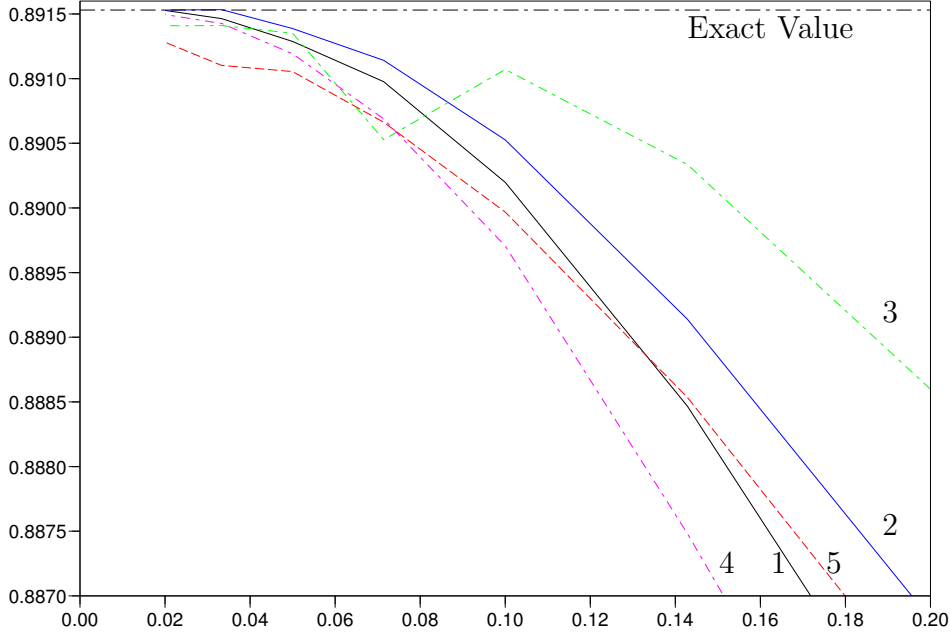


Figure 1:  $\mathbb{E}(\exp(-\hat{X}_{t_n^n}^n))$  in function of  $1/n$  with  $x_0 = 0.3$ ,  $k = 0.1$ ,  $a = 0.04$  and  $\sigma = 2$ . Exact value:  $\mathbb{E}[\exp(-X_1^x)] \approx 0.89153$ .

that uses a Gaussian variable instead of  $Y$  is not far from a parabola and presents even a bias slightly lower than the scheme 1. That is why we will prefer slightly the scheme 2 for simulation purpose.

The results of the schemes 3 and 4 show the importance of the choice of  $\mathbf{K}$ . If one takes  $\mathbf{K}$  greater than the one in Example 2.5 (scheme 4), the qualitative convergence is still quadratic. This is coherent with the theoretical results. Nonetheless, the bias is also increased and this is why it is better to take  $\mathbf{K}$  not too big. The results of the scheme 3 show on the contrary what happens if one takes  $\mathbf{K}$  too small for that our theoretical results work. The convergence is not really bad in that case, but has nothing to do with a parabola shape. Heuristically, this is because the positive part is here crucial to maintain the nonnegativity contrary to the schemes 1, 2 and 4 where the nonnegativity is quasi natural, thanks to the choice of  $\mathbf{K}$ . And this positive part induces strange effects on the convergence.

Last, let us comment the convergence of the scheme 5. Qualitatively, it is hard to say just on these results that the convergence is not truly quadratic. Nonetheless, we observe that the convergence of the scheme 5 is worse than the one for the schemes 1, 2 and 4 that all satisfy the condition  $\varphi_{1,1}(x) = -\frac{1}{6}\varphi_{3,0}(x)$ . Indeed its curve is below the curves of these three schemes when the time-step is small enough. This confirms numerically that this

condition is really important for the convergence quality.

To illustrate that most of the usual schemes are not accurate for large values of  $\sigma$ , we have also calculated the same expectation with the Full Truncation scheme proposed by Lord and al. [13]. This scheme is defined by  $\hat{X}_t^x = x + (a - kx^+)t + \sigma\sqrt{x^+}W_t$ . We give the values obtained apart in the following table, because they are outside the Figure 1. It is

$n$	5	7	10	14	20	30	50
$\mathbb{E}(\exp(-\hat{X}_{t_n}^n))$	0.80636	0.82799	0.84635	0.85974	0.8704	0.87883	0.88522

important to notice here that the number of samples for the Monte-Carlo method to get a precision up to four digits is about  $10^8$  with these parameters. Therefore, when  $\sigma^2 \gg 4a$ , the choice of the scheme is really crucial to make the calculations with limited time or computational means. This is of course also true for the Heston model.

## 4.2 Simulations for the Heston model

In this section, we want to test our scheme to price claims under the Heston model. This is the scheme described in Table 1 with the Normal variable (not  $Y$ ), and we name it scheme 1 in that section. For comparison, we introduce the following scheme which coincides for the first and the third coordinates to the one suggested by Lord and al. [13]:

$$\hat{X}_t^x = \begin{pmatrix} x_1 + (a - kx_1^+)t + \sigma\sqrt{x_1^+}W_t \\ x_2 + x_1t \\ x_3 \exp\left((r - x_1^+/2)t + \sqrt{x_1^+}(\rho W_t + \sqrt{1 - \rho^2}Z_t)\right) \\ x_4 + x_3t \end{pmatrix}.$$

This is the scheme 2.

In all the simulations, we have fixed  $T = 1$ . To test the schemes, we have calculated European put prices for different strikes with rather high values of  $\sigma$  in Figure 2 and Figure 3. It is hard to say qualitatively from the curves that the convergence is indeed quadratic for the scheme 1. Nonetheless in the European put case we can compare the value obtained with the exact value. For example in Figure 2, for a time step  $1/50$  and for each strike, the exact value is in the two standard deviations window of which width is between  $0.5 \times 10^{-3}$  and  $1.2 \times 10^{-3}$  according to the strike value. Therefore, the bias is not much big as  $(1/50)^2 = 0.4 \times 10^{-3}$  and the convergence quality is not far from being the one of a true second-order scheme. In comparison, the scheme 2 has in that case a rather linear convergence and is still far from the exact value for  $n = 50$ .

We have also plotted in Figure 4 the prices of an Asian put and of an exotic option that gives the right to earn the difference between the average stock and the stock when the realized variance is above a certain level. We have chosen here a rather low value of  $\sigma$  ( $\sigma < 4a$ ). Thus, the CIR process  $X^1$  does not spend much time near 0 and the convergence observed for the scheme 1 is qualitatively parabolic in function of the time-step. In comparison and to underline the importance of the method chosen, we have put in

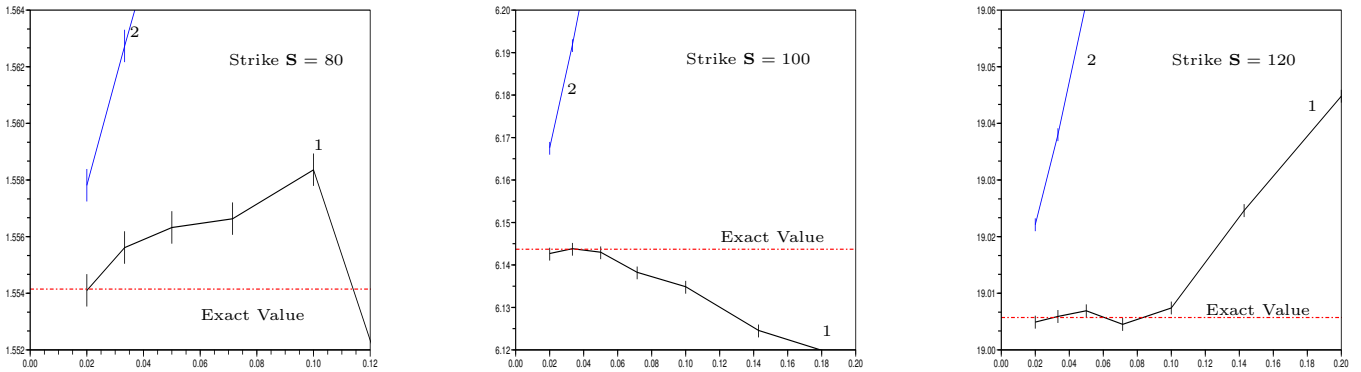


Figure 2:  $\mathbb{E}[e^{-r}(\mathbf{S} - (\hat{X}_{t_n}^n)_3)^+]$  in function of  $1/n$  with  $X_0^1 = 0.04$ ,  $k = 0.5$ ,  $a = 0.02$ ,  $\sigma = 0.4$ ,  $r = 0.02$ ,  $X_0^3 = 100$  and  $\rho = -0.5$ . The width of each point indicates the precision up to two standard deviations.

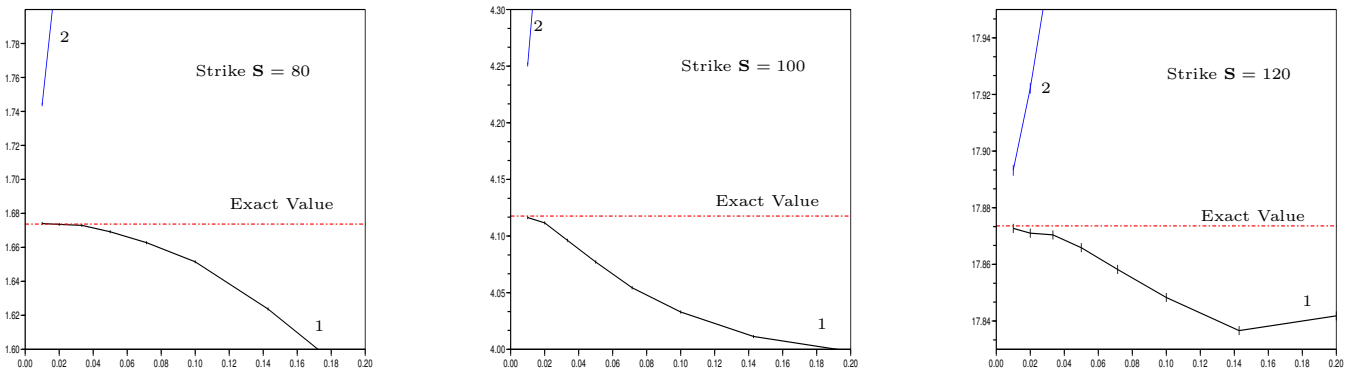


Figure 3:  $\mathbb{E}[e^{-r}(\mathbf{S} - (\hat{X}_{t_n}^n)_3)^+]$  in function of  $1/n$  with  $X_0^1 = 0.04$ ,  $k = 0.5$ ,  $a = 0.02$ ,  $\sigma = 1$ ,  $r = 0.02$ ,  $X_0^3 = 100$  and  $\rho = -0.8$ . The width of each point indicates the precision up to two standard deviations.

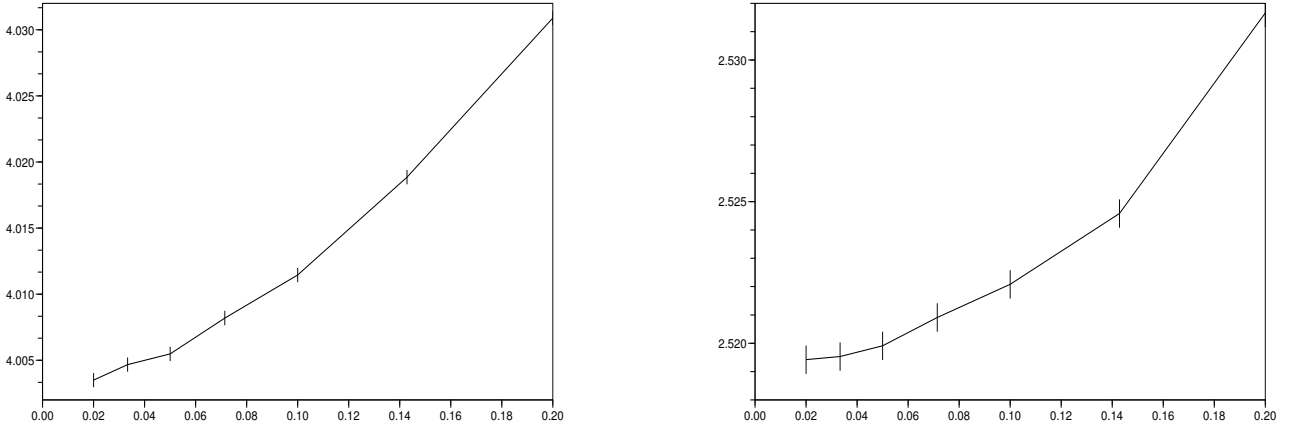


Figure 4: For the scheme 1:  $\mathbb{E}[e^{-r}(100 - (\hat{X}_{t_n^n}^n)_4)^+]$  (left) and  $\mathbb{E}[e^{-r}\mathbf{1}_{(\hat{X}_{t_n^n}^n)_2 > a/k}((\hat{X}_{t_n^n}^n)_4 - (\hat{X}_{t_n^n}^n)_3)^+]$  (right) in function of  $1/n$  with  $X_0^1 = 0.04$ ,  $k = 0.5$ ,  $a = 0.02$ ,  $\sigma = 0.2$ ,  $r = 0.02$ ,  $X_0^3 = 100$  and  $\rho = -0.3$ .

Table 2 the values obtained with the scheme 2, because they could not have been plotted on the same scale. The convergence is in that case quasi-linear.

Last, let us mention here (for a low sigma) that the convergences observed are regular, and a Romberg extrapolation may be very efficient. Let us show this on the exotic option example. For the scheme 2, we have  $2\mathbb{E}[e^{-r}\mathbf{1}_{(\hat{X}_{t_{10}^{10}}^{10})_2 > \frac{a}{k}}((\hat{X}_{t_{10}^{10}}^{10})_4 - (\hat{X}_{t_{10}^{10}}^{10})_3)^+]$  -

$\mathbb{E}[e^{-r}\mathbf{1}_{(\hat{X}_{t_5^5}^5)_2 > \frac{a}{k}}((\hat{X}_{t_5^5}^5)_4 - (\hat{X}_{t_5^5}^5)_3)^+] \approx 2.5179$ , and for the scheme 1:

$\frac{4}{3}\mathbb{E}[e^{-r}\mathbf{1}_{(\hat{X}_{t_{10}^{10}}^{10})_2 > \frac{a}{k}}((\hat{X}_{t_{10}^{10}}^{10})_4 - (\hat{X}_{t_{10}^{10}}^{10})_3)^+] - \frac{1}{3}\mathbb{E}[e^{-r}\mathbf{1}_{(\hat{X}_{t_5^5}^5)_2 > \frac{a}{k}}((\hat{X}_{t_5^5}^5)_4 - (\hat{X}_{t_5^5}^5)_3)^+] \approx 2.5189$  which is already very close to the limit observed in Figure 4.

$n$	5	7	10	14	20	30	50
$\mathbb{E}[e^{-r}(100 - (\hat{X}_{t_n^n}^n)_4)^+]$	4.6189	4.4427	4.3108	4.2235	4.1570	4.1062	4.0646
$\mathbb{E}[e^{-r}\mathbf{1}_{(\hat{X}_{t_n^n}^n)_2 > \frac{a}{k}}((\hat{X}_{t_n^n}^n)_4 - (\hat{X}_{t_n^n}^n)_3)^+]$	2.1658	2.2664	2.3418	2.3924	2.4299	2.4595	2.4833

Table 2: Results for the scheme 2. Parameters as in Figure 4. Precision up to two standard deviations:  $5 \times 10^{-4}$ .

## Conclusion

To sum up, the contribution of this paper is twofold. On the one hand, we have slightly extended the Ninomiya-Victoir scheme and proposed in a rigorous framework a general

recursive construction of potential second order schemes. On the other hand, we have introduced a scheme for the CIR process that is a weak second-order scheme without any restriction on its parameters (especially without limit on  $\sigma$ ). We have combined these results in the setting of the Heston model even though the technical required assumptions are not satisfied, and obtained a scheme that is numerically rather efficient.

A rigorous analysis of the weak error in the Heston model seems to be a challenging topic. Indeed, as it has been mentioned before, the theory used here relies mainly on the control of the moments. Because of the moment explosion in the Heston model, a new or refined approach is necessary to get theoretical results of convergence.

## A Proofs

*Proof of Lemma 2.3.* We consider  $A \leq 3$ , and without restriction we can assume  $A \geq 5/3$  for convenience. From (24), We have for  $\lambda, t \geq 0$  and  $y \in \mathbb{R}$ :

$$\begin{aligned} \varphi(\lambda t, t, \sqrt{t}y)/t &= \Psi(\lambda, y) - kt \left( \lambda + \frac{3\sigma\sqrt{\lambda}y}{8}(y^2 - 1) + \frac{1}{2}(a - k\lambda t) \right) \text{ with} \\ \Psi(\lambda, y) &= (\sqrt{\lambda} + \sigma y/2)^2 + (a - \frac{\sigma^2}{4}) + \frac{\sigma(a - \sigma^2/4)}{8\sqrt{\lambda}}y(y^2 - 1). \end{aligned}$$

There is a constant  $\alpha > 1$  such that  $\mathbf{K} = \alpha^2(\frac{\sigma A}{2} + \sqrt{|\frac{\sigma^2}{4} - a|})^2$ , so that  $\lambda \geq \mathbf{K} \iff \frac{\sqrt{\lambda}}{\alpha} \geq \frac{\sigma A}{2} + \sqrt{|\frac{\sigma^2}{4} - a|}$ . Let us fix  $\lambda \geq \mathbf{K}$  and  $y \in [-A, A]$ . We have then

$$(\sqrt{\lambda} + \sigma y/2)^2 \geq \left( \frac{\alpha - 1}{\alpha} \sqrt{\lambda} + \sqrt{|\sigma^2/4 - a|} + \frac{\sigma}{2}(A + y) \right)^2 \geq \left( \frac{\alpha - 1}{\alpha} \right)^2 \lambda + |\sigma^2/4 - a| + \frac{\sigma^2}{4}(A + y)^2$$

and we distinguish the two following cases.

- $\sigma^2/4 - a \geq 0$ . We have  $\Psi(\lambda, y) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda + \frac{\sigma^2}{4}(A + y)^2 + \frac{\sigma(a - \sigma^2/4)}{8\sqrt{\lambda}}y(y^2 - 1)$ . If  $y \in [-A, -1] \cup [0, 1]$ ,  $y(y^2 - 1) \leq 0$  and  $\Psi(\lambda, y) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda$ . If  $y \in [-1, 0] \cup [1, A]$ ,  $y(y^2 - 1) \geq 0$  and  $\Psi(\lambda, y) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda + \frac{\sigma^2}{4}((A + y)^2 - \frac{\sigma y}{\sqrt{\lambda}} \frac{y^2 - 1}{8})$ . Moreover, since  $A \geq 5/3$ , the following bounds hold:  $|\frac{\sigma y}{\sqrt{\lambda}} \frac{y^2 - 1}{8}| \leq \frac{A^2 - 1}{4}$  and  $(A + y)^2 \geq (A - 1)^2 \geq \frac{A^2 - 1}{4}$ . We then get  $\Psi(\lambda, y) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda$ .
- $\sigma^2/4 - a < 0$ . We have  $\Psi(\lambda, y) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda + 2(a - \sigma^2/4) + \frac{\sigma(a - \sigma^2/4)}{8\sqrt{\lambda}}y(y^2 - 1)$ . Since  $|\frac{\sigma(a - \sigma^2/4)}{8\sqrt{\lambda}}y(y^2 - 1)| \leq \frac{a - \sigma^2/4}{4}(A^2 - 1)$ , we have  $\Psi(\lambda, y) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda + (a - \frac{\sigma^2}{4})(2 - \frac{1}{4}(A^2 - 1)) \geq \left(\frac{\alpha-1}{\alpha}\right)^2 \lambda$  if  $A \leq 3$ .

Therefore, we have for  $t \geq 0$ ,  $\lambda \geq \mathbf{K}$ , and  $y \in [-A, A]$ ,

$$\varphi(\lambda t, t, \sqrt{t}y)/t \geq \lambda \left[ \left( \frac{\alpha - 1}{\alpha} \right)^2 - kt \frac{\lambda + \frac{3\sigma\sqrt{\lambda}y}{8}(y^2 - 1) + \frac{1}{2}(a - k\lambda t)}{\lambda} \right].$$

The fraction being bounded for  $t \in (0, 1)$ ,  $|y| \leq A$  and  $\lambda \geq \mathbf{K}$  there is a positive constant  $\eta$  such that  $\varphi(\lambda t, t, \sqrt{t}y) \geq 0$  for  $t \in (0, \eta)$ .  $\square$

*Proof of Lemma 2.4.* We write  $\varphi(x, t, \sqrt{t}Y) = x + \sigma\sqrt{xt}Y + S(t, x)$ . Since  $Y$  a bounded variable,  $S(t, x)$  satisfies:

$$\exists C > 0, \forall t \in (0, 1), |S(t, x)| \leq Ct(1 + x).$$

Therefore, expanding  $\varphi(x, t, \sqrt{t}Y)^q$ , we observe that we can write  $\varphi(x, t, \sqrt{t}Y)^q = x^q + q\sigma x^{q-1/2}\sqrt{t}Y + S_2(t, x)$  with  $|S_2(t, x)| \leq C_q t(1 + x^q)$  for some positive constant  $C_q$  and we get then the result.  $\square$

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