Diffusion Monte Carlo method: Numerical Analysis in a Simple Case*

M.El Makrini, B.Jourdain, T. Lelièvre
ENPC-CERMICS, 6-8 av Blaise Pascal,
Cité Descartes, Champs sur Marne,
77455 Marne-la-Vallée Cedex 2, France
e-mail: {makrimo,jourdain,lelievre}@cermics.enpc.fr

December 2, 2005

Abstract

The Diffusion Monte Carlo method is devoted to the computation of electronic ground-state energies of molecules. In this paper, we focus on implementations of this method which consist in exploring the configuration space with a **fixed** number of random walkers evolving according to a Stochastic Differential Equation discretized in time. We allow stochastic reconfigurations of the walkers to reduce the discrepancy between the weights that they carry. On a simple one-dimensional example, we prove the convergence of the method for a fixed number of reconfigurations when the number of walkers tends to $+\infty$ while the discretization step of the SDE tends to 0. We confirm our theoretical rates of convergence by numerical experiments.

Introduction

The computation of electronic structures of atoms, molecules and solids is a central problem in chemistry and physics. We focus here on electronic ground state calculations where the objective is the computation of the lowest eigenvalue (the so-called ground-state energy) E_0 of a self-adjoint Hamiltonian $H = -\frac{1}{2}\Delta + V$ whith domain $D_{\mathcal{H}}(H)$ on a Hilbert space $\mathcal{H} \subset L^2(\mathbb{R}^{3N})$ where N is the number of electrons (see [3] for a general introduction):

$$E_0 = \inf\{\langle \psi, H\psi \rangle,\ \psi \in D_{\mathcal{H}}(H), \|\psi\| = 1\}, \tag{1}$$

where $\langle \cdot, \cdot \rangle$ denotes the duality bracket on $L^2(\mathbb{R}^{3N})$ and $\| \cdot \|$ the $L^2(\mathbb{R}^{3N})$-norm. For simplicity, we omit the spin variables. The function V describes the interaction between the electrons, and between the electrons and the nuclei, which are supposed to be fixed point-like particles. The functions ψ are square integrable, their normalized square modulus $|\psi|^2$ being interpreted as the probability density of the particles positions in space, and they satisfy an antisymmetry condition with respect to the numbering of the electrons, due to the fermionic nature of the electrons (Pauli principle): $\mathcal{H} = \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$. We suppose that the potential V is such that E_0 is an isolated eigenvalue of H (see [4] for sufficient conditions), and we denote by ψ_0 a normalized eigenfunction associated with E_0.

Due to the high dimensionality of the problem, stochastic methods are particularly well suited to compute E_0. The Diffusion Monte Carlo (DMC) method is widely used in chemistry (see [2, 10]), but has been only recently considered from a mathematical viewpoint (see [4, 8]). This method gives an estimate of E_0 in terms of the long-time limit of the expectation of a functional of a drift-diffusion process with a

*We thank Eric Cancès (CERMICS) and Mathias Rousset (Université Paul Sabatier, Toulouse) for many fruitful discussions and Michel Caffarel (IRSAMC, Toulouse) for introducing us to the DMC method and suggesting the toy model studied in this paper.

source term. It requires an importance sampling function ψ_I which approximates the ground-state ψ_0 of H. Let us define the drift function $\boldsymbol{b} = \nabla \ln |\psi_I|$, the so-called local energy $E_L = \dfrac{H\psi_I}{\psi_I}$ and the DMC energy:

$$E_{\mathrm{DMC}}(t) = \frac{\mathbb{E}\left(E_L(\boldsymbol{X}_t) \exp\left(-\int_0^t E_L(\boldsymbol{X}_s)ds\right)\right)}{\mathbb{E}\left(\exp\left(-\int_0^t E_L(\boldsymbol{X}_s)ds\right)\right)}, \tag{2}$$

where the $3N$-dimensional process $\boldsymbol{X}_t$ satisfies the stochastic differential equation:

$$\begin{cases} \boldsymbol{X}_t = \boldsymbol{X}_0 + \displaystyle\int_0^t \boldsymbol{b}(\boldsymbol{X}_s)\, ds + d\boldsymbol{W}_t, \\ \boldsymbol{X}_0 \sim |\psi_I|^2(\boldsymbol{x})\, d\boldsymbol{x}. \end{cases} \tag{3}$$

The stochastic process $(\boldsymbol{W}_t)_{t\geq 0}$ is a standard $3N$-dimensional Brownian motion. One can then show that (see [4])

$$\lim_{t\to\infty} E_{\mathrm{DMC}}(t) = E_{\mathrm{DMC},0}, \tag{4}$$

where

$$E_{\mathrm{DMC},0} = \inf\{\langle\psi, H\psi\rangle,\ \psi \in D_{\mathcal{H}}(H), \|\psi\| = 1,\ \psi = 0 \text{ on } \psi_I^{-1}(0)\}. \tag{5}$$

We have proved in [4] that $E_{\mathrm{DMC},0} \geq E_0$, with equality if and only if the nodal surfaces of ψ_I coincide with those of a ground state ψ_0 of H. In other words, if there exists a ground state ψ_0 such that $\psi_I^{-1}(0) = \psi_0^{-1}(0)$, then $\lim_{t\to\infty} E_{\mathrm{DMC}}(t) = E_0$. The error $|E_0 - E_{\mathrm{DMC},0}|$ is related to the so-called fixed-node approximation, which is well knwon by practitioners of the field (see [3]).

In this paper, we complement the theoretical results obtained in [4] with a numerical analysis in a simple case. In practice, the longtime limit $E_{\mathrm{DMC},0}$ in (4) is approximated by taking the value of E_{DMC} at a (large) time $T > 0$. Then $E_{\mathrm{DMC}}(T)$ is approximated by using a discretization in time of the stochastic differential equation (3) and of the integral in the exponential factor in (2), and an approximation of the expectation values in (2) by an empirical mean over a large number N of trajectories. These trajectories, $(\boldsymbol{X}^i)_{1\leq i\leq N}$, also called walkers in the physical literature or particles in the mathematical literature satisfy a discretized version of (3), and interact at times $n\Delta t$ for $n \in \{1, \ldots, \nu - 1\}$ where $\Delta t = T/\nu$ for $\nu \in \mathbb{N}^*$ through a stochastic reconfiguration step aimed at reducing the discrepancy between their exponential weights. We thus obtain an interacting particle system. The number of reconfiguration steps if $\nu - 1$. The stochastic differential equation (3) is discretized with a possibly smaller step $\delta t = \Delta t/\kappa = T/(\nu\kappa)$ with $\kappa \in \mathbb{N}^*$. The total number of steps for the discretization of (3) is then $K = \nu\kappa$.

In the following, we consider an adapted version of the DMC scheme with minimal stochastic reconfiguration (see [2]):

- **Initialisation** of an ensemble of N walkers $\left(\boldsymbol{X}^j_{0\Delta t}\right)_{1\leq j\leq N}$ i.i.d. according to $|\psi_I|^2(\boldsymbol{x})\, d\boldsymbol{x}$.
- **Iterations in time:** let us be given the particle positions $\left(\boldsymbol{X}^j_{n\Delta t}\right)_{1\leq j\leq N}$ at time $n\Delta t$, for $n \in \{0, \ldots, \nu - 1\}$. The new particle positions at time $(n+1)\Delta t$ are obtained in two steps:
  1. **Walkers displacement:** for all $1 \leq j \leq N$, the successive positions $\left(\boldsymbol{X}^j_{n\Delta t+\delta t}, \ldots, \boldsymbol{X}^j_{n\Delta t+\kappa\delta t}\right)$ over the time interval $(n\Delta t, (n+1)\Delta t)$ are obtained by an appropriate discretization of (3). In the field of interacting particles system for Feynman-Kac formulae (see [5, 6]), this step is called **the mutation step**.
  2. **Stochastic reconfiguration:** The new positions[1] $\left(\boldsymbol{X}^j_{(n+1)\Delta t}\right)_{1\leq j\leq N}$ which will be used as the initial particle positions on the time interval $((n+1)\Delta t, (n+2)\Delta t)$ are obtained from

[1] With a slight abuse of notation and though $n\Delta t + \kappa\delta t = (n+1)\Delta t$, we distinguish between the particle positions $\boldsymbol{X}^j_{n\Delta t+\kappa\delta t}$ at the end of the walkers displacement on time interval $(n\Delta t, (n+1)\Delta t)$, and the new particle positions $\boldsymbol{X}^j_{(n+1)\Delta t}$ obtained after the reconfiguration step, and which are used as the initial position for the next walkers displacement on time interval $((n+1)\Delta t, (n+2)\Delta t)$. We will use a more precise notation for the analysis of the numerical scheme in Section 1, but this is not required at this stage.

independent sampling of the measure

$$\frac{\sum_{j=1}^{N} \exp\left(-\delta t \sum_{k=1}^{\kappa} E_L(\boldsymbol{X}^j_{n\Delta t+k\delta t})\right) \delta_{\boldsymbol{X}^j_{n\Delta t+\kappa\delta t}}}{\sum_{j=1}^{N} \exp\left(-\delta t \sum_{k=1}^{\kappa} E_L(\boldsymbol{X}^j_{n\Delta t+k\delta t})\right)}. \tag{6}$$

In words, the new particle positions $\left(\boldsymbol{X}^j_{(n+1)\Delta t}\right)_{1\leq j\leq N}$ are randomly chosen among the final particle positions $\left(\boldsymbol{X}^j_{n\Delta t+\kappa\delta t}\right)_{1\leq j\leq N}$, each of them being weighted with the coefficient $\exp\left(-\delta t \sum_{k=1}^{\kappa} E_L(\boldsymbol{X}^j_{n\Delta t+k\delta t})\right)$ (accordingly to the exponential factor in (2)). In the field of interacting particles system for Feynman-Kac formulae, this step is called **the selection step**.

An estimate of $E_{\mathrm{DMC}}(t_{n+1})$ is then given by:

$$E_{\mathrm{DMC}}(t_{n+1}) \simeq \frac{1}{N} \sum_{j=1}^{N} E_L\left(\boldsymbol{X}^j_{(n+1)\Delta t}\right). \tag{7}$$

There are other possible estimations of $E_{\mathrm{DMC}}(t_{n+1})$. In [2], the authors propose to use Cesaro or weighted Cesaro means of the expression (7) . In Section 1, we will use the following expression:

$$E_{\mathrm{DMC}}(t_{n+1}) \simeq \frac{\sum_{j=1}^{N} E_L(\boldsymbol{X}^j_{n\Delta t+\kappa\delta t}) \exp\left(-\delta t \sum_{k=1}^{\kappa} E_L(\boldsymbol{X}^j_{n\Delta t+k\delta t})\right)}{\sum_{j=1}^{N} \exp\left(-\delta t \sum_{k=1}^{\kappa} E_L(\boldsymbol{X}^j_{n\Delta t+k\delta t})\right)}, \tag{8}$$

in an intermediate step to prove the convergence result.

We would like to mention that a continuous in time version of the DMC scheme with stochastic reconfiguration has been proposed in [8]. The author analyzes the longtime behaviour of the interacting particle system and proves in particular a uniform in time control of the variance of the estimated energy.

We can distinguish between four sources of errors in the approximation of E_0 by $\frac{1}{N} \sum_{j=1}^{N} E_L\left(\boldsymbol{X}^j_{\nu\Delta t}\right)$:

1. the error due to the fixed node approximation $|E_0 - E_{\mathrm{DMC},0}|$,
2. the error due to finite time approximation of the limit: $\lim_{t\to\infty} E_{\mathrm{DMC}}(t) \simeq E_{\mathrm{DMC}}(T)$,
3. the error due to the time discretization of the stochastic differential equation (3) and of the integral in the exponential factor in $E_{\mathrm{DMC}}(t)$ (see (2)),
4. the error introduced by the interacting particle systems, due to the approximation of the expectation value in (2) by an empirical mean.

The error (1) due to the fixed node aproximation has been analyzed theoretically in [4].

Concerning the error (2) due to finite time approximation of the limit, the rate of convergence in time is typically exponential. Indeed if H admits a spectral gap (namely if the distance between E_0 and the remaining of the spectrum of H is strictly positive), and if ψ_I is such that $\langle \psi_I, H\psi_I\rangle < \inf \sigma_{\mathrm{ess}}(H)$, then one can show that the operator H with domain $D_{\mathcal{H}}(H) \cap \{\psi,\, \psi = 0 \text{ on } \psi_I^{-1}(0)\}$ (whose lowest eigenvalue is $E_{\mathrm{DMC},0}$, see (5)) also admits a spectral gap $\gamma > 0$. Then, by standard spectral decomposition methods, we have:

$$0 \leq |E_{\mathrm{DMC}}(t) - E_{\mathrm{DMC},0}| \leq C \exp(-\gamma t).$$

Our aim in this paper is to provide some theoretical and numerical results related to the errors (3) and (4), in the framework of a simple one-dimensional case. We therefore consider in the following that the

final time of simulation T is fixed and we analyze the error introduced by the numerical scheme on the estimate of $E_{\rm DMC}(T)$. Our convergence result is of the form:

$$\mathbb{E}\left|E_{\rm DMC}(T) - \frac{1}{N}\sum_{j=1}^{N} E_L\left(\boldsymbol{X}^j_{\nu\kappa\Delta t}\right)\right| \leq C(T)\,\delta t + \frac{C(T,\nu)}{\sqrt{N}}, \tag{9}$$

where $C(T)$ (resp. $C(T,\nu)$) denotes a constant which only depends on T (resp. on T and ν) (see Theorem 4 and Corollary 12 below).

Let us now present the toy model we consider in the following. Though our model is one-dimensional (and therefore still far from the real problem (1)), it contains one of the main difficulties related to the approximation of the ground state energy for fermionic systems, namely the explosive behavior of the drift in the stochastic differential equation. We therefore think that the convergence results we obtain are prototypical of what could be proved for more complicated systems.

We consider the hamiltonian

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + V, \text{ with } V = \frac{\omega^2}{2}x^2 + \theta x^4, \tag{10}$$

where $\omega, \theta > 0$ are two constants. The ground state energy E_0 is defined by (1), with

$$\mathcal{H} = \left\{\psi \in L^2(\mathbb{R}),\, \psi(x) = -\psi(-x)\right\}. \tag{11}$$

We restrict the functional spaces to odd functions in order to mimic the antisymmetry constraint on ψ for fermionic systems. The importance sampling ψ_I is chosen to be the ground state of $H_0 = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\omega^2}{2}x^2$ with energy $\frac{3}{2}\omega$:

$$\psi_I(x) = \sqrt{2\omega}\left(\frac{\omega}{\pi}\right)^{1/4} x e^{-\frac{\omega}{2}x^2}. \tag{12}$$

The drift function b and the local energy E_L are then defined by:

$$b(x) = \frac{\psi_I'}{\psi_I}(x) = \frac{1}{x} - \omega x, \text{ and } E_L(x) = V(x) - \frac{1}{2}\,\frac{\psi_I''}{\psi_I}(x) = \frac{3}{2}\omega + \theta x^4. \tag{13}$$

Thus, using equation (2), the DMC energy is:

$$E_{\rm DMC}(t) = \frac{3}{2}\omega + \theta\frac{\mathbb{E}\left(X_t^4 \exp\left(-\theta\int_0^t X_s^4 ds\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\int_0^t X_s^4 ds\right)\right)}, \tag{14}$$

where

$$X_t = X_0 + \int_0^t \left(\frac{1}{X_s} - \omega X_s\right) ds + W_t, \tag{15}$$

with $(W_t)_{t\geq 0}$ a Brownian motion independent from the initial variable X_0 which is distributed according to the invariant measure $2\psi_I^2(x)1_{\{x>0\}}dx$. We recall that due to the explosive part in the drift function b, the stochastic process cannot cross 0, which is the zero point of ψ_I (see [4]): $\mathbb{P}(\exists t > 0,\, X_t = 0) = 0$. This explains why the restriction of ψ_I^2 to $\mathbb{R}_+^*$ is indeed an invariant measure for (15). For $\theta > 0$, the longtime limit $E_{\rm DMC,0}$ of $E_{\rm DMC}(t)$ is not analytically known, but can be very accurately computed by a spectral method (see Section 2.1). Let us finally precise that for the numerical analysis, we use a special feature of our simple model, namely the fact that for $s \leq t$, it is possible to simulate the conditional law of X_t given X_s (see Appendix). The time discretization error is thus only related to the discretization of the integral in the exponential factor in the DMC energy (2).

The paper is organized as follows. In Section 1, we prove the convergence result, by adapting the methods of [5, 6] to analyze the dependence of the error on δt. We then check the optimality of this theoretical result by numerical experiments in Section 2, where we also analyze numerically the dependence of the results on various numerical parameters, including the number $(\nu - 1)$ of reconfiguration steps.

Notation: For any set of random variables $(Y_i)_{i\in I}$, we denote by $\sigma((Y_i)_{i\in I})$ the sigma-field generated by these random variables.
The parameters ω and θ are fixed positive constants.
By convention, any sum from one to zero is equal to zero : $\sum_{k=1}^{0} \cdot = 0$.

1 Numerical Analysis in a Simple Case

We perfom the numerical analysis in two steps: time discretization and then particle approximation.

1.1 Time discretization

We recall that $T > 0$ denotes the final simulation time, and that $\delta t = \frac{T}{K}$ is the smallest time-step. Since $Y_t = X_t^2$ is a square root process solving $dY_t = (3 - 2\omega Y_t)dt + 2\sqrt{Y_t}dW_t$, it is possible to simulate the increments $Y_{(k+1)\delta t} - Y_{k\delta t}$ and therefore $X_{(k+1)\delta t} - X_{k\delta t}$ (see Appendix or [7] p.120). We can thus simulate exactly in law the vector $(X_0, X_{\delta t}, \dots, X_{K\delta t})$. That is why we are first going to study the error related to the time discretization of the integral which appears in the exponential factors in (14).

Let us define the corresponding approximation of $E_{\mathrm{DMC}}(T)$:

$$E_{\mathrm{DMC}}^{\delta t}(T) = \frac{\mathbb{E}\left(E_L(X_T)\exp\left(-\theta\delta t\sum_{k=1}^K E_L(X_{k\delta t})\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^K E_L(X_{k\delta t})\right)\right)} = \frac{3}{2}\omega + \theta\frac{\mathbb{E}\left(X_T^4\exp\left(-\theta\delta t\sum_{k=1}^K X_{k\delta t}^4)\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^K X_{k\delta t}^4\right)\right)}. \quad (16)$$

Proposition 1

$$\forall K \in \mathbb{N}^*, \left|E_{\mathrm{DMC}}(T) - E_{\mathrm{DMC}}^{\delta t}(T)\right| \le C_T\delta t.$$

Proof : Using Hölder inequality, we have:

$$\left|E_{\mathrm{DMC}}(T) - E_{\mathrm{DMC}}^{\delta t}(T)\right| \le \frac{\theta}{\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^K X_{k\delta t}^4\right)\right)}\left(\sqrt{\mathbb{E}(X_T^8)} + \frac{\mathbb{E}\left(X_T^4\exp\left(-\theta\int_0^T X_s^4 ds\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\int_0^T X_s^4 ds\right)\right)}\right)$$
$$\left(\mathbb{E}\left(\left(\exp\left(-\theta\int_0^T X_s^4 ds\right) - \exp\left(-\theta\delta t\sum_{k=1}^K X_{k\delta t}^4\right)\right)^2\right)\right)^{1/2}.$$

The conclusion is now a consequence of Lemma 2 and the fact that the function $x \in \mathbb{R}_+ \to e^{-\theta x}$ is Lipschitz continuous with constant θ. ∎

Lemma 2 *For any $K \in \mathbb{N}^*$,*

$$\mathbb{E}\left(\left(\int_0^T X_s^4 ds - \delta t\sum_{k=1}^K X_{k\delta t}^4\right)^2\right) \le C\delta t^2(T^2 + T),$$

where $\delta t = \frac{T}{K}$.

Proof of Lemma 2 : By Itô's formula, $dX_t^4 = (10X_t^2 - 4\omega X_t^4)dt + 4X_t^3 dW_t$. With the integration by parts formula, one deduces that for any $k \in \{1, \dots, K\}$,

$$\int_{(k-1)\delta t}^{k\delta t}(X_{k\delta t}^4 - X_s^4)ds = \int_{(k-1)\delta t}^{k\delta t}(s - (k-1)\delta t)\left((10X_s^2 - 4\omega X_s^4)ds + 4X_s^3 dW_s\right).$$

Therefore denoting $\tau_s = \lfloor \frac{s}{\delta t} \rfloor \delta t$ the discretization time just before s, one obtains

$$\delta t \sum_{k=1}^{K} X_{k\delta t}^4 - \int_0^T X_s^4 ds = \int_0^T (s-\tau_s)(10X_s^2 - 4\omega X_s^4) ds + \int_0^T (s-\tau_s) 4X_s^3 dW_s.$$

Hence

$$\mathbb{E}\left(\left(\delta t \sum_{k=1}^{K} X_{k\delta t}^4 - \int_0^T X_s^4 ds \right)^2 \right) \leq 2 \int_0^T (s-\tau_s)^2 \mathbb{E}\left(T(10X_s^2 - 4\omega X_s^4)^2 + 16 X_s^6 \right) ds.$$

Since X_0 is distributed according to the invariant measure $2\psi_I^2(x) 1_{\{x>0\}} dx$, so is X_s. As a consequence, for any $p \in \mathbb{N}$, $\mathbb{E}(X_s^p)$ does not depend on s and is finite and the conclusion follows readily. ∎

In realistic situations, exact simulation of the increments $X_{(k+1)\delta t} - X_{k\delta t}$ is not possible and one has to resort to discretization schemes. The singularity of the drift coefficient prevents the process X_t from crossing the nodal surfaces of the importance sampling function ψ_I. The standard explicit Euler scheme does not preserve this property at the discretized level. For that purpose, we suggest to use the following explicit scheme proposed by [1]

$$\begin{cases} \bar{X}_0 = X_0, \\ \forall k \in \mathbb{N},\ \bar{X}_{(k+1)\delta t} = \left(\left(\bar{X}_{k\delta t}(1-\omega\delta t) + \dfrac{\Delta W_{k+1}}{1-\omega\delta t} \right)^2 + 2\delta t \right)^{1/2} \text{ with } \Delta W_{k+1} = W_{(k+1)\delta t} - W_{k\delta t}. \end{cases} \tag{17}$$

Because of the singularity at the origin of the drift coefficient in (15), we have not been able so far to prove the following weak error bound (see Remark 3 below):

$$\left| E\left(f(X_T^4) \exp\left(-\theta \int_0^T X_s^4 ds \right) \right) - \mathbb{E}\left(f(\bar{X}_T^4) \exp\left(-\theta \delta t \sum_{k=1}^{K} \bar{X}_{k\delta t}^4 \right) \right) \right| \leq C_T \delta t \text{ for } f(x) \equiv 1 \text{ and } x^4. \tag{18}$$

Such a bound is expected according to [9] and would imply that

$$\left| E_{\mathrm{DMC}}(T) - \frac{\mathbb{E}\left(E_L(\bar{X}_T) \exp\left(-\delta t \sum_{k=1}^{K} E_L(\bar{X}_{k\delta t}) \right) \right)}{\mathbb{E}\left(\exp\left(-\delta t \sum_{k=1}^{K} E_L(\bar{X}_{k\delta t}) \right) \right)} \right| \leq C_T \delta t. \tag{19}$$

Remark 3 *We would like to sketch a possible way to prove* (18)*. Because the square root in* (17) *makes expansions with respect to* δt *and* ΔW_{k+1} *complicated, it is easier to work with* $Y_t = X_t^2$ *and* $\bar{Y}_{k\delta t} = \bar{X}_{k\delta t}^2$ *which satisfy*

$$dY_t = (3 - 2\omega Y_t) dt + 2\sqrt{Y_t}\, dW_t \ \text{ and } \ \bar{Y}_{(k+1)\delta t} = \left(\sqrt{\bar{Y}_{k\delta t}}(1-\omega\delta t) + \frac{\Delta W_{k+1}}{1-\omega\delta t} \right)^2 + 2\delta t.$$

The standard approach to analyze the time discretization error of the numerator and denominator of the left hand side of (19) *is then to introduce some functions* v *and* w *solutions to the partial differential equation:*

$$\partial_t v = (3-2y)\partial_y v + 2y\partial_{yy} v - \theta y^2 v,\ (t,y) \in \mathbb{R}_+ \times (0, +\infty) \tag{20}$$

with initial conditions $v(0,y) = y^2$ *et* $w(0,y) = 1$*. Now, we write (for the numerator, for example):*

$$\begin{aligned} &\mathbb{E}\left(X_T^4 \exp\left(-\theta \int_0^T X_s^4 ds \right) \right) - \mathbb{E}\left(\bar{X}_T^4 \exp\left(-\theta \delta t \sum_{k=1}^{K} \bar{X}_{k\delta t}^4 \right) \right) \\ &= \sum_{k=0}^{K-1} \mathbb{E}\left(\left(v(T-k\delta t, \bar{Y}_{k\delta t}) - e^{-\theta\delta t \bar{Y}_{(k+1)\delta t}^2} v(T-(k+1)\delta t, \bar{Y}_{(k+1)\delta t}) \right) \exp\left(-\theta\delta t \sum_{j=0}^{k-1} \bar{Y}_{j\delta t}^2 \right) \right). \end{aligned}$$

An error bound of the form $C_T\delta t$ can now be proved by some Taylor expansions as in [9] [1], provided the existence of a sufficiently smooth solution v to (20). We have not been able to prove existence of such a solution so far.

1.2 Particle approximation

We now introduce some notation to study the particle approximation. We recall that ν denotes the number of large timesteps (the number of reconfiguration steps is $\nu - 1$), and $\Delta t = \kappa\delta t$ the time period between two reconfiguration steps. Let us suppose that we know the initial positions $(X^i_{n,0})_{1\leq i\leq N}$ of the N walkers at time $(n-1)\Delta t$, for a time index $n \in \{1, \dots, \nu\}$. The successive positions of the walkers over the time interval $((n-1)\Delta t, n\Delta t)$ are then given by $(X^i_{n,\delta t}, \dots, X^i_{n,\kappa\delta t})$, where $(X^i_{n,t})_{0\leq t\leq\Delta t}$ satisfies:

$$X^i_{n,t} = X^i_{n,0} + \int_0^t b(X^i_{n,s})\, ds + \left(W^i_{t+(n-1)\Delta t} - W^i_{(n-1)\Delta t}\right). \tag{21}$$

Here $(W^1, \dots, W^N)$ denotes a N-dimensional Brownian motion independent from the initial positions of the walkers $(X^i_{1,0})_{1\leq i\leq N}$ whixh are i.i.d. according to $2\psi_I^2(x)1_{\{x>0\}}dx$. We recall that in our framework, it is possible to simulate exactly in law all these random variables (see Appendix). We store the successive positions $(X^i_{n,\delta t}, \dots, X^i_{n,\kappa\delta t})$ of the i-th walkers over the time interval $((n-1)\Delta t, n\Delta t)$ in a so-called particle $\xi^i_n \in (\mathbb{R}^*_+)^\kappa$ (see Figure 1): $\forall i \in \{1, \dots, N\}, \forall n \in \{1, \dots, \nu\}$,

$$\xi^i_n = (X^i_{n,\delta t}, \dots, X^i_{n,\kappa\delta t}). \tag{22}$$

In the following, we will denote by $\xi_n = (\xi^1_n, \dots, \xi^N_n)$ the configuration of the ensemble of particles at time index n. We have here described **the mutation step**.

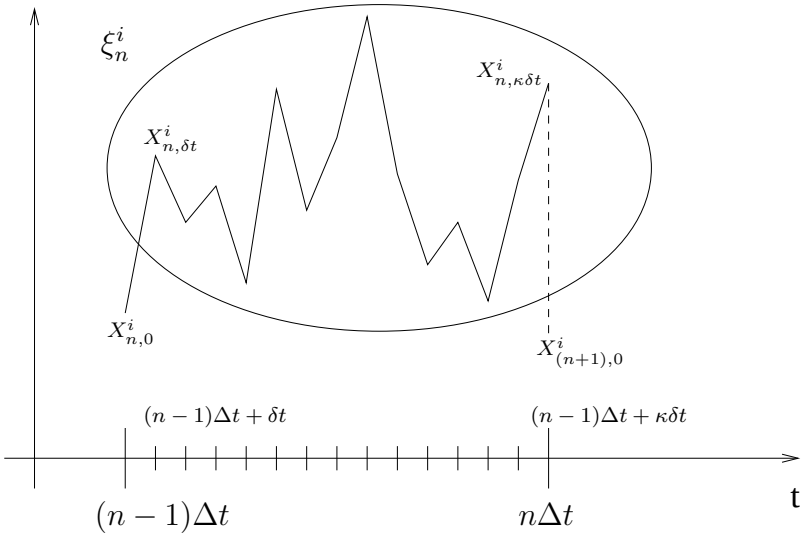

Figure 1: The i-th particle ξ^i_n at time index n is composed of the successive positions $(X^i_{n,\delta t}, \dots, X^i_{n,\kappa\delta t})$ of the i-th walker on time interval $((n-1)\Delta t, n\Delta t)$.

For a given configuration of the particles $(\xi^i_n)_{1\leq i\leq N}$ at a time index $n \in \{1, \dots, \nu\}$, **the selection step** now consists in choosing the initial positions $(X^i_{n+1,0})_{1\leq i\leq N}$ of the N walkers at time $n\Delta t$, conditionally independent, with $X^i_{n+1,0}$ distributed according to the measure

$$\epsilon_n g(\xi^i_n)\delta_{\xi^i_{n,\kappa}} + (1 - \epsilon_n g(\xi^i_n))\frac{\sum_{j=1}^N g(\xi^j_n)\delta_{\xi^j_{n,\kappa}}}{\sum_{j=1}^N g(\xi^j_n)}, \tag{23}$$

where g is defined by, for $y = (y_1, \dots, y_\kappa) \in (\mathbb{R}^*_+)^\kappa$,

$$g(y) = \exp\left(-\theta\delta t \sum_{k=1}^{\kappa} y_k^4\right), \tag{24}$$

and ϵ_n is a non negative function of ξ_n such that $\epsilon_n \leq \frac{1}{\max_{1\leq i\leq N} g(\xi_n^i)}$. In particular the following choices are possible for ϵ_n:

$$\epsilon_n = 0,\ \epsilon_n = 1 \text{ and } \epsilon_n = \frac{1}{\max_{1\leq i\leq N} g(\xi_n^i)}. \tag{25}$$

The case $\epsilon_n = 0$ corresponds to a maximum decorrelation with the former position of the particles, while with growing ϵ_n, more and more correlation is introduced.

For $n \in \{1, \ldots, \nu\}$, let us denote by $\eta_n^N = \frac{1}{N}\sum_{i=1}^N \delta_{\xi_n^i}$ the particle approximation of the measure η_n defined by: $\forall f : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}$ bounded ,

$$\eta_n(f) = \frac{\mathbb{E}\left(f\left(X_{(n-1)\Delta t+\delta t}, \ldots, X_{(n-1)\Delta t+\kappa\delta t}\right)\exp\left(-\theta\delta t\sum_{k=1}^{(n-1)\kappa}(X_{k\delta t})^4\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^{(n-1)\kappa}(X_{k\delta t})^4\right)\right)}, \tag{26}$$

where the process $(X_t)_{0\leq t\leq T}$ is defined by (15).

For $y = (y_1, \ldots, y_\kappa) \in (\mathbb{R}_+^*)^\kappa$ and $f : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}$, we set

$$Pf(y) = \mathbb{E}\left(f(X_{\delta t}^{y_\kappa}, \ldots, X_{\kappa dt}^{y_\kappa})\right) \tag{27}$$

where for $x \in \mathbb{R}_+^*$,

$$X_t^x = x + \int_0^t b(X_s^x)ds + W_t \tag{28}$$

denotes the solution of the stochastic differential equation (15) starting from x. By the Markov property, the measures $(\eta_n)_{1\leq n\leq \nu}$ satisfy the inductive relations, for any function $f : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}$ bounded, $\forall n \in \{1, \ldots, \nu-1\}$,

$$\eta_{n+1}(f) = \frac{\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^{n\kappa}(X_{k\delta t})^4\right)\mathbb{E}\left(f\left(X_{n\Delta t+\delta t}, \ldots, X_{n\Delta t+\kappa\delta t}\right)\middle|(X_{j\delta t})_{0\leq j\leq n\kappa}\right)\right)}{\eta_n(g)\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^{(n-1)\kappa}(X_{k\delta t})^4\right)\right)} \tag{29}$$

$$= \frac{1}{\eta_n(g)} \times \frac{\mathbb{E}\left(gPf\left(X_{(n-1)\Delta t+\delta t}, \ldots, X_{(n-1)\Delta t+\kappa\delta t}\right)\exp\left(-\theta\delta t\sum_{k=1}^{(n-1)\kappa}(X_{k\delta t})^4\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^{(n-1)\kappa}(X_{k\delta t})^4\right)\right)} = \frac{\eta_n(gPf)}{\eta_n(g)}, \tag{30}$$

where g is defined by (24). Moreover, we can express $E_{\mathrm{DMC}}^{\delta t}(T)$ defined by (16) as:

$$E_{\mathrm{DMC}}^{\delta t}(T) = \frac{3}{2}\omega + \theta\frac{\eta_\nu(gy_\kappa^4)}{\eta_\nu(g)}. \tag{31}$$

Therefore the particle approximation of $E_{\mathrm{DMC}}(T)$ is given by

$$E_{\mathrm{DMC}}^{N,\nu,\kappa}(T) = \frac{3}{2}\omega + \theta\frac{\eta_\nu^N(gy_\kappa^4)}{\eta_\nu^N(g)}. \tag{32}$$

This approximation of $E_{\mathrm{DMC}}(T)$ corresponds to the expression (8) given in the introduction. We will also prove in Corollary 12 below the convergence of the approximation which corresponds to the expression (7) given in the introduction (see Equation (41) below).

The convergence of the approximation $E_{\mathrm{DMC}}^{N,\nu,\kappa}(T)$ is ensured by our main result :

Theorem 4

$$\mathbb{E}\left|E_{\mathrm{DMC}}(T) - E_{\mathrm{DMC}}^{N,\nu,\kappa}(T)\right| \leq \frac{C}{\nu\kappa} + \frac{C_\nu}{\sqrt{N}}, \tag{33}$$

where the constant C only depends on T and the constant C_ν on T and ν.

Remark 5 *The number of selection steps is $\nu - 1$. For instance, when $\nu = 1$, there is no selection involved in the expression of $E_{\mathrm{DMC}}^{N,\nu,\kappa}(T)$ and the particles remain independent. In this case, the first term in the right hand side of (33) corresponds to the time discretization error proved in Proposition 1, while the second term is the classical error estimate related to the law of large numbers. For a fixed number of selection steps, the theorem ensures the convergence of the particle approximation $E_{\mathrm{DMC}}^{N,\nu,\kappa}(T)$ as the time-step $\delta t = T/(\nu\kappa)$ used for the discretization of the stochastic differential equation (15) tends to 0 while the number N of particles tends to $+\infty$. But this result does not specify the dependence of C_ν on ν and gives no hint on the optimal choice of the number of selection steps in terms of error minimization. We are going to deal with this important issue in the numerical study (see Section 2).*

According to the above expressions (31) and (32) of $E_{\mathrm{DMC}}^{\delta t}(T)$ and $E_{\mathrm{DMC}}^{N,\nu,\kappa}(T)$, this theorem is easily proved by combining Proposition 1 and the following result :

Proposition 6

$$\mathbb{E}\left|\frac{\eta_\nu^N(gy_\kappa^4)}{\eta_\nu^N(g)} - \frac{\eta_\nu(gy_\kappa^4)}{\eta_\nu(g)}\right| \leq \frac{C_\nu}{\sqrt{N}}. \tag{34}$$

Proof of Proposition 6 : One has

$$\begin{aligned}\mathbb{E}\left|\frac{\eta_\nu^N(gy_\kappa^4)}{\eta_\nu^N(g)} - \frac{\eta_\nu(gy_\kappa^4)}{\eta_\nu(g)}\right| \leq & \frac{\mathbb{E}|\eta_\nu^N(gy_\kappa^4) - \eta_\nu(gy_\kappa^4)|}{\eta_\nu(g)} \\ & + \left(\mathbb{E}\left(\frac{\eta_\nu^N(gy_\kappa^4)}{\eta_\nu^N(g)}\right)^2\right)^{1/2} \frac{\left(\mathbb{E}\left(\eta_\nu^N(g) - \eta_\nu(g)\right)^2\right)^{1/2}}{\eta_\nu(g)}.\end{aligned}$$

According to Proposition 7 and Lemma 11 below, the first term of the right-hand-side and the quotient in the second term are smaller than $C_\nu/\sqrt{N}$. Since by Jensen's inequality, $\left(\frac{\eta_\nu^N(gy_\kappa^4)}{\eta_\nu^N(g)}\right)^2 \leq \frac{\eta_\nu^N(gy_\kappa^8)}{\eta_\nu^N(g)}$, the boundedness of $\mathbb{E}\left(\frac{\eta_\nu^N(gy_\kappa^4)}{\eta_\nu^N(g)}\right)^2$ follows from Lemma 8 below. ∎

Proposition 7 *For any bounded function $f : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}$,*

$$\forall n \in \{1, \ldots, \nu\},\ \mathbb{E}((\eta_n^N(f) - \eta_n(f))^2) \leq \frac{C_n}{N}\|f\|_\infty^2, \tag{35}$$

where the constant C_n does not depend on κ.

For any function $f : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}$ such that for some $p \geq 2$, $\|f\|_{\kappa,p} = \sup_{y \in \mathbb{R}_+^\kappa} \frac{|f(y)|}{1 + y_\kappa^p}$ is finite,

$$\forall n \in \{1, \ldots, \nu\},\ \mathbb{E}|\eta_n^N(f) - \eta_n(f)| \leq \frac{C_n}{\sqrt{N}}\|f\|_{\kappa,p}, \tag{36}$$

where the constant C_n does not depend on κ.

For f bounded, the first estimate (35) is proved in [6]. In order to prove Proposition 6, we need to apply Proposition 7 with $f(y) = g(y)$ and $f(y) = g(y)y_\kappa^4$, which are bounded functions with L^∞ norm respectively equal to 1 and $\frac{C}{\delta t}$ where C is a constant not depending on δt. But we want to obtain the convergence when δt tends to 0. This is why we need the second estimate (36), that we use with $f(y) = g(y)y_\kappa^4$ for which $\|f\|_{\kappa,p}$ is bounded and does not depend on δt.

Notice that for f bounded, Corollary 2.20 in [6] states the convergence in law of $\sqrt{N}(\eta_n^N(f) - \eta_n(f))$ to a centered Gaussian variable and gives an expression of the variance of this limit variable. Because of the complexity of this expression, using this result with $f(y) = g(y)y_\kappa^4$ did not really help us to understand the dependence of C_ν on ν (see Remark 5 above).

Proof : For f bounded, the first estimate (35) is proved by induction on n in [6] (see Proposition 2.9). Since we follow the same inductive reasoning to deal with f such that $\|f\|_{\kappa,p} < +\infty$, we give at the same time the proof for f bounded.

Since the initial positions $(\xi_1^i)_{1\leq i\leq N}$ are independent and identically distributed with $\xi_{1,\kappa}^i$ distributed according to $2\psi_I^2(x)1_{\{x>0\}}dx$, the statement holds for $n=1$.
To deduce the statement at rank $n+1$ from the statement at rank n, we remark that according to (30),

$$\eta_{n+1}^N(f) - \eta_{n+1}(f) = T_{n+1} + \frac{1}{\eta_n(g)}\left((\eta_n^N(gPf) - \eta_n(gPf)) + \frac{\eta_n^N(gPf)}{\eta_n^N(g)}(\eta_n(g) - \eta_n^N(g))\right) \tag{37}$$

where we recall that P is defined by (27), and

$$T_{n+1} = \eta_{n+1}^N(f) - \frac{\eta_n^N(gPf)}{\eta_n^N(g)}.$$

To deal with this term T_{n+1}, one remarks that all the possible choices of ϵ_n given in (25) are $\sigma(\xi_n)$-measurable. As a consequence, for $i \in \{1,\dots,N\}$,

$$\mathbb{E}(f(\xi_{n+1}^i)|\xi_n) = \epsilon_n g(\xi_n^i)Pf(\xi_n^i) + (1-\epsilon_n g(\xi_n^i))\frac{\sum_{j=1}^N g(\xi_n^j)Pf(\xi_n^j)}{\sum_{j=1}^N g(\xi_n^j)}.$$

Multiplying this equality by $\frac{1}{N}$ and summing over i, one deduces

$$\mathbb{E}(\eta_{n+1}^N(f)|\xi_n) = \frac{\sum_{i=1}^N g(\xi_n^i)Pf(\xi_n^i)}{\sum_{i=1}^N g(\xi_n^i)} = \frac{\eta_n^N(gPf)}{\eta_n^N(g)}. \tag{38}$$

Since the variables $(\xi_{n+1}^i)_{1\leq i\leq N}$ are independent conditionally on ξ_n, one deduces that

$$\mathbb{E}((T_{n+1})^2|\xi_n) = \frac{1}{N^2}\sum_{i=1}^N \mathbb{E}\left(\left(f(\xi_{n+1}^i) - \mathbb{E}(f(\xi_{n+1}^i)|\xi_n)\right)^2|\xi_n\right) \leq \frac{1}{N}\mathbb{E}\left(\eta_{n+1}^N(f^2)|\xi_n\right).$$

Therefore

$$\mathbb{E}((T_{n+1})^2) \leq \frac{1}{N}\mathbb{E}(\eta_{n+1}^N(f^2)). \tag{39}$$

When f is bounded, $\eta_{n+1}^N(f^2) \leq \|f\|_\infty^2$, $\left|\frac{\eta_n^N(gPf)}{\eta_n^N(g)}\right| \leq \|Pf\|_\infty$, and $\|Pf\|_\infty \leq \|f\|_\infty$. Hence by (37),

$$\mathbb{E}((\eta_{n+1}^N(f) - \eta_{n+1}(f))^2) \leq 3\left(\frac{\|f\|_\infty^2}{N} + \frac{\mathbb{E}((\eta_n^N(gPf) - \eta_n(gPf))^2) + \|f\|_\infty^2\mathbb{E}((\eta_n^N(g) - \eta_n(g))^2)}{(\eta_n(g))^2}\right)$$

with the second term of the right-hand-side smaller than $C\|f\|_\infty^2/N$ by the induction hypothesis and Lemma 11 below.

When $\|f\|_{\kappa,p} < +\infty$, combining (37) and (39), one obtains

$$\begin{aligned}\mathbb{E}\left|\eta_{n+1}^N(f) - \eta_{n+1}(f)\right| \leq & \frac{\mathbb{E}(\eta_{n+1}^N(f^2))^{1/2}}{\sqrt{N}} + \frac{\mathbb{E}\left|\eta_n^N(gPf) - \eta_n(gPf)\right|}{\eta_n(g)} \\ & + \left(\mathbb{E}\left(\frac{\eta_n^N(gPf)}{\eta_n^N(g)}\right)^2\right)^{1/2}\frac{\left(\mathbb{E}(\eta_n^N(g) - \eta_n(g))^2\right)^{1/2}}{\eta_n(g)}.\end{aligned}$$

Since $\|f^2\|_{k,2p} \leq 2\|f\|_{k,p}^2$ (by using the inequality $f^2(y) \leq 2\|f\|_{\kappa,p}^2(1+y_\kappa^{2p})$), the first term of the right-hand-side is smaller than $C_n\|f\|_{\kappa,p}/\sqrt{N}$ by Lemma 8 below. Since, according to Lemma 9 below, $\|Pf\|_{\kappa,p} \leq e^{C_p\Delta t}\|f\|_{\kappa,p}$, the second term is smaller than $C_n\|f\|_{\kappa,p}/\sqrt{N}$ by the induction hypothesis and Lemma 11. Last, by using successively Cauchy Schwartz inequalities, (38) for f^2 and Lemma 8, one obtains that $\mathbb{E}\left(\frac{\eta_n^N(gPf)}{\eta_n^N(g)}\right)^2 \leq \mathbb{E}\left(\frac{\eta_n^N(g(Pf)^2)}{\eta_n^N(g)}\right) \leq \mathbb{E}\left(\frac{\eta_n^N(gPf^2)}{\eta_n^N(g)}\right) \leq \mathbb{E}(\eta_{n+1}^N(f^2)) \leq C_n\|f\|_{\kappa,p}^2$. And it follows

from the Proposition statement for f bounded and Lemma 11 that $\frac{\left(\mathbb{E}(\eta_n^N(g)-\eta_n(g))^2\right)^{1/2}}{\eta_n(g)}$ is smaller than $C_n/\sqrt{N}$. ∎

Lemma 8 *Let $h : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}_+$ be such that for some $p \geq 2$, $\|h\|_{\kappa,p} < +\infty$. Then,*

$$\forall n \in \{1,\ldots,\nu\},\ \max\left(\mathbb{E}(\eta_n^N(h)), \mathbb{E}\left(\frac{\eta_n^N(gh)}{\eta_n^N(g)}\right)\right) \leq e^{C_p n\Delta t}\|h\|_{\kappa,p}(1+\mathbb{E}(X_0)^p),$$

where X_0 is distributed according to the measure $2\psi_I^2(x)1_{\{x>0\}}dx$ (see (15)).

Proof : As the variables $\xi_{1,\kappa}^i, 1 \leq i \leq N$ are distributed according to the invariant measure $2\psi_I^2(x)1_{\{x>0\}}dx$, one has $\mathbb{E}(\eta_1^N(h)) \leq \|h\|_{\kappa,p}(1+\mathbb{E}(X_0)^p)$. In addition for $n \geq 1$, according to (38), $\mathbb{E}(\eta_{n+1}^N(h)) = \mathbb{E}\left(\frac{\eta_n^N(gPh)}{\eta_n^N(g)}\right)$ where $\|Ph\|_{\kappa,p} \leq e^{C_p\Delta t}\|h\|_{k,p}$ by Lemma 9. Therefore it is enough to check the bound for $\mathbb{E}\left(\frac{\eta_n^N(gh)}{\eta_n^N(g)}\right)$.

For $n \geq 0$, one has

$$\mathbb{E}\left(\frac{\eta_{n+1}^N(gh)}{\eta_{n+1}^N(g)}\right) \leq \|h\|_{\kappa,p}\left(1+\mathbb{E}\left(\frac{\sum_{i=1}^N \exp\left(-\theta\delta t\sum_{k=1}^\kappa(\xi_{n+1,k}^i)^4\right)(\xi_{n+1,\kappa}^i)^p}{\sum_{j=1}^N \exp\left(-\theta\delta t\sum_{k=1}^\kappa(\xi_{n+1,k}^j)^4\right)}\right)\right). \tag{40}$$

Let us denote in this proof $\xi_{n+1,0}^i = X_{n+1,0}^i$, where $0 \leq n \leq \nu-1$ and $1 \leq i \leq N$. Let us set $\mathcal{F} = \sigma(\xi_{n+1,k}^i,\ 1 \leq i \leq N,\ 0 \leq k \leq \kappa-1)$. By Lemma 10 below,

$$\begin{aligned}
\mathbb{E}\left(\frac{\sum_{i=1}^N \exp\left(-\theta\delta t\sum_{k=1}^\kappa(\xi_{n+1,k}^i)^4\right)(\xi_{n+1,\kappa}^i)^p}{\sum_{j=1}^N \exp\left(-\theta\delta t\sum_{k=1}^\kappa(\xi_{n+1,k}^j)^4\right)}\middle|\mathcal{F}\right) &\leq \frac{\sum_{i=1}^N \exp\left(-\theta\delta t\sum_{k=1}^{\kappa-1}(\xi_{n+1,k}^i)^4\right)\mathbb{E}((\xi_{n+1,\kappa}^i)^p|\mathcal{F})}{\sum_{j=1}^N \exp\left(-\theta\delta t\sum_{k=1}^{\kappa-1}(\xi_{n+1,k}^j)^4\right)},\\
&= \frac{\sum_{i=1}^N \exp\left(-\theta\delta t\sum_{k=1}^{\kappa-1}(\xi_{n+1,k}^i)^4\right)\mathbb{E}((X_{\delta t}^x)^p)|_{x=\xi_{n+1,\kappa-1}^i}}{\sum_{j=1}^N \exp\left(-\theta\delta t\sum_{k=1}^{\kappa-1}(\xi_{n+1,k}^j)^4\right)},\\
&\leq e^{C_p\delta t}\frac{\sum_{i=1}^N \exp\left(-\theta\delta t\sum_{k=1}^{\kappa-1}(\xi_{n+1,k}^i)^4\right)(\xi_{n+1,\kappa-1}^i)^p}{\sum_{j=1}^N \exp\left(-\theta\delta t\sum_{k=1}^{\kappa-1}(\xi_{n+1,k}^j)^4\right)} + e^{C_p\delta t} - 1,
\end{aligned}$$

where we have used the definition of the mutation step (see (21)) and the Markov property for the stochastic differential equation (28) to obtain the equality, and then Lemma 9 for the last inequality. Notice that this estimate also holds for $\kappa = 1$, in which case the right hand side reduces to $\frac{e^{C_p\delta t}}{N}(\xi_{n+1,0}^i)^p + e^{C_p\delta t} - 1$.

Taking expectations and iterating the reasoning, one deduces that

$$\mathbb{E}\left(\frac{\sum_{i=1}^N \exp\left(-\theta\delta t\sum_{k=1}^\kappa(\xi_{n+1,k}^i)^4\right)(\xi_{n+1,\kappa}^i)^p}{\sum_{j=1}^N \exp\left(-\theta\delta t\sum_{k=1}^\kappa(\xi_{n+1,k}^j)^4\right)}\right) \leq \frac{e^{C_p\Delta t}}{N}\sum_{i=1}^N \mathbb{E}((\xi_{n+1,0}^i)^p) + (e^{C_p\delta t}-1)\sum_{k=0}^{\kappa-1} e^{C_pk\delta t}.$$

Inserting this bound in (40), one concludes that

$$\mathbb{E}\left(\frac{\eta_{n+1}^N(gh)}{\eta_{n+1}^N(g)}\right) \leq e^{C_p\Delta t}\|h\|_{\kappa,p}\left(1+\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^N(\xi_{n+1,0}^i)^p\right)\right).$$

For $n=0$, one deduces that $\mathbb{E}\left(\frac{\eta_1^N(gh)}{\eta_1^N(g)}\right) \leq e^{C_p\Delta t}\|h\|_{\kappa,p}(1+\mathbb{E}(X_0^p))$, where X_0 is distributed according to the measure $2\psi_I^2(x)1_{\{x>0\}}dx$.

For $n \geq 1$, since by a reasoning similar to the one made to obtain (38), $\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^N(\xi_{n+1,0}^i)^p\right) = \mathbb{E}\left(\frac{\eta_n^N(g(y)y_\kappa^p)}{\eta_n^N(g(y))}\right)$, one also deduces that

$$\mathbb{E}\left(\frac{\eta_{n+1}^N(gh)}{\eta_{n+1}^N(g)}\right) \leq e^{C_p\Delta t}\|h\|_{\kappa,p}\mathbb{E}\left(\frac{\eta_n^N(g(1+y_\kappa^p))}{\eta_n^N(g)}\right).$$

The proof is completed by an obvious inductive reasoning. ∎

Lemma 9 *For any $p \geq 2$, there is a constant C_p such that*

$$\forall x \in \mathbb{R}_+^*,\ \forall t \geq 0,\ \mathbb{E}((X_t^x)^p) \leq (1+x^p)e^{C_p t} - 1,$$

where X_t^x is defined by (28). Therefore, if $h : (\mathbb{R}_+^*)^\kappa \to \mathbb{R}$ is such that $\|h\|_{\kappa,p} < +\infty$ then $\|Ph\|_{\kappa,p} \leq e^{C_p\Delta t}\|h\|_{\kappa,p}$, where the operator P is defined by (27).

Proof : By Itô's formula, $d(X_t^x)^p = \left(\frac{p(p+1)}{2}(X_t^x)^{p-2} - \omega p(X_t^x)^p\right)dt + p(X_t^x)^{p-1}dW_t$. Hence

$$(X_t^x)^p \leq x^p + \int_0^t \left(\frac{p(p+1)}{2} + \frac{p(p+1-2\omega)}{2}(X_s^x)^p\right)ds + p\int_0^t (X_s^x)^{p-1}dW_s.$$

Formally, taking expectations in this inequality, one obtains

$$\mathbb{E}((X_t^x)^p) \leq x^p + \int_0^t \frac{p(p+1)}{2} + \frac{p(p+1-2\omega)}{2}\mathbb{E}((X_s^x)^p)ds,$$

and check by Gronwall's lemma that the conclusion holds with $C_p = \frac{p(p+1)}{2}$. This formal argument can be made rigorous by a standard localization procedure.
For $h : \mathbb{R}_+^\kappa \to \mathbb{R}$ such that $\|h\|_{\kappa,p} < +\infty$ one deduces that

$$\forall y \in \mathbb{R}_+^\kappa,\ |Ph(y)| \leq \mathbb{E}|h(X_{\delta t}^{y_\kappa}, \ldots, X_{\kappa\delta t}^{y_\kappa})| \leq C\|h\|_{\kappa,p}(1+\mathbb{E}((X_{\kappa\delta t}^{y_\kappa})^p)) \leq e^{C_p\Delta t}\|h\|_{\kappa,p}(1+y_\kappa^p).$$

∎

Lemma 10

$$\forall (z_1,\ldots,z_N),(a_1,\ldots,a_N) \in \mathbb{R}_+^N \text{ with } \sum_{i=1}^N a_i > 0,\ \forall p \geq 0,\ \forall c \geq 0,\ \frac{\sum_{i=1}^N a_i z_i^p e^{-cz_i^4}}{\sum_{i=1}^N a_i e^{-cz_i^4}} \leq \frac{\sum_{i=1}^N a_i z_i^p}{\sum_{i=1}^N a_i}.$$

Proof : Let us set $f(c) = \frac{\sum_{i=1}^N a_i z_i^p e^{-cz_i^4}}{\sum_{i=1}^N a_i e^{-cz_i^4}}$. By Hölder's inequality, the derivative

$$f'(c) = \left(\frac{\sum_{i=1}^N a_i z_i^p e^{-cz_i^4}}{\sum_{i=1}^N a_i e^{-cz_i^4}}\frac{\sum_{i=1}^N a_i z_i^4 e^{-cz_i^4}}{\sum_{i=1}^N a_i e^{-cz_i^4}}\right) - \frac{\sum_{i=1}^N a_i z_i^{p+4} e^{-cz_i^4}}{\sum_{i=1}^N a_i e^{-cz_i^4}}$$

is non positive. Hence for any $c \geq 0$, $f(c) \leq f(0) = \frac{\sum_{i=1}^N a_i z_i^p}{\sum_{i=1}^N a_i}$. ∎

Lemma 11 *The sequence $(\eta_n(g))_{1\leq n\leq \nu}$ is bounded from below by a positive constant non depending on κ.*

Proof : Since

$$\eta_n(g) = \frac{\mathbb{E}\left(\exp\left(-\theta\delta t \sum_{k=1}^{n\kappa} X_{k\delta t}^4\right)\right)}{\mathbb{E}\left(\exp\left(-\theta\delta t \sum_{k=1}^{(n-1)\kappa} X_{k\delta t}^4\right)\right)} \leq 1$$

the sequence $(\eta_n(g))_{1\leq n\leq \nu}$ is bounded from below by

$$\prod_{n=1}^{\nu} \eta_n(g) = \mathbb{E}\left(\exp\left(-\theta\delta t \sum_{k=1}^{\nu\kappa} X_{k\delta t}^4\right)\right).$$

According to Lemma 2, this expectation converges to $\mathbb{E}\left(\exp\left(-\theta \int_0^T X_s^4 ds\right)\right) > 0$ when κ tends to $+\infty$, which concludes the proof. ∎

We can now prove, as a corollary of Theorem 4, the convergence of the approximation $\overline{E_{\rm DMC}^{N,\nu,\kappa}}(T)$ of $E_{\rm DMC}(T)$, defined by:

$$\overline{E_{\rm DMC}^{N,\nu,\kappa}}(T) = \frac{3}{2}\omega + \frac{\theta}{N}\sum_{i=1}^{N}(X_{\nu+1,0}^i)^4. \tag{41}$$

Corollary 12

$$\mathbb{E}\left|E_{\rm DMC}(T) - \overline{E_{\rm DMC}^{N,\nu,\kappa}}(T)\right| \leq \frac{C}{\nu\kappa} + \frac{C_\nu}{\sqrt{N}},$$

where the constant C only depends on T and the constant C_ν on T and ν.

Proof : By using the result of Theorem 4 and Cauchy Schwartz inequality, it is sufficient to prove the estimate $\mathbb{E}\left(E_{\rm DMC}^{N,\nu,\kappa}(T) - \overline{E_{\rm DMC}^{N,\nu,\kappa}}(T)\right)^2 \leq \frac{C_\nu}{N}$. Let us denote in this proof $\xi_{\nu+1,0}^i = X_{\nu+1,0}^i$ for $1 \leq i \leq N$. We have:

$$E_{\rm DMC}^{N,\nu,\kappa}(T) - \overline{E_{\rm DMC}^{N,\nu,\kappa}}(T) = \theta\left(\frac{\eta_\nu^N(g\, y_\kappa^4)}{\eta_\nu^N(g)} - \frac{1}{N}\sum_{i=1}^{N}(\xi_{\nu+1,0}^i)^4\right) = \theta\left(\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^{N}(\xi_{\nu+1,0}^i)^4\middle|\xi_\nu\right) - \frac{1}{N}\sum_{i=1}^{N}(\xi_{\nu+1,0}^i)^4\right)$$

by using the fact that, for any function $f : \mathbb{R}_+^* \to \mathbb{R}_+$,

$$\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^{N} f(\xi_{\nu+1,0}^i)\middle|\xi_\nu\right) = \frac{\eta_\nu^N(g(y)\, f(y_\kappa))}{\eta_\nu^N(g(y))}, \tag{42}$$

which is obtained by a reasoning similar to the one made to prove (38). Now, using the same method as to obtain (39), one easily gets the estimate:

$$\mathbb{E}\left(E_{\rm DMC}^{N,\nu,\kappa}(T) - \overline{E_{\rm DMC}^{N,\nu,\kappa}}(T)\right)^2 \leq \frac{\theta^2}{N}\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^{N}(\xi_{\nu+1,0}^i)^8\right) = \frac{\theta^2}{N}\mathbb{E}\left(\frac{\eta_\nu^N(g(y)\,(y_\kappa)^8)}{\eta_\nu^N(g(y))}\right),$$

by using again (42). Lemma 8 completes the proof. ∎

We end this Section by proving that Proposition 6 also holds for the numerical scheme (17).

Proposition 13 *Let us consider the Markov chain $(\bar{X}_{j\delta t})_{0\leq j\leq K}$ generated by the explicit scheme* (17) *and denote by Q its transition kernel. We now define the measure η_n by replacing $(X_{j\delta t})_{0\leq j\leq K}$ with $(\bar{X}_{j\delta t})_{0\leq j\leq K}$ in (26), and we define accordingly the evolution of the particle system: conditionally on ξ_n,*

the vectors $(X^i_{n+1,0}, X^i_{n+1,\delta t}, \ldots, X^i_{n+1,\kappa\delta t})_{1\le i\le N}$ *are independent, with* $X^i_{n+1,0}$ *distributed according to* (23) *and* $(X^i_{n+1,j\delta t})_{0\le j\le\kappa}$ *a Markov chain with transition kernel* Q*. Then, we have:*

$$\mathbb{E}\left|\frac{\eta^N_\nu(gy^4_\kappa)}{\eta^N_\nu(g)} - \frac{\eta_\nu(gy^4_\kappa)}{\eta_\nu(g)}\right| \le \frac{C_\nu}{\sqrt{N}}.$$

Proof : Looking carefully at the proof of Proposition 6 above, one remarks that (34) holds in this framework as soon as Lemma 11 holds, and the following property, which replaces Lemma 9, is satisfied:

$$\exists C>0,\ \forall x\in\mathbb{R}_+,\ Qf(x)\le e^{C\delta t}(1+f(x))-1 \text{ for } f(x)\equiv x^4 \text{ and } f(x)\equiv x^8. \tag{43}$$

Let us first prove (43). We have: $Qf(x)=\mathbb{E}\left(f\left(\bar{X}^x_{\delta t}\right)\right)$ where $\bar{X}^x_{\delta t}=\left((1-\omega\delta t)^2x^2+2xW_{\delta t}+\frac{W^2_{\delta t}}{(1-\omega\delta t)^2}+2\delta t\right)^{1/2}$. Now, for $q\in\mathbb{N}^*$,

$$(\bar{X}^x_{\delta t})^{2q}=\sum_{j_1+j_2+j_3=q}\frac{q!}{j_1!j_2!j_3!}(1-\omega\delta t)^{2j_1}\,2^{j_2}\,x^{2j_1+j_2}\,W^{j_2}_{\delta t}\left(\frac{W^2_{\delta t}}{(1-\omega\delta t)^2}+2\delta t\right)^{j_3},$$

where the indices (j_1,j_2,j_3) are non negative integers. Remarking that the expectation of the terms with j_2 odd vanishes and then using Young's inequality, one deduces that for $\delta t\le\frac{1}{2\omega}$,

$$\begin{aligned}
\mathbb{E}\left((\bar{X}^x_{\delta t})^{2q}\right) &\le (1-\omega\delta t)^{2q}x^{2q}+\mathbb{E}\left(\left(\frac{W^2_{\delta t}}{(1-\omega\delta t)^2}+2\delta t\right)^q\right)+C_q\sum_{\substack{j_1+j_2+j_3=q\\ j_1<q, j_2\ even\ , j_3<q}} x^{2\left(q-\frac{j_2+2j_3}{2}\right)}\delta t^{\frac{j_2+2j_3}{2}},\\
&\le x^{2q}+C_q\delta t+C_q\sum_{\substack{j_1+j_2+j_3=q\\ j_1<q, j_2\ even\ , j_3<q}}\left(x^{2q}\delta t+\delta t^{1+q\left(1-\frac{2}{j_2+2j_3}\right)}\right),\\
&\le (1+C_q\delta t)x^{2q}+C_q\delta t\le e^{C_q\delta t}(1+x^{2q})-1.
\end{aligned}\tag{44}$$

Let us now prove Lemma 11 for the scheme (17). As noticed in the proof of Lemma 11 above, it is sufficient to bound from below $\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^{\nu\kappa}\bar{X}^4_{k\delta t}\right)\right)$. By Jensen inequality, we have $\mathbb{E}\left(\exp\left(-\theta\delta t\sum_{k=1}^{\nu\kappa}\bar{X}^4_{k\delta t}\right)\right)\ge\exp\left(-\theta\frac{T}{\nu\kappa}\sum_{k=1}^{\nu\kappa}\mathbb{E}\left(\bar{X}^4_{k\delta t}\right)\right)$. By using (44), it is easy to prove by induction that $\mathbb{E}\left(\bar{X}^4_{k\delta t}\right)\le e^{C_2k\delta t}(1+\mathbb{E}\left(\bar{X}^4_0\right))-1$ and this concludes the proof of Lemma 11 in this framework. ∎

In order to obtain a complete convergence result of the form (33) for the scheme (17), it remains to prove the complementary bound (19), that we have not obtained so far. However, we will check by numerical simulations that (33) still holds.

2 Numerical results

2.1 Computation of a reference solution by a spectral method

In this section, we would like to explain how we can obtain a very precise reference solution by using a partial differential equation approach to compute $E_{\mathrm{DMC}}(T)$ (see [4]).

2.1.1 A partial differential equation approach to compute $E_{\mathrm{DMC}}(T)$

Let us introduce the solution ϕ to the following partial differential equation for :

$$\begin{cases}\dfrac{\partial\phi}{\partial t}=-H\phi,\ (t,x)\in\mathbb{R}_+\times\mathbb{R}\\ \phi(0,x)=\psi_I(x),\ x\in\mathbb{R}\end{cases}\tag{45}$$

where H (resp. ψ_I) is defined by (10) (resp. (12)). Since $\psi_I \in \mathcal{H}$, it is a standard result that this problem admits a unique solution $\phi \in C^0(\mathbb{R}_+, \mathcal{H}) \cap C^0(\mathbb{R}_+^*, D_{\mathcal{H}}(H)) \cap C^1(\mathbb{R}_+^*, \mathcal{H})$. The function ϕ is regular and odd, and therefore is such that $\phi(t,0) = 0$ for all $t \geq 0$. Therefore the function ϕ is also solution to the following partial differential equation:

$$\begin{cases} \dfrac{\partial \phi}{\partial t} = -H\phi, \ (t,x) \in \mathbb{R}_+ \times \mathbb{R} \\ \phi(t,0) = 0, \ t \geq 0 \\ \phi(0,x) = \psi_I(x), \ x \in \mathbb{R}. \end{cases} \tag{46}$$

In [4], we have shown that since ϕ satisfies (46), we can express $E_{\mathrm{DMC}}(t)$ (defined by (2)) using the function ϕ (see Proposition 11 in [4]):

$$E_{\mathrm{DMC}}(t) = \frac{\langle H\psi_I, \phi(t)\rangle}{\langle \psi_I, \phi(t)\rangle}. \tag{47}$$

Our reference solution $E_{\mathrm{DMC}}(T)$ will rely on formula (47) after discretization of (45) by a spectral method.

2.1.2 Computation of the wave function ϕ

We will briefly present the spectral method developed to compute an approximation of ϕ. We recall that the Hermite polynomials are defined by :

$$\forall n \in \mathbb{N}, \ h_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}).$$

We introduce the eigenfunctions of the operator H_0, normalized for the $L^2(\mathbb{R})$ norm associated with the eigenvalues $E_n = \omega(n+1/2)$ for $n \geq 0$,

$$\varphi_n(x) = h_n(\sqrt{\omega}x) \exp(-\frac{1}{2}\omega x^2) \left(\frac{(\omega/\pi)^{1/4}}{\sqrt{2^n n!}} \right).$$

It is well known that the vector space spanned by the set of functions $\{\varphi_{2k+1}\}_{k\geq 0}$ is dense in $\mathcal{V}_0 = \{\varphi \in H^1(\mathbb{R}) \cap \mathcal{H} \mid x\varphi \in L^2\}$, which is the domain of the quadratic form associated with H_0.

Let us now introduce the functional space $\mathcal{V} = \{\varphi \in H^1(\mathbb{R}) \cap \mathcal{H} \mid x^2\varphi \in L^2\}$, which is the domain of the quadratic form associated with H. The set of functions $\{\varphi_{2k+1}\}_{k\geq 0}$ is also a basis of $\mathcal{V}$.

Let $\mathcal{V}_n = Span(\varphi_1, \varphi_3, \ldots, \varphi_{2n-1})$. We use this approximation space to build the following Galerkin scheme for (45): find $\phi_n \in C^0(\mathbb{R}_+, \mathcal{V}_n)$ such that[2] $\phi_n(0,x) = \psi_I$, and $\forall \varphi \in \mathcal{V}_n$

$$\left\langle \frac{\partial \phi_n(t)}{\partial t}, \varphi \right\rangle = -\left\langle H\phi_n(x,t), \varphi \right\rangle. \tag{48}$$

We diagonalize the operator H restricted to $\mathcal{V}_n$. We denote $(\varphi_0^n, \varphi_2^n, \ldots, \varphi_{n-1}^n)$ the eigenfunctions and $E_0^n, E_2^n, \ldots, E_{n-1}^n$ the associated eigenvalues. Because of the symmetry of H, it is easy to check that $\mathcal{V}_n$ can also be spanned by $(\varphi_0^n, \varphi_2^n, \ldots, \varphi_{n-1}^n)$:

$$\mathcal{V}_n = Span(\varphi_0^n, \varphi_2^n, \ldots, \varphi_{n-1}^n). \tag{49}$$

Since for $t \geq 0$, $\phi_n(t,.) \in \mathcal{V}_n$, there exists $u_k(t), \ k = 0, \ldots, n-1$, such that

$$\phi_n = \sum_{k=0}^{n-1} u_k(t)\varphi_k^n. \tag{50}$$

In view of (49) and (50), (48) is equivalent to the equations: $\forall i = 0, \ldots, n-1$,

$$\begin{aligned} \sum_{k=0}^{n-1} \frac{\partial u_k(t)}{\partial t} \langle \varphi_k^n, \varphi_i^n \rangle &= -\left\langle H \sum_{k=0}^{n-1} u_k(t)\varphi_k^n, \varphi_i^n \right\rangle, \\ &= -\sum_{k=0}^{n-1} E_k^n u_k(t) \langle \varphi_k^n, \varphi_i^n \rangle. \end{aligned}$$

[2] Notice that $\psi_I = \varphi_1 \in \mathcal{V}_n$.

We deduce that $\forall k = 0, \ldots, n-1$,

$$\frac{\partial u_k(t)}{\partial t} = -E_k^n u_k(t),$$

so that

$$\phi_n(t,x) = \sum_{k=0}^{n-1} u_k(0) \exp(-E_k^n t) \varphi_k^n(x), \tag{51}$$

where $u_k(0) = \langle \psi_I, \varphi_k^n \rangle$.

Remark 14 *The eigenfunctions of H are obtained by diagonalization of the matrix $A = (a_{ij})_{i,j=0,\ldots,n-1}$ with $\forall i, j = 0, \ldots, n-1$:*

$$\begin{aligned} a_{ij} &= \langle H\varphi_{2i+1}, \varphi_{2j+1} \rangle, \\ &= \langle H_0\varphi_{2i+1}, \varphi_{2j+1} \rangle + \theta \left\langle x^4 \varphi_{2i+1}, \varphi_{2j+1} \right\rangle, \\ &= \delta_{ij}\, \omega\, (2i + \tfrac{3}{2}) + \theta \left\langle x^4 \varphi_{2i+1}, \varphi_{2j+1} \right\rangle. \end{aligned}$$

We can use the n–point Gauss-Hermite formula to deal with the integration of the second term on the right. We recall that this method provides an exact result for $\int_{-\infty}^{+\infty} p(x) \exp(-x^2) dx$ as long as p is a polynomial of degree $2n-1$ or less.

2.1.3 Approximation of $E_{\mathrm{DMC}}(T)$

We now use formula (47) to approximate $E_{\mathrm{DMC}}(T)$. By an elementary calculation, we obtain the following approximation:

$$E_{\mathrm{DMC}}(T) \simeq \frac{E_0^n + \sum_{i=1}^{n-1} \frac{u_i(0) \langle \varphi_i^n, \varphi_1 \rangle}{u_0(0) \langle \varphi_1^n, \varphi_1 \rangle} E_i^n \exp(-(E_i^n - E_0^n)T)}{1 + \sum_{i=1}^{n-1} \frac{u_i(0) \langle \varphi_i^n, \varphi_1 \rangle}{u_0(0) \langle \varphi_1^n, \varphi_1 \rangle} \exp(-(E_i^n - E_0^n)T)}. \tag{52}$$

In our test cases, we have observed that $n = 40$ is enough to reach convergence.

Notice that for a given n, the convergence in time to the lowest eigenvalue E_0^n is exponentially fast, with an exponent equal to the spectral gap $E_1^n - E_0^n$.

2.2 Numerical results of Monte Carlo simulations

In all the computations, we take $T = 5$.

We represent on Figure 2, the expectation e and the variance v of the error : $\left| E_{\mathrm{DMC}}^{N,\nu,T/(\nu\delta t)}(T) - E_{\mathrm{DMC}}(T) \right|$ as a function of the number of walkers N, the time step δt and the number of reconfigurations $\nu - 1$, where $E_{\mathrm{DMC}}(T)$ is approximated using (52) and $E_{\mathrm{DMC}}^{N,\nu,T/(\nu\delta t)}(T)$ is defined by (32).
The top figures represent the expectation of the error and its variance according to the number of walkers. To compute these quantities, we perform 2000 independent realizations, with the number of reconfigurations $\nu - 1 = 50$, a small time step $\delta t = 5.10^{-3}$ and $\theta = 0.5$. The simulations confirm the theoretical result : the error decreases as $C/\sqrt{N}$.
The effect of the time step is shown on the two figures in the center. The numerical parameters are: a large number of particles $N = 5000$, number of configurations $\nu - 1 = 30$, $\theta = 2$ and 300 independent realizations. We can see on the figure on the left that the error decreases linearly as the time step decreases. We also remark that the error is smaller with the approximate scheme (17) than when using the exact simulation of the SDE (15) proposed in the Appendix. This rather amazing result can be interpreted as follows. When using the exact simulation of the SDE, there is only one source of error related to the time discretization, namely the approximation of the integral in the exponential factor in (2). When using the scheme (17), we add a weak error term which seems to partly compensate the previous one.

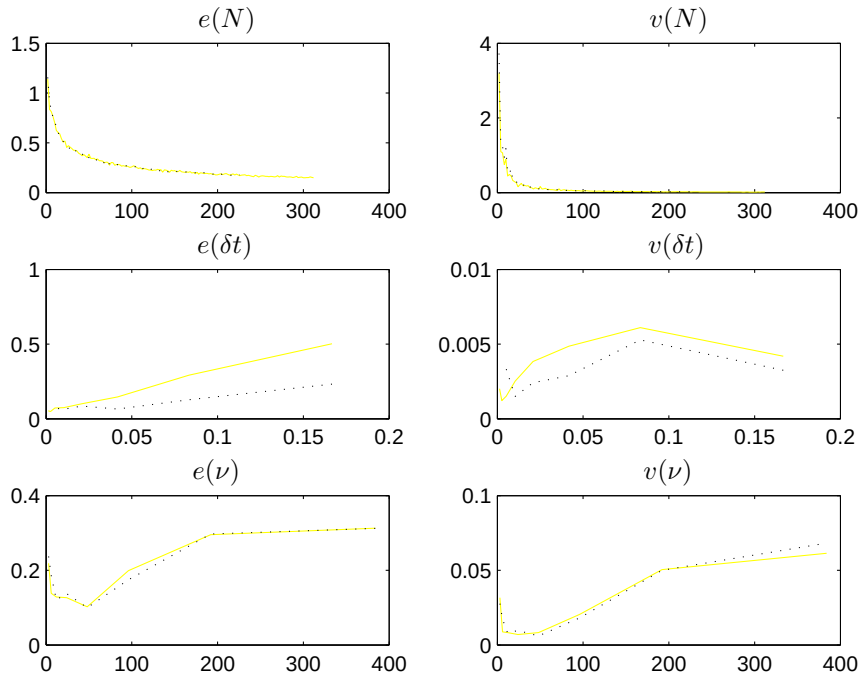

Figure 2: Expectation and variance of the error when (15) is discretized according to the method described in Appendix (solid curve) and according to the scheme (17) (dotted curve).

The last figures represent the effect of the number of reconfiguration steps. The numerical parameters are: time step $\delta t = 5.10^{-3}$, number of particles $N = 5000$, $\theta = 2$ and 300 independent realizations. The curve representing the variation of the error according to the number of reconfigurations has the shape of a basin. We deduce that on the one hand a small number of reconfigurations has the disadvantage that walkers with increasingly differing weights are kept. On the other hand a large number of reconfigurations introduces much noise. An optimal number of reconfiguration seems to lie between 20 and 50.

On Figure 3, we check that the optimal number of reconfigurations in terms of the variance $\tilde{v}$ of $E_{\mathrm{DMC}}^{N,\nu,T/(\nu\delta t)}(T)$ (and not of the error) is also obtained for a number of reconfiguration which seems to lie between 20 and 50. The numerical parameters are those considered for the figures below in Figure 2: time step $\delta t = 5.10^{-3}$, number of particles $N = 5000$, $\theta = 2$ and 300 independent realizations. We have not studied how the optimal number of reconfigurations varies according to the other numerical parameters.

We have investigated a practical method to estimate numerically the optimal number of reconfigurations. On Figure 4 we represent the variance of $E_{\mathrm{DMC}}^{N,1,t/\delta t}(t)$ according to time t, without any reconfiguration step $\nu = 1$. The other numerical parameters are again those considered for the figures below in Figure 2. We can see that the variance is minimal at $t^* \approx 0.25$ before it starts to raise again. We remark that $\nu = T/t^* = 20$ is close to the optimal number of reconfigurations obtained on the previous Figures. Therefore, it seems that the optimal number of reconfiguration is related to T/t^* where t^* minimizes the variance of $E_{\mathrm{DMC}}^{N,1,t/\delta t}(t)$.

Conclusion

In this paper, we have proved on a simple example convergence of numerical implementations of the DMC method with a fixed number of walkers. The observed theoretical rates of convergence are confirmed by

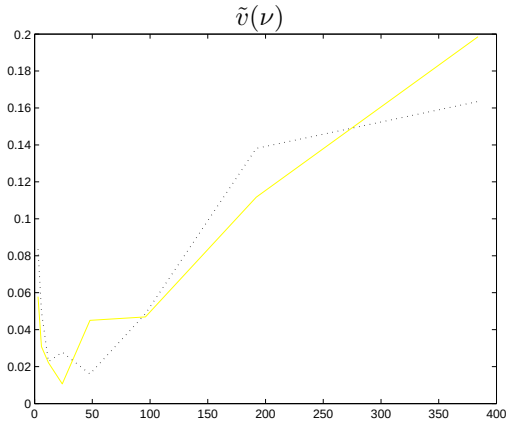

Figure 3: Variance of $E_{\mathrm{DMC}}^{N,\nu,T/(\nu\delta t)}(T)$ in function of the number of reconfigurations when (15) is discretized according to the method described in Appendix (solid curve) and according to the scheme (17) (dotted curve).

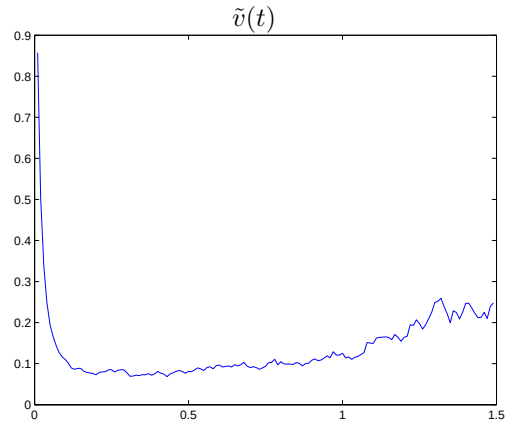

Figure 4: Variance of $E_{\mathrm{DMC}}^{N,1,t/\delta t}(t)$ according to time t.

numerical experiments and is likely to hold in more general situations. We have also checked numerically the existence of an optimal number of reconfiguration steps. For future work, we plan to investigate criteria devoted to the choice of the number of reconfiguration steps. One interesting direction is the use of automatic criteria based on a measure of the discrepancy between the weights carried by the walkers to decide when to perform a reconfiguration step.

Appendix : Simulation of the stochastic differential equation (15)

In this appendix, we show that it is possible to simulate exactly in law the $(K+1)$-plet $(X_0, X_{\delta t}, \ldots, X_{K\delta t})$, where X_t is defined by (15). Let (G, U) denote a couple of independent random variables with G normal and U uniformly distributed on the interval $[0, 1]$.

Simulation of the increment $X_t - X_s$, for $t \geq s$.

The square R_t of the norm of a 3-dimensional Brownian motion $\boldsymbol{W}_t = \left(\boldsymbol{W}_t^1, \boldsymbol{W}_t^2, \boldsymbol{W}_t^3\right)$ solves $dR_t = 3dt + 2\sqrt{R_t}dB_t$ where $B_t = \displaystyle\int_0^t \frac{\boldsymbol{W}_s \cdot d\boldsymbol{W}_s}{\|\boldsymbol{W}_s\|}$ is a one-dimensional Brownian motion. Hence $\rho_t = \dfrac{R_t}{1+2\omega t}$ solves

$$d\rho_t = (3 - 2\omega\rho_t)\frac{dt}{1+2\omega t} + 2\sqrt{\rho_t}\frac{dB_t}{\sqrt{1+2\omega t}}. \tag{53}$$

It is easy to check that $\left(\int_0^{\frac{1}{2\omega}(e^{2\omega t}-1)} \frac{dB_s}{\sqrt{1+2\omega s}}\right)_t$ is a Brownian motion. Hence, performing a time-change in (53), one obtains that $\rho_{\frac{1}{2\omega}(e^{2\omega t}-1)} = e^{-2\omega t} R_{\frac{1}{2\omega}(e^{2\omega t}-1)}$ is a weak solution of the equation $dY_t = (3 - 2\omega Y_t)dt + 2\sqrt{Y_t}\, dW_t$ satisfied by $Y_t = X_t^2$. Therefore $e^{-\omega t}\sqrt{R_{\frac{1}{2\omega}(e^{2\omega t}-1)}}$ is a weak solution of (15).

For $v \geq u$, R_v has the same distribution as $\left(\sqrt{R_u} + \boldsymbol{W}_v^1 - \boldsymbol{W}_u^1\right)^2 + (\boldsymbol{W}_v^2 - \boldsymbol{W}_u^2)^2 + (\boldsymbol{W}_v^3 - \boldsymbol{W}_u^3)^2$, and therefore as $(\sqrt{R_u} + G\sqrt{v-u})^2 - 2(v-u)\log(U)$ with (G, U) independent from R_u. Hence for $t \geq s$, X_t has the same distribution as

$$\left(e^{-2\omega t}\left(\left(e^{\omega s}X_s + \frac{G}{\sqrt{2\omega}}(e^{2\omega t} - e^{2\omega s})^{1/2}\right)^2 - 2\frac{1}{2\omega}(e^{2\omega t} - e^{2\omega s})\log(U)\right)\right)^{1/2}$$
$$= \left(\left(e^{-\omega(t-s)}X_s + \frac{G}{\sqrt{2\omega}}(1 - e^{-2\omega(t-s)})^{1/2}\right)^2 - \frac{1}{\omega}(1 - e^{-2\omega(t-s)})\log(U)\right)^{1/2}$$

where the couple (G, U) is independent from X_s.

Simulation of X_0 with distribution $2\psi_I^2(x)1_{\{x>0\}}dx$.

The random variable $\frac{1}{\sqrt{2\omega}}\left(G^2 - 2\log(U)\right)^{1/2}$ is distributed according to the invariant measure $2\psi_I^2(x)1_{\{x>0\}}dx$, as suggested by letting the time increment $t - s$ tend to $+\infty$ in the previous simulation. Indeed, $G^2 - 2\log(U)$ is a Gamma random variable with density $\frac{1}{2^{3/2}\Gamma(3/2)}1_{\{z>0\}}\sqrt{z}e^{-z/2}$. And one deduces the density of $\frac{1}{\sqrt{2\omega}}\left(G^2 - 2\log(U)\right)^{1/2}$ by an easy change of variables.

References

[1] A. Alfonsi, *On the discretization schemes for the CIR (and Bessel squared) processes*, Preprint Cermics 2005-279.

[2] R. Assaraf, M. Caffarel and A. Khelif, *Diffusion Monte Carlo with a fixed number of walkers*, Phys. Rev. E 61 (2000) 4566-4575.

[3] E. Cancès, M. Defranceschi, W. Kutzelnigg, C. Le Bris, and Y. Maday, *Computational Quantum Chemistry: a Primer*, in: Handbook of Numerical Analysis, Special volume, Computational Chemistry, volume X, Ph. G. Ciarlet and C. Le Bris (eds), North-Holland 2003, p. 3-270.

[4] E. Cancès, B. Jourdain and T. Lelièvre, *Quantum Monte Carlo simulations of fermions. A mathematical analysis of the fixed-node approximation*, Preprint Cermics 2004-270.

[5] P. Del Moral, *Feynman-Kac Formulae : Genealogical and Interacting Particle Systems with Applications*, Springer-Verlag (2004).

[6] P. Del Moral and L. Miclo *Branching and Interacting Particle Systems. Approximation of Feynman-Kac Formulae with Applications to Non-Linear Filtering*, in Séminaire de Probabilités XXXIV, Lecture Notes in Mathematics 1729, pp1-145, Springer-Verlag (2000).

[7] P. Glasserman, *Monte Carlo methods in financial engineering*, Springer-Verlag (2004).

[8] M. Rousset, *On the Control of an Interacting Particle Approximation of Schrödinger Groundstates*, Preprint (2005).

[9] D. Talay and L. Tubaro, *Expansion of the global error for numerical schemes solving stochastic differential equations*, Stochastic Analysis and Applications, 8(4):94–120, 1990.

[10] C.J. Umrigar, M.P. Nightingale and K.J. Runge, *A Diffusion Monte Carlo algorithm with very small time-step errors*, J. Chem. Phys., 99(4):2865–2890, 1993.