ON THE CONTROL OF AN INTERACTING PARTICLE ESTIMATION OF SCHRÖDINGER GROUND STATES

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Abstract. We consider a general Schrödinger operator $L + V$ on a domain $E \subset \mathbb{R}^d$, and its associated positive ground state h solution to the maximal eigenvalue problem $L(h) + Vh = \lambda h$. In this work, an interacting particle model approximating the pair (h, λ) is studied. When $V \leq 0$, a basic version of this particle system consists of N walkers evolving independently according to the Markov generator L, each walker dying at a rate given by the value of the potential $|V|$ at the walker's current location; when a walker dies, any other one splits in two. The long time distribution of the particle system is then an estimator of h.
Under some reasonable assumptions (with examples for $E = \mathbb{R}^d$), we get a non-asymptotic control of the $\mathbb{L}^p$ deviations (resp. the bias) of this estimator with the genuine rate of convergence in $1/\sqrt{N}$ (resp.$1/N$). We also compute explicitly the asymptotic standard deviation of the estimation of λ, which remains bounded in usual mild situations.

Key words. Schrödinger ground states, stochastic particle methods, long time behavior, Quantum Monte Carlo

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Introduction. Our motivation can be split in two steps:

1. Control the long time behavior of an interacting particle approximation of Feynman-Kac formulas with genuine rate of convergence.
2. Use the long time distribution of the particle system as a Monte Carlo estimator of the ground state of Schrödinger operators.

The last question is of very high practical interest in Quantum Physics and Chemistry, where one uses such Diffusion Monte Carlo methods to compute observable of systems (see [3], [2] and references therein). In the difficult yet crucial case of Fermi systems, the so-called Fixed Node Approximation is used ([3],[2]), where one is resorting to the ground state of a general Schrödinger operator on a domain of $\mathbb{R}^d$.

We have focused in this work on the interacting particle system (IPS) studied by P.Del Moral and L.Miclo in the article [7]. In its diffusive time-continuous version, it is particularly well suited to this context. Indeed, the fixed number of particles and the selection mechanism make it liable to be stable on the long run, and to give rise to finite variance. Note that it has not yet inspired as such practitioners' heuristics. Several keys are given here to design it in practice, and some toy simulations will be soon available on the author's web page, and in [12].

We have used for the analysis some semi-group and martingale techniques inherited from [7]. However, this paper is mostly self-contained. The good rate of convergence of the long time distribution of the IPS is a new result, technically demanding, and proved in a very reasonable setting which includes examples in $\mathbb{R}^d$. Intermediate results can be used to precise some proofs of [7] (see remark 4.5). For the stability questions, we have used a Foster-Lyapounov drift criterion to prove uniform exponential convergence of Schrödinger semi-groups (proposition 1.2) under a quite general assumption, which seems to be a new point also.

If $K(x, dy)$ is an integral kernel, φ a test function, and μ a probability measure, we will use the notation: $\mu K(\varphi) = \int \varphi(y) K(x, dy) \mu(dx)$. $(\quad)^+$ and $(\quad)^-$ denote respectively the positive and negative part.

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Let us give now the main results of this paper. Suppose we are given an irreducible strong Feller diffusion X_t in an open connected domain $E \subset \mathbb{R}^d$ with generator L, reversible with respect to a probability measure $\mu(dx) = \frac{h_I^2(x)dx}{\int h_I^2(x)dx}$ for some $h_I \geq 0$. V denotes a potential function such that the Feynman-Kac semi-group

$$P_t^V(\varphi)(x) = \mathbb{E}\left(\varphi(X_t)e^{\int_0^t V(X_s)ds} | X_0 = x\right) \quad \varphi \in \mathbb{L}^2(\mu)$$

is strongly continuous in $\mathbb{L}^2(\mu)$ and Fellerian ($x \mapsto P_t^V(\varphi)(x)$ is continuous for φ bounded, see [8]). It gives rise to its associated self-adjoint Schrödinger operator

$$(L+V)(\varphi) = \lim_{t \to 0^+} \frac{P_t^V(\varphi) - \varphi}{t} \quad \in \mathbb{L}^2(\mu)$$

defined on its domain $\mathcal{D}(L+V)$ where the latter limit exists (see [8]).
Our main example (detailed in section 1.1), which arises in many practical situations of interest (again in [3]), is some importance sampling transformation of the usual Schrödinger operator (with $h_I > 0$)

$$(L+V)(.) = h_I^{-1}(\frac{\Delta}{2} + V_0)(h_I.) \ , \tag{0.1}$$

which leaves the spectrum of $\frac{\Delta}{2} + V_0$ invariant, and multiply eigenfunctions by h_I^{-1}. X_t is then a Brownian motion with local drift $\nabla \ln h_I$.
We will work under the following usual assumption:

Assumption 1. *The spectrum of $L+V$ is bounded by a greatest eigenvalue λ, and has a spectral gap $\lambda^* > 0$. λ is associated with a unique eigenfunction $h \in \mathbb{L}^2(\mu)$ (the ground state), which is continuous and strictly positive.*

Note that assumption 1 is very general and idiomatic, see [8] chapter 3, [4], [9], [11], and the example of section 1.1.
By spectral theory, we get that

$$P_t^{V-\lambda}(\varphi) \xrightarrow[t \to +\infty]{\exp} h\mu(h\varphi) \quad \text{in } \mathbb{L}^2(\mu)$$

with rate $\lambda^\star > 0$. If the initial probability law η_0 of X_0 has a density in $\mathbb{L}^2(\mu)$, the Cauchy-Schwarz inequality gives that

$$\eta_0 P_t^{V-\lambda}(\varphi) \xrightarrow[t \to +\infty]{\exp} \eta_0(h)\mu(h\varphi) \ .$$

This is not sufficient to compute h numerically, since of course λ is unknown. That's why we resort to the renormalized version of the semigroup

$$\eta_t = \frac{\eta_0 P_t^V(\varphi)}{\eta_0 P_t^V(1)} = \frac{\eta_0 P_t^{V-\lambda}(\varphi)}{\eta_0 P_t^{V-\lambda}(1)} \ .$$

This probability flow verifies from the discussion above

$$\eta_t(\varphi) \xrightarrow[t \to +\infty]{\exp} \frac{\mu(h\varphi)}{\mu(h)} = \eta_\infty(\varphi) \ ,$$

the ground state eigenvalue λ can be recovered from η_∞ by the identity

$$\eta_\infty(V) = \frac{\mu(-L(h) + \lambda h)}{\mu(h)} = \lambda \ ,$$

and the Feynman-Kac semi-group can be recovered from η_t by

$$\eta_0 P_t^V(\varphi) = \eta_t(\varphi) \exp\left(\int_0^t \eta_s(V)ds\right) .$$

Thus a stochastic particle approximation of η_t enables the computation of P_t^V, of λ, and of h under a re-normalized weak form.
Now we consider continuous and bounded potentials $V \in \mathcal{C}_b(E)$ and smooth test functions $\varphi \in \mathcal{C}_b^\infty(E)$, and we remark then that η_t is a weak solution to the "non-linear" Fokker-Planck equation

$$\begin{aligned} \partial_t \eta_t(\varphi) &= \eta_t \left(L(\varphi) + (V - \eta_t(V))\varphi\right) \\ &= \eta_t(L_{\eta_t}(\varphi)) . \end{aligned} \tag{0.2}$$

The "nonlinear" Markov generator L_η is a jump perturbation of L defined by (other choices are possible as in the abstract, see subsection 2.1)

$$L_\eta(\varphi)(x) = L(\varphi)(x) + \int_E (\varphi(y) - \varphi(x)) \left((V(x) - \eta(V))^- + (V(y) - \eta(V))^+\right) \eta(dy) .$$

To compute η_t, we construct a particle system associated to this mean-field interpretation. The latter is denoted $\xi_t = (\xi_t^1, ..., \xi_t^N) \in E^N$ with initial law $\eta_0^{\otimes N}$, and its Markov generator is given by

$$\mathcal{L}(\psi)(\xi) = \sum_{i=1}^N L_{m(\xi)}^{(i)}(\psi)(\xi) \quad \text{with} \quad m(\xi) = \frac{1}{N}\sum_{j=1}^N \delta_{\xi^j} \tag{0.3}$$

for any $\xi = (\xi^1, ..., \xi^N) \in E^N$. The exponent (i) means that the operator acts on the i-th coordinate of the test function $\psi \in \mathcal{C}_b^\infty(E^N)$. The empirical measure of the particle system ξ_t denoted

$$\eta_t^N = m(\xi_t) = \frac{1}{N}\sum_{j=1}^N \delta_{\xi_t^j}$$

is then a stochastic approximation of η_t and converges to the ground state η_∞ on the long run.
ξ_t consists of N walkers evolving independently according to the Markov generator L, but constrained by the following birth and death mechanism:

1. with rate $(V(\xi_t^i) - \eta_t^N(V))^-$, each walker ξ_t^i jumps to the location of a uniformly randomly chosen walker.
2. with rate $(V(\xi_t^i) - \eta_t^N(V))^+$, a uniformly randomly chosen walker jumps to the location of each walker ξ_t^i.

Under some localization assumptions (assumptions 1, 2 and 3; with examples in $\mathbb{R}^d$), we prove a strong control on the long time behavior of this IPS,

$$\begin{aligned} \sup_{T\geq 0} \mathbb{E}(|\eta_T^N(\varphi) - \eta_T(\varphi)|^p)^{1/p} &\leq \frac{C_p\|\varphi\|_\infty}{\sqrt{N}} \\ \sup_{T\geq 0} |\mathbb{E}(\eta_T^N(\varphi)) - \eta_T(\varphi)| &\leq \frac{C\|\varphi\|_\infty}{N} \\ \sup_{T\geq 0} \|\mathrm{Law}(\xi_T^i) - \eta_T\|_{tv} &\leq \frac{C}{N} . \end{aligned}$$

To get a more quantitative result, we then consider the asymptotic standard deviation of the estimator of λ

$$\mathrm{Ad}^2(V) = \lim_{N\to+\infty} \overline{\lim_{T\to+\infty}} N\mathbb{E}\left((\eta_T^N(V)-\lambda)^2\right) \ , \tag{0.4}$$

and wee give an explicit upper bound on the latter which remains finite in usual mild situations with general unbounded potentials V.

1. Assumptions and examples. We begin with our main example (see also [3]), which motivates the results of the paper.

1.1. Example. We say that a positive function h has exponential fall-off at infinity as soon as $-\ln h$ goes to infinity at least linearly.

Let E be a bounded open domain of $\mathbb{R}^d$ with boundary ∂E. Classically, we consider the Schrödinger operator $\frac{\Delta}{2}+V_0$, with V_0 continuous on $\bar{E}$ and going to $-\infty$ at infinity $\lim_{+\infty} V_0 = -\infty$.
$\frac{\Delta}{2}+V_0$ is then self-adjoint for the core $\mathcal{C}_c^\infty(E)$ of smooth test functions with compact support in E (Dirichlet conditions), and has compact resolvent (see [11] ch.XIII). The operator has thus a discrete spectrum with maximal eigenvalue λ, a spectral gap λ^*, and a ground state $h_0 > 0$ on E. h_0 is continuous on $\bar{E}$ with $h_0|_{\partial E} = 0$, and has exponential fall-off at infinity (see [1]).
Now we consider the importance sampling transformation (0.1) for $h_I \in \mathcal{C}^\infty \cap \mathbb{L}^2(\bar{E})$, with $h_I > 0$ on E, $h_I|_{\partial E} = 0$ and exponential fall-off. The resulting operator $L+V$ then reads

$$L = \frac{\Delta}{2} + \nabla \ln h_I \nabla$$
$$V = V_0 + h_I^{-1}\frac{\Delta}{2}h_I \ .$$

$L+V$ is self-adjoint for the core $\mathcal{C}_c^\infty(E)$ in $\mathbb{L}^2(\mu)$, with $\mu(dx) = \frac{h_I^2(x)dx}{\int h_I^2(x)dx}$, it has the same spectrum as $\frac{\Delta}{2}+V_0$, but with continuous ground state $h = h_0 h_I^{-1} > 0$. As a consequence, $L+V$ satisfies assumption 1.
To stick to our probabilistic setting we additionally ask that

1. $\nabla h_I \neq 0$ on ∂E,
2. For some constant a and b, $x.\nabla \ln h_I(x) \leq a|x|^2 + b$ for all $x \in \bar{E}$,
3. V or $h_I^{-1}\frac{\Delta}{2}h_I$ is bounded above.

By proposition 7 of [3], L defines then a non-explosive strong Feller diffusion X_t in E, verifying the EDS (for some Brownian motion $t \mapsto W_t$)

$$dX_t = dW_t + \nabla \ln h_I(X_t)dt \ ,$$

and reversible with respect to μ.
Here are two examples satisfying assumptions 2 and 3:

Remark 1.1. Within the context of section 1.1, assumption 2 and 3 are satisfied as soon as V_0 is Hölder continuous, and that there is an $\epsilon > 0$ such that, outside some compact set

$$\epsilon \leq h = h_I h_0^{-1} \leq \epsilon^{-1} \ , \tag{1.1}$$

$$-\epsilon^{-1} \leq h_I^{-1}\frac{\Delta}{2}h_I - h_0^{-1}\frac{\Delta}{2}h_0 \leq -\epsilon \ . \tag{1.2}$$

Heuristically, this means that h_I and h_0 must have similar behaviors outside compact sets; h_I being chosen slightly more concave than h_0.

First example for bounded domains. Suppose now that E is bounded and V_0 is Hölder. The Schrödinger operator is regularizing and h_0 is smooth. Note this classical fact [1]: $\nabla h_0 \neq 0$ on ∂E. It is now always possible to construct explicitly a h_I satisfying (1.1) and (1.2), and thus assumptions 1, 2 and 3.

Proof. On the boundary ∂E, ∇h_0 and ∇h_I are non-degenerated and directed along the normal vector of ∂E. This ensures (1.1). Now adjust the concavity of h_I near the boundary so that (1.2) is satisfied. □

Second example for unbounded domains. This case is slightly more intricate, so we only give a particular explicit example:
Suppose that $E = \mathbb{R}^d$, V_0 Hölder, and that h_0 has the following expression

$$h_0(x) = \mathrm{e}^{-\frac{|x|^4}{4} + \epsilon_0(x)} ,$$

where ϵ_0 is smooth and bounded with bounded first derivatives.
Now if we choose h_I such that, outside some compact set,

$$h_I(x) = \mathrm{e}^{-\frac{|x|^4}{4} + \epsilon_0(x) - \frac{C}{|x|^2}}$$

for some $C > 0$; (1.1) and (1.2), and thus assumptions 1, 2 and 3 are satisfied.

Proof. (1.1) is obvious. A straightforward computation shows that at infinity $V(x) - \lambda = -4C + o(|x|^{-2})$, which gives (1.2). □

Third example for general situations. Here is our last example, less restrictive (neither V nor h^{-1} shall be bounded). Assumptions 2 and 3 are not satisfied, but the expression of the asymptotic standard deviation of the eigenvalue estimation $Ad(V)$ (defined by (0.4)) remains finite, which is a very favorable indication of practical efficiency.
Take $E = \mathbb{R}^d$ and suppose V_0 behaves polynomially at infinity. Choose h_I such that:

1. $\ln h_I$ and its two first derivatives are of polynomial behavior.
2. $h = h_0 h_I^{-1}$ is bounded with exponential fall-off.

then the expression of $Ad(V)$ remains bounded. Note that it is practically easy to choose such a h_I, since the exponential fall-off of h_0 is known from V_0 (see [1]).

Proof. Remark that: $V = V_0 + \frac{\Delta}{2}\ln(h_I) + \frac{1}{2}(\nabla \ln(h_I))^2$ is polynomially dominated, and that $\frac{d\eta_\infty}{d\mu}(x) \propto h(x) = h_0(x)h_I^{-1}(x)$, $\frac{d\eta_\infty}{dx}(x) \propto h_0(x)h_I(x)$, and $\frac{d\mu}{dx}(x) \propto h_I^2(x)$ are bounded with exponential fall-off. The result follows then from proposition 3.5. □

This latter case could be generalized to non-continuous potentials V_0 lying locally in the Kato class (see [5]).

1.2. Convergence of semi-groups in the uniform sense. We define the non-linear propagator associated to η_t by

$$\Phi_{t,T}(\nu) = \frac{\nu P^V_{T-t}}{\nu P^V_{T-t}(1)} \in \mathcal{P}(E) .$$

By the semi-group property, it verifies the propagation equation $\eta_T = \Phi_{t,T}(\eta_t)$.

In this subsection, we give an assumption for the uniform convergence of $P_t^{V-\lambda}$ and its consequence for the stability of $\Phi_{t,T}$. This will be crucial for the stability of the particle approximation. The only assumption we need is the following:

[1] consider theorem 4.7 and 4.19 of [5], and an integration by part between $\frac{\Delta}{2}h_0$ and positive solutions of the Dirichlet Boundary Value Problem.

Assumption 2. *V is bounded above and there is an $\epsilon > 0$ such that the subset $K_\epsilon = \{x \in E \mid V(x) - \lambda \geq -\epsilon\}$ is relatively compact in E.*

This is a natural physical assumption, which ensures that h is a "strict bound" state in the sense that V is a strict potential barrier outside some compact set.
We then have:

Proposition 1.2. *Under assumptions 1 and 2, the Feynman-Kac semi-group is uniformly exponentially converging, in the sense that there is some $C \geq 0$ and $0 < \rho < 1$ such that for any test function φ,*

$$\|P_t^{V-\lambda}(\varphi) - h\mu(h\varphi)\|_\infty \leq \|\varphi\|_\infty C\rho^t \ .$$

Proof. We use the results developed by R.L. Tweedie and its collaborators for instance in [6]. We consider the following strong Feller irreducible Markov diffusion semi-group

$$P_t^h(\varphi) = h^{-1}P_t^{V-\lambda}(h\varphi) \ ,$$

its associated diffusion process X_t^h, and its extended generator $L^h = h^{-1}(L + V - \lambda)(h.)$, reversible with respect to $h^2(x)\mu(dx)$. We show that h^{-1} is a strict Lyapounov function for L^h outside $\bar{K}_\epsilon$ (in the sense of condition $(\tilde{\mathcal{D}})$ of [6]). Indeed we have that:

1. $\bar{K}_\epsilon$ is compact and thus is a petite set for X_t^h (see [13] theorem 7.1 and 5.1).
2. $L^h(h^{-1}) + \epsilon h^{-1} = (V - \lambda + \epsilon)h^{-1}$ is bounded on $\bar{K}_\epsilon$ and negative outside.

So by theorem 5.2 of [6], X_t^h is h^{-1}-uniformly ergodic which means that:

$$\sup_{|g|\leq h^{-1}} |P_t^h(g)(x) - \mu(h^2 g)| \leq h^{-1}(x)C\rho^t \ ,$$

and gives the result for $\varphi = gh$. □

We then harvest the uniform stability of $\Phi_{t,T}$:

Corollary 1.3. *Under assumption 1 and 2, we have for some $C \geq 0$, $0 < \rho < 1$ and any $\nu \in \mathcal{P}(E)$*

$$|\Phi_{t,T}(\varphi)(\nu) - \eta_\infty(\varphi)| \leq \|\varphi\|_\infty \frac{C}{\nu(h)}\rho^{T-t} \ .$$

Proof. We take $\|\varphi\|_\infty \leq 1$ and use the Landau symbol "O" uniformly with respect to t, T, ν and φ. From proposition 1.2 we get

$$\begin{aligned}\Phi_{t,T}(\varphi)(\nu) = \frac{\nu P_{T-t}^{V-\lambda}(\varphi)}{\nu P_{T-t}^{V-\lambda}(1)} &= \frac{\nu(h)\mu(h\varphi) + O(\rho^{T-t})}{\nu(h)\mu(h) + O(\rho^{T-t})} \\ &= \frac{\mu(h\varphi) + O(\frac{\rho^{T-t}}{\nu(h)})}{\mu(h) + O(\frac{\rho^{T-t}}{\nu(h)})} \ ,\end{aligned}$$

which gives the result. □

1.3. A last assumption. To construct the particle system and carry out the long time analysis, we will need some more boundedness and regularity hypotheses:

Assumption 3.

1. *V is continuous and bounded*
2. *$\ln h$ is continuous and bounded*

3. *For* $\varphi \in \mathcal{C}_b^\infty(E)$*,* $(t,x) \mapsto P_t^V(\varphi)(x)$ *is* $\mathcal{C}_b^{1,2}(E \times \mathbb{R}^+)$

Remark 1.4. $\mathcal{C}_b^{1,2}(E \times \mathbb{R}^+)$ denotes bounded continuous functions of E with continuous first time derivative and continuous twice space derivatives. The regularity assumption is probably necessary only for intermediate technical purpose.
The second assumption could be replaced by $\sup_{t,N} \mathbb{E}\left(\frac{1}{(\eta_t^N(h))^p}\right) < +\infty$.
The regularity of $P_t^V(\varphi)$ and V gives the backward Fokker-Planck equation in a pointwise sense:

LEMMA 1.5. *For all* $\varphi \in \mathcal{C}_b^\infty(E)$*, we have*

$$\begin{aligned}\partial_t P_{T-t}^V(\varphi) &= -P_{T-t}^V(L(\varphi) + V\varphi) \\ &= -L(P_{T-t}^V(\varphi)) + V P_{T-t}^V(\varphi) \ .\end{aligned}$$

2. The Interacting Particle System approximation.

2.1. The generator of the IPS. In this subsection, we design the interacting particle interpretation of the flow $(\eta_t)_{t\geq 0}$, with initial probability $\eta_0 \in \mathcal{P}(E)$. The bounded potential being given, we first consider two continuous bounded applications $(\mathcal{P}(E), \text{weak topology}) \to (\mathcal{C}_b(E), \| \ \|_\infty)$, whose images are nonnegative functions denoted

$$\eta \mapsto V_\eta^b \geq 0 \ , \quad \eta \mapsto V_\eta^d \geq 0$$

and verifying

$$V_\eta^b(x) - V_\eta^d(x) = V(x) + C_\eta \ ,$$

where C_η does not depend on x (as explained in section 2.2, “b” stands for “birth” and “d” for “death”).
We define:

$$V_\eta^* = V_\eta^b + V_\eta^d \ .$$

Example 2.1. Here are several possible choices of the above functions:

1. $V^b = 0 \ , \quad V^d = \sup(V) - V$ (as in the abstract)
2. $V^b = V^+ \ , \quad V^d = V^-$
3. $V_\eta^b = (V - \eta(V))^+ \ , \quad V_\eta^d = (V - \eta(V))^-$

The last choice is of fundamental importance since it is invariant by the transformation $V \mapsto V + C$ which leaves η_t invariant.

Recall from (0.2) that η_t satisfies the following fundamental non-linear Markovian evolution equation

$$\partial_t \eta_t(\varphi) = \eta_t(L_{\eta_t}(\varphi)) \ ,$$

but here the non-linear Markov generator is more generally defined by

$$L_\eta(\varphi)(x) = L(\varphi)(x) + \int (\varphi(y) - \varphi(x))(V_\eta^b(y) + V_\eta^d(x))\, \eta(dy) \ .$$

Indeed we have that

$$\begin{aligned}\eta(L_\eta(\varphi)) &= \eta(L(\varphi)) + \eta(V_\eta^b \varphi) - \eta(V_\eta^d \varphi) + \eta(V_\eta^d)\eta(\varphi) - \eta(V_\eta^b)\eta(\varphi) \\ &= \eta(L(\varphi) + V\varphi) - \eta(\varphi)\eta(V) \ .\end{aligned}$$

If A is a linear operator, the associated formal "carré du champ" Γ_A is a bilinear operator defined by

$$\Gamma_A(\varphi,\varphi) = A(\varphi^2) - 2\varphi A(\varphi).$$

Recall that when A is the generator of a Markov process X_t, $\Gamma_A(\varphi,\varphi) \geq 0$ and $\int_0^t \Gamma_A(\varphi,\varphi)(X_s)ds$ is the predictable quadratic variation of the martingale part of $\varphi(X_t)$.
We can define then

$$\begin{aligned}\Gamma_{L_\eta}(\varphi,\varphi)(x) = {} & \Gamma_L(\varphi,\varphi)(x) \\ & + \int (\varphi(y)-\varphi(x))^2 (V_\eta^b(y) + V_\eta^d(x))\eta(dy) \ ,\end{aligned}$$

and remark that

$$\begin{aligned}\eta(\Gamma_{L_\eta}(\varphi,\varphi)) &= \eta(\Gamma_L(\varphi,\varphi)) + \eta(\varphi^2 V_\eta^*) + \eta(\varphi^2)\eta(V_\eta^*) - 2\eta(V_\eta^*\varphi)\eta(\varphi) \\ &= \eta(\Gamma_L(\varphi,\varphi)) + \eta\left((\varphi-\eta(\varphi))^2(V_\eta^* + \eta(V_\eta^*))\right) \ .\end{aligned}$$

We now consider the interacting particle model $(\xi_t)_{t\in\mathbb{R}^+}$ associated to the nonlinear operator L_η as defined in the introduction by its initial law $\eta_0^{\otimes N}$ and its Markov generator $\mathcal{L}$ given in (0.3). The IPS is a Markov process resulting of a bounded jump perturbation of N independent copies of X_t, and thus is well defined.
When we use as a test function the empirical mean $m(.)(\varphi) \in \mathcal{C}_b^\infty(E^N)$ of a $\varphi \in \mathcal{C}_b^\infty(E)$, we have the following simple form of the generator and its associated carré-du-champs:

Lemma 2.2.

$$\mathcal{L}(m(.)(\varphi)) = m(.)(L_{m(.)}(\varphi))$$

$$\Gamma_\mathcal{L}(m(.)(\varphi), m(.)(\varphi)) = \frac{1}{N} m(.)(\Gamma_{L_{m(.)}}(\varphi,\varphi)).$$

Proof. The first identity is by definition. The second one is a straightforward formal computation. We use the linearity of $A \mapsto \Gamma_A$ to get

$$\Gamma_\mathcal{L}(\psi,\psi) = \sum_{i=1}^N \Gamma^{(i)}_{L_{m(.)}}(\psi,\psi) \ ,$$

and since $L_\eta(\text{constant}) = 0$, for any $\xi \in E^N$, we have

$$\begin{aligned}\Gamma^{(i)}_{L_{m(\xi)}}(m(.)(\varphi), m(.)(\varphi))(\xi) &= \frac{1}{N^2} 2 \sum_{j\neq i} \varphi(\xi^j) L_{m(\xi)}(\varphi)(\xi^i) + \frac{1}{N^2} L_{m(\xi)}(\varphi^2)(\xi^i) \\ &\qquad - 2\left(\frac{1}{N}\sum_j \varphi(\xi^j)\right)\frac{1}{N} L_{m(\xi)}(\varphi)(\xi^i) \\ &= \frac{1}{N^2}\Gamma^{(i)}_{m(\xi)}(\varphi,\varphi)(\xi^i) \ ,\end{aligned}$$

and the result follows. ∎

Now we can state our key tool:
PROPOSITION 2.3. *For all $\varphi_. \in \mathcal{C}_b^{1,2}(E \times \mathbb{R}^+)$, the process*

$$\mathcal{M}_t(\varphi_.) = \eta_t^N(\varphi_t) - \eta_0^N(\varphi_0) - \int_0^t \eta_s^N \left(\partial_s \varphi_s + L_{\eta_s^N}(\varphi_s)\right) ds$$

is a local martingale, with predictable quadratic variation given by

$$\left\langle \mathcal{M}(\varphi_.)\right\rangle_0^t = \frac{1}{N}\int_0^t \eta_s^N \left(\Gamma_{L_{\eta_s^N}}(\varphi_s, \varphi_s)\right) ds \ ,$$

and jumps estimated by

$$|\Delta \mathcal{M}_t(\varphi_.)| \leq \frac{2\|\varphi_t\|}{N} \ .$$

We recall that

$$\eta_s^N(L_{\eta_s^N}(\varphi)) = \eta_s^N \left(L(\varphi) + (V - \eta_s^N(V))\varphi\right)$$

and

$$\eta_s^N(\Gamma_{L_{\eta_s^N}}(\varphi, \varphi)) = \eta_s^N(\Gamma_L(\varphi, \varphi)) + \eta_s^N \left((\varphi - \eta_s^N(\varphi))^2 (V^*_{\eta_s^N} + \eta_s^N(V^*_{\eta_s^N}))\right) \ .$$

Proof. This is a particular case of the usual martingale problem associated to the Markov process ξ_t. The statement can be proved with a standard application of Itô formula, with Markov property arguments for the jump part.
The estimate on the jumps follows from the fact that each jump concerns only one particle (see the probabilistic construction in subsection 2.2). □

From the above proposition we immediately get the stochastic differential equation

$$d\eta_t^N(\varphi) = \eta_t^N(L_{\eta_t^N}(\varphi))dt + d\mathcal{M}_t(\varphi) \ ,$$

which is a perturbation of the equation (0.2) of the dynamic of η_t by a martingale whose jumps and predictable quadratic variation of order $\frac{1}{N}$. In this sense, we already see that η_t^N is a natural approximation of the flow η_t. Of course, this point of view is to elementary to enable an asymptotic analysis mainly because of the non-linearity of (0.2).

2.2. Probabilistic construction and genetic interpretation. We start with a more explicit expression for the IPS generator:

PROPOSITION 2.4. *We have $\mathcal{L} = \mathcal{L}^{mut} + \mathcal{L}^{sel}$ with the pair mutation/selection generators defined by*

$$\begin{aligned}
\mathcal{L}^{mut}(\psi)(\xi) &= \sum_{i=1}^N L^{(i)}(\psi)(\xi) \\
\mathcal{L}^{sel}(\psi)(\xi) &= \sum_{i=1}^N \ V^d_{m(\xi)}(\xi^i)\frac{1}{N}\sum_{j=1}^N (\psi(\xi^{i\to j}) - \psi(\xi)) \\
&\quad + \sum_{i=1}^N \ V^b_{m(\xi)}(\xi^i)\frac{1}{N}\sum_{j=1}^N (\psi(\xi^{j\to i}) - \psi(\xi)) \ ,
\end{aligned}$$

where if $\xi' = \xi^{i\to j}$ *then* $\xi'^k = \xi^k$ *except for* $k = i$ *where* $\xi'^i = \xi^j$.

Proof. The jump part of $\mathcal{L}$ is by definition

$$\mathcal{L}^{\text{sel}}(\psi)(\xi) = \sum_{i=1}^{N} V^d_{m(\xi)}(\xi^i)(\frac{1}{N}\sum_{j=1}^{N}\psi(\xi^{i\to j}) - \psi(\xi)) + \sum_{i=1}^{N}\frac{1}{N}\sum_{j=1}^{N} V^b_{m(\xi)}(\xi^j)(\psi(\xi^{i\to j}) - \psi(\xi)) \ ,$$

and the result follows by exchanging the indexes i and j in the second part of the right hand side of the identity. ∎

Thus the N walkers evolve according to the following birth and death mechanism, for any $i \in [1, N]$ ($\tau^{d/b,i}_{n+1}$ designing independent exponential clocks of mean 1):

1. Between each jump time, the walkers evolve independently according to the mutation generator L.

2. At random times $T^{d,i}_n$ defined by $\int_{T^{d,i}_n}^{T^{d,i}_{n+1}} V^d_{\eta^N_s}(\xi^i_s)ds = \tau^{d,i}_{n+1}$, a walker is uniformly randomly chosen, and the i-th walker then jumps to its location.

3. At random times $T^{b,i}_n$ defined by $\int_{T^{b,i}_n}^{T^{b,i}_{n+1}} V^b_{\eta^N_s}(\xi^i_s)ds = \tau^{b,i}_{n+1}$, a walker is uniformly randomly chosen, and then jumps to the location of the i-th walker.

This explains how the selection generator tends to "get rid of" walkers with relatively high potential $V^d_{\eta^N_t}$, and tends to "reproduce" walkers with relatively high potential $V^b_{\eta^N_t}$. The effect of selection being then to favor walkers with relatively high potential $V = V^b_{\eta^N_t} - V^d_{\eta^N_t} - C_{\eta^N_t}$. In this sense, the IPS can be seen as a continuous time genetic algorithm with fitness function V and mutations of generator L.
Moreover this structure enables a nice parallelized implementation, where walkers are individually collecting information from V, but yet learns globally the structure of the ground state h.
In practice, one may use some Euler discretization scheme, and may approximate integrals with sums. This requires at least the continuity of the potential V.

3. Long time behavior of the IPS.

3.1. Non-asymptotic control. We give directly the main theoretical results of this paper, the proof being postponed to section 4:

THEOREM 3.1 (Time-uniform $\mathbb{L}^p$ estimate). *We suppose that assumptions 1, 2 and 3 are verified.*
There are constants C_p *such that, for all test function* $\varphi \in \mathcal{C}_b(E)$ *with* $\|\varphi\|_\infty \leq 1$

$$\sup_{T\geq 0} \mathbb{E}\big(|\eta^N_T(\varphi) - \eta_T(\varphi)|^p\big)^{1/p} \leq \frac{C_p}{\sqrt{N}} \ .$$

and

THEOREM 3.2 (Bias estimate/Time-uniform convergence of a particle). *We suppose that assumptions 1, 2 and 3 are verified.*
There is a constant C *such that, for all* $\varphi \in \mathcal{C}_b(E)$ *with* $\|\varphi\|_\infty \leq 1$*:*

$$\sup_{T\geq 0} \big|\mathbb{E}\big(\eta^N_T(\varphi)\big) - \eta_T(\varphi)\big| \leq \frac{C}{N} \ ,$$

$$\sup_{T\geq 0} \| Law(\xi_T^i) - \eta_T \|_{tv} \leq \frac{C}{N} \ .$$

Remark 3.3. One can easily show that the particle system ξ_t is recurrent and ergodic. If the invariant measure is finite, it converges in law to a random variable ξ_∞ (this always happens when E is compact). η_∞^N is then the natural estimator of η_∞ and we have the almost sure convergence

$$\eta_\infty^N \xrightarrow[N\to+\infty]{a.s.} \eta_\infty \quad \text{in the weak topology}$$

which follows the $\mathbb{L}^p$ estimate for $p = 4$ with a Borel-Cantelli argument.
This situation is probably true in general for N large enough, although the positivity seems difficult to prove. Anyway, one can take for η_∞^N any adherent limit (which is a positive measure) of η_t^N under the weak topology of evanescent functions.

We want to lay the emphasis on the difficulty of the proof of these results, which comes from the non-linear propagation of the error made by the particle approximation.

We also propose an asymptotic study of the standard deviation:

3.2. Long time asymptotic standard deviation. The asymptotic standard deviation gives a quantitative information of the IPS approximation. We show in proposition 3.5 that the latter is likely to remain bounded in many mild situations of interest.

Theorem 3.4. *Under assumptions 1, 2 and 3, we have for any $\varphi \in \mathcal{C}_b(E)$ ($\bar\varphi = \varphi - \eta_\infty(\varphi)$)*

$$\begin{aligned}&\lim_{N\to+\infty} \overline{\lim_{T\to+\infty}} N\mathbb{E}\left((\eta_T^N(\varphi) - \eta_\infty(\varphi))^2\right)\\ &= Ad^2(\varphi) = \eta_\infty(\bar\varphi^2) + 2\int_0^{+\infty} \eta_\infty\left(P_s^{V-\lambda}(\bar\varphi)^2(V_{\eta_\infty}^b + \eta_\infty(V_{\eta_\infty}^d))\right) ds \ .\end{aligned}$$

Note that by proposition 1.2, the local noise introduced by interactions

$$s \mapsto \eta_\infty\left(P_s^{V-\lambda}(\bar\varphi)^2(V_{\eta_\infty}^b + \eta_\infty(V_{\eta_\infty}^d))\right)$$

is exponentially decreasing with s.

We're interested at clarifying this quantity for the meaningful case $\varphi = V$, which corresponds to the eigenvalue estimation. We will take $V_\eta^b = (V - \eta(V))^+$ and $V_\eta^d = (V - \eta(V))^-$.

Proposition 3.5. *Under assumption 1 only, we have*

$$Ad^2(V) \leq \eta_\infty((V-\lambda)^2) + \frac{1}{\lambda^*}\left\| \frac{d\eta_\infty}{d\mu} \times \left((V-\lambda)^+ + \eta_\infty((V-\lambda)^-)\right)\right\|_\infty \mu((V-\lambda)^2) \ .$$

Proof. Since $\bar\varphi = \varphi - \eta_\infty(\varphi)$ is orthogonal to h in $\mathbb{L}^2(\mu)$, we have by spectral theory: $\mu(P_t^{V-\lambda}(\bar\varphi)^2) \leq e^{-2\lambda^* t}\mu(\bar\varphi^2)$. The result follows from theorem 3.4 for $\varphi = V$ with $\eta_\infty(V) = \lambda$. ∎

When $\frac{d\eta_\infty}{d\mu} = \frac{h}{\mu(h)}$ is bounded with exponential fall-off, this upper bound is expected to remain finite in almost any situation of interest (see the third example of section 1.1).

4. Proofs. In all this section we will use the following notations:

1. $T > 0$ will be a deterministic horizon time and we will take $t \in [0, T]$.
2. $n \geq 0$ $p \geq 1$ are integers.
3. $\| \ \|$ is the uniform norm.
4. $\varphi \in \mathcal{C}_b^\infty(E)$ is a test function such that $\|\varphi\| \leq 1$, and $\bar{\varphi} = \varphi - \eta_T(\varphi)$.
5. $C > 0$ a constant independent of test functions, of the time parameters t, T and of the number of particles N. In the same spirit, we will use the Landau notation "O" uniformly with these variables. Note: The constant C and the "O" notation may depend on integers n and p.

We recall that $\|V\| \leq C$ and $\sup_\eta \|V^*_\eta\| \leq C$.

The proofs are based on the use of a "linearized" version of the propagator of η_t defined by

$$Q_{t,T}(\varphi) = \frac{P^V_{T-t}(\varphi)}{\eta_t P^V_{T-t}(1)}$$

which verifies the propagation equation

$$\eta_T(\varphi) = \eta_t Q_{t,T}(\varphi) \ .$$

The main idea is to analyze the martingale part and the predictable part of the process $t \mapsto \eta^N_t Q_{t,T}(\bar{\varphi})$ for $\bar{\varphi} = \varphi - \eta_T(\varphi)$. Because we have $\eta_t(Q_{t,T}(\bar{\varphi})) = 0$, it can be interpreted as a stochastic perturbation of the identically null process. Note that $\eta^N_T(Q_{T,T}(\bar{\varphi})) = \eta^N_T(\varphi) - \eta_T(\varphi)$ which is the quantity we wish to control when $T \to +\infty$.

In computations, the test function φ will be omitted to lighten.

Throughout these proofs, we will use the following stability results:

Lemma 4.1. *The propagator $Q_{t,T}$ verify the following properties: n being given, there is a C such that for any test function φ*

$$\|Q_{t,T}(\varphi)\| \leq C$$
$$\int_t^T \|Q_{s,T}(\varphi)\|^{2^n} ds \leq C(T - t) \ .$$

Moreover there is some $0 < \rho < 1$ such that for any $\bar{\varphi} = \varphi - \eta_T(\varphi)$

$$\|Q_{t,T}(\bar{\varphi})\| \leq C\rho^{T-t}$$
$$\int_t^T \|Q_{s,T}(\bar{\varphi})\|^{2^n} ds \leq C \ .$$

Proof. First we write

$$Q_{t,T}(\varphi) = \frac{P^{V-\lambda}_{T-t}(\varphi)(x)}{\eta_t P^{V-\lambda}_{T-t}(1)} \ .$$

We claim that

$$\frac{1}{\eta_t P^{V-\lambda}_{T-t}(1)} \leq C \ .$$

Indeed by definition and semi-group property we have $\eta_t P^{V-\lambda}_{T-t}(1) = \frac{\eta_0 P^{V-\lambda}_T(1)}{\eta_0 P^{V-\lambda}_t(1)}$, and $t \mapsto \eta_0 P^{V-\lambda}_t(1)$ is continuous, positive, and goes from 1 to $\eta_0(h)\mu(h) > 0$.

By proposition 1.2, we get then for any φ: $\|Q_{t,T}(\varphi)\| \leq C$.
For $\bar{\varphi} = \varphi - \eta_T(\varphi)$ we use the decomposition

$$|Q_{t,T}(\bar{\varphi})| = \frac{1}{(\eta_t P_{T-t}^{V-\lambda}(1))^2} |\eta_t P_{T-t}^{V-\lambda}(1) P_{T-t}^{V-\lambda}(\varphi) - \eta_t P_{T-t}^{V-\lambda}(\varphi) P_{T-t}^{V-\lambda}(1)| \ ,$$

and again proposition 1.2 gives a $0 < \rho < 1$ such that for any $\bar{\varphi}$: $\|Q_{t,T}(\bar{\varphi})\| \leq C\rho^{T-t}$.
□

Note the control on the initial error:
LEMMA 4.2. *We have for any φ*

$$\mathbb{E}((\eta_0^N(\varphi) - \eta_0(\varphi))^p) \leq \frac{C}{N^{p/2}} \ .$$

Proof. Since, at time $t = 0$, all particles are sampled independently with law η_0, $\eta_0^N(\varphi)$ is a sum of N zero-mean i.i.d. variables. The result is then Burkholder-Davies-Gundy inequality for i.i.d. variables. □

4.1. Precise L^p-estimate of the key martingales. We want to apply proposition 2.3 to the collection $(Q_{t,T}(\varphi)^{2^n})_{n\geq 0} \equiv (Q_{t,T}^{2^n})_{n\geq 0}$. Recall that $\eta_t(P_{T-t}^V(1)) = \frac{\eta_0 P_T^V(1)}{\eta_0 P_t^V(1)}$ and so

$$\begin{aligned}
\partial_t \eta_t \left(P_{T-t}^V(1)\right) &= -\frac{\eta_0 P_T^V(1)}{\eta_0 P_t^V(1)^2} \eta_0 P_t^V(V) \\
&= -\eta_t \left(P_{T-t}^V(1)\right) \eta_t(V) \ ,
\end{aligned}$$

this yields using lemma 1.5

$$\begin{aligned}
\partial_t Q_{t,T} &= -L(Q_{t,T}) - VQ_{t,T} + \frac{1}{\eta_t(P_{T-t}^V(1))^2} \eta_t \left(P_{T-t}^V(1)\right) \eta_t(V) \\
&= -L(Q_{t,T}) - (V - \eta_t(V))Q_{t,T} \ ,
\end{aligned}$$

and

$$\partial_t Q_{t,T}^{2^n} = -2^n Q_{t,T}^{2^n-1} L(Q_{t,T}) - 2^n Q_{t,T}^{2^n} \times (V - \eta_t(V)) \ .$$

From proposition 2.3, we obtain a collection of difference of martingales between t and T indexed by n:

$$\begin{aligned}
\mathcal{M}_t^T(Q_{.,T}^{2^n}) &= \mathcal{M}_T(Q_{.,T}^{2^n}) - \mathcal{M}_t(Q_{.,T}^{2^n}) \\
&= \eta_T^N(Q_{T,T}^{2^n}) - \eta_t^N(Q_{t,T}^{2^n}) - \int_t^T \eta_s^N \left(L(Q_{s,T}^{2^n}) - 2^n Q_{s,T}^{2^n-1} L(Q_{s,T})\right) ds \\
&\quad - \int_t^T \eta_s^N \left(Q_{s,T}^{2^n} \times \left(V - \eta_s^N(V) - 2^n(V - \eta_s(V))\right)\right) ds \qquad (4.1)
\end{aligned}$$

with predictable quadratic variation given by

$$\begin{aligned}
&N\langle \mathcal{M}(Q_{.,T}^{2^n})\rangle_t^T = \\
&\int_t^T \eta_s^N \left(\Gamma_L\left(Q_{s,T}^{2^n}, Q_{s,T}^{2^n}\right)\right) + \eta_s^N \left(\left(Q_{s,T}^{2^n} - \eta_s^N(Q_{s,T}^{2^n})\right)^2 \left(V^* + \eta_s^N(V^*)\right)\right) ds \ . \quad (4.2)
\end{aligned}$$

We can get rid of the carré du champs term and get the following bounds up to a martingale:

LEMMA 4.3. *For all $n \geq 0$ and any test function φ we have*

$$N\big\langle \mathcal{M}(Q^{2^n}_{.,T}(\varphi))\big\rangle_t^T \leq C(T-t+1) - \mathcal{M}_t^T(Q^{2^{n+1}}_{.,T}(\varphi)) \ ,$$

and for any centered test function $\bar\varphi = \varphi - \eta_T(\varphi)$

$$N\big\langle \mathcal{M}(Q^{2^n}_{.,T}(\bar\varphi))\big\rangle_t^T \leq C - \mathcal{M}_t^T(Q^{2^{n+1}}_{.,T}(\bar\varphi)) \ .$$

Proof. The formal carré-du-champs upper bound (lemma 5.1) gives

$$\int_t^T \eta_s^N\left(\Gamma_L(Q^{2^n}_{s,T}, Q^{2^n}_{s,T})\right) ds \leq \quad (= \text{ for } n=0)$$
$$\int_t^T \eta_s^N\left(L(Q^{2^{n+1}}_{s,T}) - 2^{n+1}Q^{2^{n+1}-1}_{s,T}L(Q_{s,T})\right) ds \ .$$

From (4.2), we use the above inequality and (4.1) at rank $n+1$ to find the upper bound

$$\begin{aligned} N\big\langle \mathcal{M}(Q^{2^n}_{.,T})\big\rangle_t^T \overset{(= \text{ for } n=0)}{\leq} & -\mathcal{M}_t^T(Q^{2^{n+1}}_{.,T}) + \eta_T^N(Q^{2^{n+1}}_{T,T}) - \eta_t^N(Q^{2^{n+1}}_{t,T}) \\ & - \int_t^T \eta_s^N\left(Q^{2^{n+1}}_{s,T}\big(V - \eta_s^N(V) - 2^{n+1}(V - \eta_s(V))\big)\right) ds \\ & + \int_t^T \eta_s^N\left(\big(Q^{2^n}_{s,T} - \eta_s^N(Q^{2^n}_{s,T})\big)^2\big(V^* + \eta_s^N(V^*)\big)\right) ds \ . \end{aligned} \tag{4.3}$$

The result follows then from lemma 4.1. ∎

The case $n = 0$ is of crucial importance. From (4.1) or proposition 2.3 we can get

$$d\eta_t^N(Q_{t,T}) = d\mathcal{M}_t(Q_{.,T}) + \big(\eta_s(V) - \eta_s^N(V)\big)\,\eta_s^N(Q_{s,T})ds \ , \tag{4.4}$$

which gives for centered test functions, by integrating on $[0,T]$,

$$\begin{aligned} \eta_T^N(\varphi) - \eta_T(\varphi) = & \ \eta_0^N(Q_{0,T}(\bar\varphi)) + \mathcal{M}_T(Q_{.,T}(\bar\varphi)) \\ & + \int_0^T \big(\eta_s(V) - \eta_s^N(V)\big)\big(\eta_s^N(Q_{s,T}(\bar\varphi)) - \eta_s(Q_{s,T}(\bar\varphi))\big) ds \ . \end{aligned} \tag{4.5}$$

The martingale part and the initial error $\eta_0^N(Q_{0,T}(\bar\varphi))$ is expected to be of order $\frac{1}{\sqrt{N}}$, and the predictable part of order $\frac{1}{N}$.

Note that by developing the right hand side of (4.3) with the identity $V = V^b_{\eta_s^N} - V^d_{\eta_s^N} + C_{\eta_s^N}$, the predictable quadratic variation of the martingale gives

$$\begin{aligned} N\big\langle \mathcal{M}(Q_{.,T})\big\rangle_0^T = & -\mathcal{M}_T(Q^2_{.,T}) + \eta_T^N(Q^2_{T,T}) - \eta_0^N(Q^2_{0,T}) \\ & +2\int_0^T \eta_s^N(Q^2_{s,T}V^b_{\eta_s^N}) + \eta_s^N(Q^2_{s,T})\eta_s(V^d_{\eta_s^N}) \\ & -\eta_s^N(Q_{s,T})\eta_s^N(Q_{s,T}V^*_{\eta_s^N}) + \eta_s^N(Q^2_{s,T})\big(\eta_s^N(V^b_{\eta_s^N}) - \eta_s(V^b_{\eta_s^N})\big) ds \ . \end{aligned} \tag{4.6}$$

We can now state the first result of this section, which is the control of all moments of these martingales:

THEOREM 4.4. *For all $p \geq 1$, all $n \geq 0$ and all test functions φ,*

$$\mathbb{E}\left(\left(\left[\mathcal{M}(Q^{2^n}_{\cdot,T}(\varphi)\right]^T_t\right)^p\right) \leq \frac{C(T-t+1)^p}{N^p} ,$$

and for centered test functions $\bar{\varphi}$,

$$\mathbb{E}\left(\left(\left[\mathcal{M}(Q^{2^n}_{\cdot,T}(\bar{\varphi})\right]^T_t\right)^p\right) \leq \frac{C}{N^p} .$$

Proof. Note that by localization, we can suppose that we work with bounded martingales.
Thanks to Jensen inequality, it is sufficient to prove the inequalities for all $p = 2^q$. We are going to use an induction on q to prove that

$$\begin{aligned}
&\forall n \geq 0, \\
&\quad \mathbb{E}\left(\left(\langle\mathcal{M}(Q^{2^n}_{\cdot,T})\rangle^T_t\right)^{2^q}\right) \leq \frac{C(T-t+1)^{2^q}}{N^{2^q}} \\
&\quad \mathbb{E}\left(\left(\left[\mathcal{M}(Q^{2^n}_{\cdot,T})\right]^T_t\right)^{2^q}\right) \leq \frac{C(T-t+1)^{2^q}}{N^{2^q}} .
\end{aligned}$$

For $q = 0$, these inequalities are a direct consequence of lemma 4.3.
Suppose the inequality true at order q and lower. Again from lemma 4.3, we get

$$\begin{aligned}
&\mathbb{E}\left(N^{2^{q+1}}\left(\langle\mathcal{M}(Q^{2^n}_{\cdot,T})\rangle^T_t\right)^{2^{q+1}}\right) \\
&\qquad \leq C(T-t+1)^{2^{q+1}} + C\mathbb{E}\left(\mathcal{M}^T_t(Q^{2^{n+1}}_{\cdot,T})^{2^{q+1}}\right) \\
&\qquad \leq C(T-t+1)^{2^{q+1}} + C\mathbb{E}\left(\left(\left[\mathcal{M}(Q^{2^{n+1}}_{\cdot,T})\right]^T_t\right)^{2^q}\right) \quad \text{(by BDG inequality).}
\end{aligned}$$

By induction, this proves the first upper bound at rank $q+1$.
Now we use the alternate BDG inequality stated in lemma 5.2 to the martingale $\mathcal{M}(Q^{2^n}_{\cdot,T})$, whose jumps verify by proposition 2.1: $a \leq \frac{2\|Q^{2^n}_{t,T}\|}{N} \leq \frac{C}{N}$. This gives

$$\mathbb{E}\left(\left(\left[\mathcal{M}(Q^{2^n}_{\cdot,T})\right]^T_t\right)^{2^{q+1}}\right) \leq C\sum_{k=0}^{q+1}\frac{1}{N^{2^{q+2}-2^{k+1}}}\mathbb{E}\left(\left(\langle\mathcal{M}(Q^{2^n}_{\cdot,T})\rangle^T_t\right)^{2^k}\right) .$$

By induction,

$$\begin{aligned}
\mathbb{E}\left(\left(\left[\mathcal{M}(Q^{2^n}_{\cdot,T})\right]^T_t\right)^{2^{q+1}}\right) &\leq C\sum_{k=0}^{q+1}\frac{(T-t)^{2^k}}{N^{2^{q+2}-2^{k+1}+2^k}} \\
&\leq \frac{C(T-t)^{2^{q+1}}}{N^{2^{q+1}}} ,
\end{aligned}$$

which proves the second upper bound at rank $q+1$.
The case of centered test functions is identical. ∎

Remark 4.5. Some results of [7] use $\mathbb{L}^p$ estimates of a similar martingales (lemma 3.23) whose proof is using Itô formula but may be incorrect. Resorting to Itô formula seems to be intractable, and the techniques used for theorem 4.4 enable to clarify these results.

4.2. Proof of theorem 3.1. First of all let's define the following quantity:

$$I_p(N) = \sup_{T,\varphi} \mathbb{E}\left((\eta_T^N(\varphi) - \eta_T(\varphi))^p\right) \ .$$

In this subsection, we will prove the time-uniform estimate: $I_p(N) \leq \frac{C}{N^{p/2}}$. And before, we start with our first key lemma:

LEMMA 4.6. *There is an $\epsilon > 0$ independent of p such that*

$$I_p(N) \leq \frac{C}{N^{\epsilon p/2}} \ .$$

Proof. Let's fix T and use the decomposition

$$\eta_T^N(\varphi) - \eta_T(\varphi) = \underbrace{\eta_T^N(\varphi) - \Phi_{t,T}(\eta_t^N)(\varphi)}_{a(t)} + \underbrace{\Phi_{t,T}(\eta_t^N)(\varphi) - \eta_T(\varphi)}_{b(t)} \ .$$

$a(t)$ can be controlled by the stochastic errors made by the particle approximation between t and T. $b(t)$ can be controlled by the stability property of the limiting propagator Φ between t and T. $b(0)$ can also be controlled by the error made by the initial condition. We then optimize the whole in t.

Control of $a(t)$. Let us define the continuous finite variation process

$$A_{t_1}^{t_2} = \exp\left(\int_{t_1}^{t_2} (\eta_s^N(V) - \eta_s(V))ds\right) \ .$$

An elementary integration by parts for $s \in [t,T]$ gives

$$\begin{aligned} d\big(A_t^s\, \eta_s^N(Q_{s,T})\big) &= \eta_s^N(Q_{s,T})\, A_t^s\, (\eta_s^N(V) - \eta_s(V))\, ds \\ &\quad + A_t^s\, d\eta_s^N(Q_{s,T}) \\ &= A_t^s\, d\mathcal{M}_s(Q_{.,T}) \quad \text{(by (4.4))}. \end{aligned}$$

Integrating from t to T and simplifying by $(A_t^T)^{-1}$ gives

$$\eta_T^N(\varphi) - (A_t^T)^{-1}\eta_t^N(Q_{t,T}(\varphi)) = (A_t^T)^{-1} \int_t^T A_t^s\, d\mathcal{M}_s(Q_{.,T}(\varphi)) \ . \tag{4.7}$$

Now, recalling that $\Phi_{t,T}(\eta_t^N)(\varphi) = \frac{(A_t^T)^{-1}\eta_t^N(Q_{t,T}(\varphi))}{(A_t^T)^{-1}\eta_t^N(Q_{t,T}(1))}$, we write $a(t)$ as follows:

$$a(t) = \eta_T^N(\varphi) - (A_t^T)^{-1}\eta_t^N(Q_{t,T}(\varphi)) - \Phi_{T-t}(\eta_t^N)(\varphi)\big(1 - (A_t^T)^{-1}\eta_t^N(Q_{t,T}(1))\big) \ ,$$

which using (4.7) gives the upper bound

$$|a(t)| \leq (A_t^T)^{-1}\Big(\Big|\int_t^T A_t^s\, d\mathcal{M}_s(Q_{.,T}(\varphi))\Big| + \Big|\int_t^T A_t^s\, d\mathcal{M}_s(Q_{.,T}(1))\Big|\Big) \ ,$$

and thus

$$\begin{aligned}
\mathbb{E}\left(|a(t)|^p\right) &\leq Ce^{2\|V\|p(T-t)}\mathbb{E}\Big(\Big|\int_t^T A_t^s\, d\mathcal{M}_s(Q_{.,T}(\varphi))\Big|^p\Big)\\
&\leq Ce^{2\|V\|p(T-t)}\mathbb{E}\Big(\Big|\int_t^T (A_t^s)^2\, d\big[\mathcal{M}(Q_{.,T}(\varphi))\big]_s\Big|^{p/2}\Big) \quad \text{(by BDG inequality)}\\
&\leq Ce^{4\|V\|p(T-t)}\mathbb{E}\big(\big|\big[\mathcal{M}(Q_{.,T}(\varphi))\big]_t^T\big|^{p/2}\big)\\
&\leq Ce^{4\|V\|p(T-t)}\frac{(T-t+1)^{p/2}}{N^{p/2}} \quad \text{(by theorem 4.4)}\\
&\leq C\frac{R^{p(T-t)}}{N^{p/2}} \quad (\text{for } R = \mathrm{e}^{4\|V\|+1} > 1).
\end{aligned}$$

Control of $b(t)$. We have for some $0<\rho<1$, as a direct consequence of corollary 1.3,

$$\begin{aligned}
\mathbb{E}(|b(t)|^p) &= \mathbb{E}\big(\big|\Phi_{t,T}(\eta_t^N)(\varphi) - \Phi_{t,T}(\eta_t)(\varphi)\big|^p\big)\\
&\leq (\mathbb{E}(\frac{1}{\eta_t^N(h)^p}) + 1)C\rho^{T-t}\\
&\leq C\rho^{T-t} \quad \text{by assumption 3.}
\end{aligned}$$

Control of $b(0)$. We remark that $\eta_0(Q_{0,T}(1)) = 1$ and write $b(0)$ as follows:

$$b(0) = \big(\eta_0^N(Q_{0,T}(\varphi)) - \eta_0(Q_{0,T}(\varphi))\big) + \Phi_{0,T}(\eta_0^N)(\varphi)\big(\eta_0(Q_{0,T}(1)) - \eta_0^N(Q_{0,T}(1))\big)\ ,$$

which gives by lemma 4.2

$$\mathbb{E}(|b(0)|^p) \leq \frac{C}{N^{p/2}}\ .$$

Global control. We have

$$\begin{aligned}
\mathbb{E}((a(0)+b(0))^p) &\leq C\frac{R^{pT}+1}{N^{p/2}}\\
\mathbb{E}((a(t)+b(t))^p) &\leq C\frac{R^{p(T-t)}}{N^{p/2}} + C\rho^{p(T-t)} \quad (\forall t\in[0,T]).
\end{aligned}$$

Now we take $\epsilon = \frac{-\ln\rho}{-\ln\rho+\ln R}$, and remark that

$$\frac{R^{\frac{1}{2}\frac{\ln N}{\ln R-\ln\rho}}}{N^{1/2}} = \frac{1}{N^{\epsilon/2}}\ ,$$

and

$$\rho^{\frac{1}{2}\frac{\ln N}{\ln R-\ln\rho}} = \frac{1}{N^{\epsilon/2}}\ .$$

We get then $\mathbb{E}((\eta_T^N(\varphi) - \eta_T(\varphi))^p) \leq \frac{C}{N^{\epsilon p/2}}$ from the first inequality when $T \leq \frac{1}{2}\frac{\ln N}{\ln R-\ln\rho}$, and from the second one otherwise for $T-t = \frac{1}{2}\frac{\ln N}{\ln R-\ln\rho}$. □

Now we go back to equation (4.5) which readily gives

$$\begin{aligned}
\big(\eta_T^N(\varphi) - \eta_T(\varphi)\big)^p \leq\ & C\big(\eta_0^N(Q_{0,T}(\bar\varphi))\big)^p + C\mathcal{M}_T^p(Q_{.,T})\\
& + C\Big(\int_0^T |\eta_s^N(V) - \eta_s(V)||\eta_s^N(Q_{s,T}(\bar\varphi))|ds\Big)^p\ .
\end{aligned}$$

From lemma 4.2:

$$\mathbb{E}(\eta_0^N(Q_{0,T}(\bar{\varphi}))^p) \leq \frac{C}{N^{p/2}} \ .$$

From theorem 4.4:

$$\mathbb{E}\big(\mathcal{M}_T^p(Q_{.,T}(\bar{\varphi}))\big) \leq \frac{C}{N^{p/2}} \ .$$

On the other hand, using Hölder inequality, we also have

$$\begin{aligned}
&\Big(\int_0^T |\eta_s^N(V) - \eta_s(V)||\eta_s^N(Q_{s,T}(\bar{\varphi}))|ds\Big)^p \\
&\leq \int_0^T |\eta_s^N(V) - \eta_s(V)|^p \Big|\eta_s^N\Big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\Big)\Big|^p \|Q_{s,T}(\bar{\varphi})\| ds \Big(\int_0^T \|Q_{s,T}(\bar{\varphi})\| ds\Big)^{p-1} \\
&\leq C \int_0^T \Big|\eta_s^N\Big(\frac{V}{\|V\|}\Big) - \eta_s\Big(\frac{V}{\|V\|}\Big)\Big|^p \Big|\eta_s^N\Big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\Big) - \eta_s\Big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\Big)\Big|^p \|Q_{s,T}(\bar{\varphi})\| ds \ .
\end{aligned}$$

Taking expectations, and then using Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}
\mathbb{E}\Big(\Big(\int_0^T |\eta_s^N(V) - \eta_s(V)||\eta_s^N(Q_{s,T}(\bar{\varphi}))|ds\Big)^p\Big) &\leq C \int_0^T I_{2p}(N) \|Q_{s,T}(\bar{\varphi})\| ds \\
&\leq C I_{2p}(N) \ , \qquad (4.8)
\end{aligned}$$

which gives on the whole for all $p \leq 1$

$$I_p(N) \leq \frac{C}{N^{p/2}} + I_{2p}(N) \ .$$

Applying this result to lemma 4.6 gives:

$$I_p(N) \leq \frac{C}{N^{\inf(2\epsilon,1)p/2}} \ ,$$

and by induction we get

$$I_p(N) \leq \frac{C}{N^{p/2}} \ ,$$

which ends the proof.

4.3. Proof of theorem 3.2. We take expectation in (4.5) to find

$$\mathbb{E}(\eta_T^N(\varphi)) - \eta_T(\varphi) = \int_0^T \mathbb{E}\left(\big(\eta_s(V) - \eta_s^N(V)\big)\eta_s^N\Big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\Big)\right) \|Q_{s,T}(\bar{\varphi})\| ds \ .$$

As above, we use Cauchy-Schwarz inequality, and find that

$$\begin{aligned}
|\mathbb{E}(\eta_T^N(\varphi)) - \eta_T(\varphi)| &\leq C \int_0^T I_2(N) \|Q_{s,T}(\bar{\varphi})\| ds \\
&\leq C I_2(N) \leq \frac{C}{N} \ , \qquad (4.9)
\end{aligned}$$

which gives the estimate on the bias.
The second result is a direct consequence of exchangeability of particles.

4.4. Proof of theorem 3.4. The study of the asymptotic standard deviation rely on the following asymptotic behavior:

LEMMA 4.7. *For all $T > 0$, and $\bar{\varphi} = \varphi - \eta_T(\varphi)$,*

$$\begin{aligned}\mathbb{E}\left((\eta_T^N(\varphi) - \eta_T(\varphi))^2\right) &= \frac{1}{N}\mathbb{E}(\eta_T^N(\bar{\varphi})^2) \\ &+ \frac{2}{N}\mathbb{E}\Big(\int_0^T \eta_s^N\left(Q_{s,T}^2(\bar{\varphi})V_{\eta_s^N}^b\right) + \eta_s^N\left(Q_{s,T}^2(\bar{\varphi})\right)\eta_s(V_{\eta_s^N}^d)ds\Big) + O(\frac{1}{N^{3/2}}) \ .\end{aligned}$$

Proof. Again we start from equation (4.5):

$$\begin{aligned}\eta_T^N(\varphi) - \eta_T(\varphi) = &\underbrace{\eta_0^N(Q_{0,T}(\bar{\varphi})) + \mathcal{M}_T(Q_{.,T}(\bar{\varphi}))}_{a} \\ &+ \underbrace{\int_0^T \left(\eta_s(V) - \eta_s^N(V)\right)\eta_s^N(Q_{s,T}(\bar{\varphi}))\,ds}_{b} \ ,\end{aligned}$$

which gives

$$\mathbb{E}((\eta_T^N(\varphi) - \eta_T(\varphi))^2) = \mathbb{E}(a^2) + \mathbb{E}(b^2) + 2\mathbb{E}(ab)$$

Now we note by the results of the previous section, that is to say by equation (4.8), that

$$\mathbb{E}(b^2) = \mathbb{E}\Big(\Big|\int_0^T (\eta_s(V) - \eta_s^N(V))\eta_s^N\Big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\Big)\|Q_{s,T}(\bar{\varphi})\|ds\Big|^2\Big) = O(\frac{1}{N^2}) \ ,$$

and by theorem 4.4 and lemma 4.2

$$\mathbb{E}(a^2) = \mathbb{E}\left(\mathcal{M}_T(Q_{.,T}(\bar{\varphi}))^2\right) + \mathbb{E}\left(\eta_0^N(Q_{0,T}(\bar{\varphi}))^2\right) = O(\frac{1}{N}) \ .$$

So we get

$$\mathbb{E}\left((\eta_T^N(\varphi) - \eta_T(\varphi))^2\right) = \mathbb{E}\left(\eta_0^N(Q_{0,T}(\bar{\varphi}))^2\right) + \mathbb{E}\big(\langle\mathcal{M}(Q_{.,T}(\bar{\varphi}))\rangle_0^T\big) + O(\frac{1}{N^{3/2}}) \ .$$

Now we shall use the identity (4.6) to compute the asymptotic (with respect to N) value of $\mathbb{E}(\langle\mathcal{M}(Q_{.,T}(\bar{\varphi}))\rangle_0^T)$. For this purpose, we note that by theorem 3.1

$$\begin{aligned}\Big|\mathbb{E}\Big(\eta_s^N\big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\big)\eta_s^N\big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}V_{\eta_s^N}^*\big)\Big)\Big| &\le C\mathbb{E}\Big(\Big|\eta_s^N\big(\frac{Q_{s,T}(\bar{\varphi})}{\|Q_{s,T}(\bar{\varphi})\|}\big)\Big|\Big) \\ &= O(\frac{1}{N^{1/2}}) \ ,\end{aligned}$$

and the same way

$$\Big|\mathbb{E}\Big(\eta_s^N\big(\frac{Q_{s,T}^2(\bar{\varphi})}{\|Q_{s,T}^2(\varphi)\|}\big)\big(\eta_s^N(V_{\eta_s^N}^b) - \eta_s(V_{\eta_s^N}^b)\big)\Big)\Big| = O(\frac{1}{N^{1/2}}) \ .$$

Finally we remark that $\eta_0^N(Q_{0,T}(\bar{\varphi}))$ is a sum of centered i.i.d. random variables, and thus

$$\mathbb{E}\left(\eta_0^N(Q_{0,T}^2(\bar{\varphi}))\right) = \eta_0(Q_{0,T}^2(\bar{\varphi})) = \mathbb{E}\left(\eta_0^N(Q_{0,T}(\bar{\varphi}))^2\right) \ ,$$

which ends the proof. ◻

Now recall that theorem 3.1 implies by a Borel-Cantelli argument:

$$\eta_s^N \xrightarrow{a.s.} \eta_s \quad \text{(in the weak sense)}$$

We take the limit first when $N \to +\infty$ in lemma 4.7 uniformly with respect to T, and then when $T \to +\infty$. Of course, the two limits commute. This gives by Lebesgue convergence therorem

$$\lim_{N\to+\infty} N\mathbb{E}\left((\eta_T^N(\varphi) - \eta_T(\varphi))^2\right) = \eta_T\left((\varphi - \eta_T(\varphi))^2\right)$$
$$+2\int_0^T \eta_s\big(Q^2_{s,T}(\bar\varphi)V^b_{\eta_s}\big) + \eta_s(Q^2_{s,T}(\bar\varphi))\eta_s(V^d_{\eta_s})ds \; .$$

Now we do the change of variables $s \mapsto T - s$ in the above integrand, and take the limit $T \to +\infty$. We have

$$\begin{aligned} \eta_{T-s} &\to \eta_\infty \\ \bar\varphi = \varphi - \eta_T(\varphi) &\to \bar\varphi = \varphi - \eta_\infty(\varphi) \\ Q_{T-s,T}(\bar\varphi) &\to \frac{P_s^V(\bar\varphi)}{\eta_\infty P_s^V(1)} = P_s^{V-\lambda}(\bar\varphi) \; , \end{aligned}$$

which gives the asymptotic standard deviation.

5. Two general lemmas.

Lemma 5.1 (An upper bound for the "carré du champ" operator). *Let L be a Markov generator and Γ be its associated "carré du champs" operator defined by $\Gamma(\varphi,\varphi) = L(\varphi^2) - 2\varphi L(\varphi)$. Then we have the upper bound for all $n \geq 0$*

$$\Gamma(\varphi^{2^n},\varphi^{2^n}) \leq L(\varphi^{2^{n+1}}) - 2^{n+1}\varphi^{2^{n+1}-1}L(\varphi) \; .$$

Proof. Check out by induction the formal identity

$$\Gamma(\varphi^{2^n},\varphi^{2^n}) = L(\varphi^{2^{n+1}}) - 2^{n+1}\varphi^{2^{n+1}-1}L(\varphi)$$
$$-\sum_{k=1}^{n} 2^{n+1-k}\varphi^{2^{n+1}-2^k}\Gamma(\varphi^{2^{k-1}},\varphi^{2^{k-1}}) \; ,$$

and use the positivity property $\Gamma(\varphi,\varphi) \geq 0$. ◻

Lemma 5.2 (BDG inequalities). *Let M be a quasi-left-continuous (i.e. with continuous predictable increasing process) locally square-integrable martingale with $M_0 = 0$ and bounded jumps $\sup_t |\Delta M_t| \leq a < +\infty$. Then there is a constant C (dependant on q) such that*

$$\mathbb{E}\big(\sup_t M_t^{2^{q+1}}\big) \leq C\mathbb{E}\big([M]_\infty^{2^q}\big) \leq C\sum_{k=0}^{q} a^{2^{q+1}-2^{k+1}}\mathbb{E}\big(\langle M\rangle_\infty^{2^k}\big) \; .$$

Proof. The first inequality is the classical Burkholder-Davis-Gundy (BDG) inequality (p. 350 of [10]).

For the second, by localization, we can suppose that M is a square-integrable martingale. We are to use the martingale $N = \big[M\big] - \big\langle M \big\rangle$. Because $\big\langle M \big\rangle$ is continuous $\Delta N = \Delta\big[M\big] = (\Delta M)^2$. Moreover, N has finite variation so

$$\begin{aligned}
\big[N\big] &= \sum_{s\leq .}(\Delta N_s)^2 = \sum_{s\leq .}(\Delta M_s)^4 \\
&\leq a^2 \sum_{s\leq .}(\Delta M_s)^2 \leq a^2\big[M\big] \\
&\leq a^2(N + \big\langle M \big\rangle) \ .
\end{aligned} \tag{5.1}$$

We will also us the general fact (C depends of q):

$$\forall x, y, \quad (x+y)^{2^q} \leq C(x^{2^q} + y^{2^q}) \ . \tag{5.2}$$

By definition of N and (5.2) we get

$$\mathbb{E}\big(\big[M\big]_\infty^{2^q}\big) \leq C\mathbb{E}\big(\sup_t N_t^{2^q}\big) + C\mathbb{E}\big(\big\langle M \big\rangle_\infty^{2^q}\big) \ .$$

Now it remains to prove for any $q \geq 1$

$$\mathbb{E}\big(\sup_t N_t^{2^q}\big) \leq \sum_{k=0}^{q-1} C a^{2^{q+1}-2^{k+1}} \mathbb{E}\big(\big\langle M \big\rangle_\infty^{2^k}\big) \ , \tag{5.3}$$

which we are going to do by induction on q. For $q = 1$, (5.3) follows from BDG inequality applied to N_t, with (5.1). Suppose (5.3) true for a given q. Applying again BDG inequality to N_t, and using (5.1) and (5.2), we get

$$\mathbb{E}\big(\sup_t N_t^{2^{q+1}}\big) \leq C a^{2^{q+1}} \mathbb{E}\big(\sup_t N_t^{2^q}\big) + C a^{2^{q+1}} \mathbb{E}\big(\big\langle M \big\rangle_\infty^{2^q}\big) \ .$$

(5.3) at rank $q+1$ follows then from the induction hypothesis. $\square$

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