Quantum Monte Carlo simulations of fermions. A mathematical analysis of the fixed-node approximation

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8th October 2004

Abstract

The Diffusion Monte Carlo (DMC) method is a powerful strategy to estimate the ground state energy E_0 of a N-body Schrödinger hamiltonian $H = -\frac{1}{2}\Delta + V$ with high accuracy. Briefly speaking, it consists in writing E_0 as the long-time limit of the expectation value of a drift-diffusion process with source term, and in numerically simulating this process by means of a collection of random walkers. As for a number of stochastic methods, a DMC calculation makes use of an importance sampling function ψ_I which hopefully approximates some ground state ψ_0 of H. In the fermionic case, it has been observed that the DMC method is biased, except in the special case when the nodal surfaces of ψ_I coincide with those of a ground state of H. The approximation arising from the fact that, in practice, the nodal surfaces of ψ_I differ from those of the ground states of H, is refered to as the Fixed Node Approximation (FNA). Our purpose in this article is to provide a mathematicial analysis of the FNA. We prove that, under some hypotheses, a DMC calculation performed with the importance sampling function ψ_I, provides an estimation of the infimum of the energy $\langle \psi, H\psi \rangle$ on the set of the fermionic test functions ψ that vanish on the nodal surfaces of ψ_I.

1 Introduction

Calculating the ground state of fermionic systems is a major concern in Computational Chemistry and Physics. In particular, this issue is the heart of the matter in Quantum Chemistry and in *ab initio* Molecular Dynamics (see e.g. [16, 19] and [5] for a more mathematical presentation). In both cases, the purpose is to determine electronic structures.

In absence of magnetic field, the electronic structure of a piece of matter consisting of M nuclei and N electrons is described by a hamiltonian of the form

$$H = -\frac{1}{2}\Delta + V$$

operating on the antisymmetrized tensor product

$$\mathcal{H}_e = \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3).$$

The above notation means that $\mathcal{H}_e$ is the Hilbert space of square integrable functions

$$\psi \ : \ \mathbb{R}^3 \times \cdots \times \mathbb{R}^3 \equiv \mathbb{R}^{3N} \to \mathbb{R} \text{ or } \mathbb{C}$$

satisfying the antisymmetry condition

$$\psi(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \epsilon(\sigma)\, \psi(x_1, \cdots, x_N) \tag{1}$$

for all permutation $\sigma \in \mathfrak{S}_N$ and almost all $(x_1, \cdots, x_N) \in \mathbb{R}^3 \times \cdots \times \mathbb{R}^3$ ($\epsilon(\sigma)$ denotes the signature of σ). The antisymmetry condition (1) accounts for the fermionic nature of the electrons. For simplicity, we do not take the spin variables into account, but all the results below can be straightforwardly extended to spin-dependent models. The particular form of V will be made precise in Section 2. Let us just mention for the moment that V is a real-valued local potential, symmetric with respect to renumbering of particules (i.e. $V(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = V(x_1, \cdots, x_N)$), and that the linear operator H, defined on a convenient domain $D(H) \subset \mathcal{H}_e$, is self-adjoint on $\mathcal{H}_e$.

We assume in the sequel that H is bounded from below and that the lower bound of its spectrum, denoted by E_0, corresponds to an isolated eigenvalue. We denote by ψ_0 a normalized eigenfunction of H associated with E_0. By definition, E_0 is the ground state energy and ψ_0 a ground state of the system. Recall that, under some technical assumptions on V (satisfied in particular by the potentials V defined in Section 2),

$$E_0 = \inf \left\{ \frac{1}{2} \int_{\mathbf{R}^{3N}} |\nabla \psi|^2 + \int_{\mathbf{R}^{3N}} V|\psi|^2, \quad \psi \in D(q_H), \quad \|\psi\|_{L^2} = 1 \right\} \tag{2}$$

where $D(q_H)$ is the domain of the energy functional, i.e. of the quadratic form

$$\langle \psi, H\psi \rangle = \frac{1}{2} \int_{\mathbf{R}^{3N}} |\nabla \psi|^2 + \int_{\mathbf{R}^{3N}} V|\psi|^2$$

associated with H (recall that $D(H) \subset D(q_H) \subset \mathcal{H}_e$ with dense embeddings). Besides, the ground state ψ_0 is a minimizer of (2) and satistifies the time-independent Schrödinger equation

$$H\psi_0 = E_0 \psi_0. \tag{3}$$

In practice, and in particular in electronic structure calculations [16, 19, 5], determining the ground state amounts to computing the ground state energy E_0, and possibly some functions of ψ_0 of the form $\langle \psi_0, A\psi_0 \rangle$ where A is a self-adjoint operator on $\mathcal{H}_e$. Let us notice that, as the potential V is real-valued and as we focus on solutions of the time-*independent* Schrödinger equation (3), it is sufficient to consider real-valued functions ψ only.

Tackling directly problem (2) or equation (3) with deterministic numerical methods is out of reach for values of N larger than 6 or 7. Most of the fermionic ground state calculations are in fact performed either with the Hartree-Fock model [20] or with the Kohn-Sham model [11]. The Hartree-Fock model is a variational approximation of problem (2) consisting in minimizing the energy functional $\langle \psi, H\psi \rangle$ on the subset of $\{\psi \in D(q_H), \ \|\psi\|_{L^2} = 1\}$ consisting of Slater determinants, i.e. on the set

$$\left\{ \psi \in D(q_H), \quad \psi(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!}} \det\left(\phi_i(x_j)\right), \quad \phi_i \in L^2(\mathbb{R}^3), \quad \int_{\mathbf{R}^3} \phi_i \phi_j = \delta_{ij} \right\}.$$

The Hartree-Fock ground state can be computed numerically for systems containing as many as several hundreds of particles on a today available personal computer. The Hartree-Fock model can be interpreted as a mean-field model. For this reason, the (non-negative) difference between the Hartree-Fock energy of the system and the exact ground state energy E_0 is called the correlation energy. In some systems, the correlation energy may play an essential role, and the Hartree-Fock model is then inefficient. The Kohn-Sham model is an attempt to calculate E_0 without calculating ψ_0, which originates from the Density Functional Theory [10]. It usually outperforms the Hartree-Fock model, but may fail in some cases. It is out of our purpose to describe the Kohn-Sham model, and we therefore refer the reader to the literature (see for instance [11, 5]). Let us only mention that the Kohn-Sham model is not a variational approximation of (2) and that, depending on the system under study, it gives an estimation of the ground state energy which can be either lower or higher than E_0. In addition, no error bound for the Kohn-Sham model is available so far. More sophisticated deterministic models, refered to as post Hartree-Fock models, have been developed (Møllet-Plesset perturbation method, configuration interaction, multi-configuration self-consistent field, coupled cluster, ...), but the computational cost of them is prohibitive for large systems.

Quantum Monte Carlo (QMC) methods [14, 15, 21] provide an alternative elegant and powerful way to solve problem (2). They are (obviously!) stochatics methods. We focus here on the so-called Diffusion Monte Carlo (DMC) method, which has many advantages: first, it aims at directly solving the N-body problem (2), without resorting to a mean-field model; second, as any Monte Carlo method, it provides confidence intervals that can be, in some sense, considered as *a posteriori* error bounds; third, it is far much easier to implement than deterministic methods, such as the Hartree-Fock, Kohn-Sham or post Hartree-Fock methods. Despite these numerous advantages, the DMC method has not been widely used by practitioners in the past decades, mainly for the following two reasons. First, DMC calculations are more demanding in terms of CPU time than, for instance, Kohn-Sham calculations. In fact, DMC calculations cannot be run from scratch; they only allow to improve on the result of a previous deterministic or Variational Monte Carlo (see e.g. [2]) calculation. Second, and contrarily to deterministic methods, DMC calculations did not offer until recently, the possibility to efficiently compute the gradient of the ground state energy E_0 with respect to external parameters, such that, in electronic structure calculations, the positions $\{\bar{x}_k\}$ of the nuclei. This was a main drawback because electronic structure calculations often are the inner loop of an algorithm aiming either in optimizing the nuclear configuration of the system (molecular mechanics), or in making the nuclei evolve in the effective potential generated by the electrons (molecular dynamics). In both cases, the gradient of E_0 with respect to the $\{\bar{x}_k\}$ is needed. The situation is likely to dramatically change in a near future, for the above two difficulties are about to be overcome. Indeed, the computational cost of the DMC method scales linearly with the number of particles, so that the efficiency of DMC increases at least as fast as computer performances. Besides, M. Caffarel and co-workers have proposed in [3] a promissing method for efficiently computing the derivatives of E_0 with respect to nuclear positions.

It is our hope that this article will help applied mathematicians to get aware of the specific problems encountered in Quantum Monte Carlo simulations of fermions, and that it will encourage some of them to contribute to the field. This article focus on the theory underlying DMC calculations. We intend to investigate the numerical aspects in a future work.

2 Properties of fermionic ground states

Before entering the presentation of the DMC method, let us recall some important properties of fermionic ground states.

In most applications, and in particular in electronic structure calculations, the potential V felt by the N fermions under consideration, can be split into two parts:

$$V(x) = \sum_{i=1}^{N} V_1(x_i) + \sum_{1\leq i<j\leq N} V_2(x_i - x_j) \qquad\qquad x = (x_1, \cdots, x_N) \in \mathbb{R}^{3N},$$

the function V_2 being such that $V_2(-y) = V_2(y)$ (usually, V_2 is in fact a function of $|y|$). The first term accounts for the interaction of the particles with an external potential V_1. The second term is a two-body interaction term. In this paper, we focus on two settings:

1. the simple case of N non-interacting fermions trapped in a harmonic potential, for which analytical results can be obtained (see Section 6);
2. the one of electronic structure calculations, which is of high practical interest.

In the former setting, the potentials V_1 and V_2 are given by

$$\forall y \in \mathbb{R}^3, \qquad V_1(y) = \sum_{j=1}^{3} \frac{1}{2}\omega_j^2 y_j^2 \qquad \text{and} \qquad V_2(y) = 0, \tag{4}$$

with (for instance) $0 < \omega_1 \le \omega_2 \le \omega_3$.

In the latter setting, the hamiltonian H models the dynamics of the N electrons of some molecular system. The potentials V_1 and V_2 account for the nuclei-electron and electron-electron electrostatic interactions respectively. In atomic units [5], they read

$$V_1 = -\sum_{k=1}^{M} \rho_k \star \frac{1}{|x|} \qquad \text{and} \qquad V_2(y) = \frac{1}{|y|}. \tag{5}$$

The symbol $\star$ denotes the convolution product in $\mathbb{R}^3$ and ρ_k is the positive charge distribution modelling the k-th nucleus. Nuclei are generally represented as classical point-like particles, i.e. by $\rho_k = z_k \delta_{\bar{x}_k}$ where $z_k \in \mathbb{N}^*$ and $\bar{x}_k \in \mathbb{R}^3$ respectively denote the charge and the position of the k-th nucleus. Point-like nuclei create attractive singularities of the potential that are difficult to deal with in Quantum Monte Carlo simulations, both on the theoretical and numerical viewpoints. We concentrate here on the problems issued from the fermionic nature of the electrons. That is why, when necessary, we get rid of the above mentioned difficulty by smearing the nuclear distribution. More precisely, we will assume in some of our results related to DMC calculations (in particular in Proposition 6 below), that the ρ_k are localized regular functions such that $\rho_k \ge 0$ and $\displaystyle\int_{\mathbb{R}^3} \rho_k = z_k$. In the present section however, this simplification is not needed.

It is of course possible to extend our results to more general potentials V with prescribed local regularities and behaviors at infinity, but we will not proceed further in this direction here.

Let us first recall some well-known results of existence and local regularity.

Theorem 1 (Existence of a ground state).

1. *For V_1 and V_2 given by (4), the hamiltonian H, defined on the domain $D(H) = \left\{ u \in \mathcal{H}_e,\ -\frac{1}{2}\Delta u + V u \in \mathcal{H}_e \right\}$ is self-adjoint on $\mathcal{H}_e$ and has a ground state.*
2. *For V_1 and V_2 given by (5) with $N \le Z = \displaystyle\sum_{k=1}^{M} z_k$ (neutral molecule or positive ion), the hamiltonian H, defined on the domain $D(H) = \mathcal{H}_e \cap H^2(\mathbb{R}^{3N})$, is self-adjoint on $\mathcal{H}_e$ and has a ground state.*

The first statement is straightforward: when the potential V is quadratic, the hamiltonian $H = -\frac{1}{2}\Delta + V$ has a purely discrete spectrum and its eigenpairs are known analytically (see Section 6 or any textbook of Quantum Mechanics). The second statement is by far less obvious. It has been established by G.M. Zhislin in [27]. Let us also mention that for V_1 and V_2 given by (4), $D(q_H) = \mathcal{H}_e \cap H^1(\mathbb{R}^{3N}) \cap \mathcal{F}\left(H^1(\mathbb{R}^{3N})\right)$ where $\mathcal{F}$ denotes the Fourier transform, and that for V_1 and V_2 given by (5), $D(q_H) = \mathcal{H}_e \cap H^1(\mathbb{R}^{3N})$.

Proposition 2 (Local regularity).

1. *For V_1 and V_2 given by (4), any ground state ψ_0 of H belongs to $C^\infty(\mathbb{R}^{3N})$.*
2. *For V_1 and V_2 given by (5) with $\rho_k = z_k\delta_{\bar{x}_k}$ (point-like nuclei) or $\rho_k \in C^\infty(\mathbb{R}^3)$ (smeared nuclei), any ground state ψ_0 of H is in $C_\theta(\mathbb{R}^{3N})$ for any $0 < \theta < 1$ where*

$$C_\theta(\mathbb{R}^{3N}) = \left\{\psi \in L^\infty(\mathbb{R}^{3N}), \quad \exists C \geq 0, \quad \forall (x,y) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}, \quad |\psi(x) - \psi(y)| \leq C\,|x-y|^\theta \right\}.$$

   In addition, $\psi_0 \in C^\infty\left(\mathbb{R}^{3N} \setminus (\gamma_n \cup \gamma_e)\right)$ for point-like nuclei and $\psi_0 \in C^\infty\left(\mathbb{R}^{3N} \setminus \gamma_e\right)$ for smeared nuclei, where

$$\gamma_e = \left\{(x_1, \cdots, x_N) \in \mathbb{R}^{3N}, \quad \exists (i,j) \in |[1,N]| \times |[1,N]|, \quad i \neq j, \quad x_i = x_j\right\}$$

   and

$$\gamma_n = \left\{(x_1, \cdots, x_N) \in \mathbb{R}^{3N}, \quad \exists (i,k) \in |[1,N]| \times |[1,M]|, \quad x_i = \bar{x}_k\right\}.$$

The first statement is a direct consequence of basic elliptic regularity arguments (see e.g. [9]). The proof of the second statement results from a straighforward adaptation of the proof of the Kato-Simon theorem (see e.g. [22], page 193).

Let us now focus on an interesting property of fermionic ground states among antisymmetric functions, which plays a crucial role in Monte Carlo simulations (see Remark 13 below).
If ψ is an antisymmetric non-zero continuous function on $\mathbb{R}^{3N}$, then the open set $\mathbb{R}^{3N} \setminus \psi^{-1}(0)$ obviously has at least two connected components. For any connected component $\mathcal{C}$, and any permutation $\sigma \in \mathfrak{S}_N$,

$$\mathcal{C}_\sigma = \left\{x_\sigma = (x_{\sigma(1)}, x_{\sigma(2)}, \cdots, x_{\sigma(N)}) \in \mathbb{R}^{3N}, \quad x = (x_1, x_2, \cdots, x_N) \in \mathcal{C}\right\}$$

is also a connected component. Indeed, if $x, y \in \mathcal{C}$ then there exists a continuous function $f : [0,1] \to \mathcal{C}$ such that $f(0) = x$ and $f(1) = y$. One has $\forall s \in [0,1]$, $\psi_I(x)\psi_I(f(s)) > 0$. Therefore by antisymmetry of ψ_I, $\forall s \in [0,1]$, $\psi_I(x_\sigma)\psi_I(f(s)_\sigma) > 0$ and x_σ and y_σ belong to the same connected component. Hence $\mathcal{C}_\sigma$ is included in a connected component denoted by $\tilde{\mathcal{C}}_\sigma$. Similarly, $(\tilde{\mathcal{C}}_\sigma)_{\sigma^{-1}}$ is included in a connected component which contains $\mathcal{C}$. Hence $(\tilde{\mathcal{C}}_\sigma)_{\sigma^{-1}} = \mathcal{C}$ and $\tilde{\mathcal{C}}_\sigma = \mathcal{C}_\sigma$.

Definition 3. *Let $\psi \in \mathcal{H}_e \cap C^0(\mathbb{R}^{3N})$ and $U = \mathbb{R}^{3N} \setminus \psi^{-1}(0)$. The function ψ is said to satisfy the tiling property if for any connected component $\mathcal{C}$ of U,*

$$U = \bigcup_{\sigma \in \mathfrak{S}_N} \mathcal{C}_\sigma.$$

The tiling property therefore means that all the connected components of U can be obtained from one of them by permutating the indices of the particles. It follows that all these connected components are isometric. In addition, the cardinal $N_{\rm inv}$ of the subgroup of permutations on the numbering of the particles which let a given connected component invariant does not depend on the connected component, and therefore, the number N_c of connected components of U verifies $N_c = N!/N_{\rm inv}$.

Theorem 4 (Tiling property). *For V_1 and V_2 given by (4) or by (5), with point-like or smeared nuclei, any ground state ψ_0 of H satisfies the tiling property.*

Theorem 4 is a rigorous formulation of a formal result due to Ceperley [7]. As we are not aware of any mathematical proof of it, we provide one in Section 5. In some sense, this result is the counterpart for the fermionic case of the well-known result stating that the ground state of $-\frac{1}{2}\Delta + V$ on $L^2(\mathbb{R}^{3N})$ has a sign.

Corollary 5. *Let ψ_0 be a ground state of H and $\mathcal{C}$ a connected component of $U_0 = \mathbb{R}^{3N} \setminus \psi_0^{-1}(0)$. For V_1 and V_2 given either by (4) or by (5), with point-like or smeared nuclei, the ground state energy E_0 satisfies*

$$E_0 = \inf \left\{ \frac{1}{2} \int_{\mathcal{C}} |\nabla \psi|^2 + \int_{\mathcal{C}} V \psi^2, \quad \psi \in H_0^1(\mathcal{C}), \quad \int_{\mathcal{C}} \psi^2 = 1 \right\}.$$

The proof of Corollary 5 is postponed until Section 5.

3 Presentation of the DMC method

For the sake of simplicity, we assume in this section that the ground state energy E_0 is an isolated *single* eigenvalue of H, and we denote by γ the spectral gap, namely the distance between E_0 and the rest of the spectrum of H.

The DMC method is based on the following remark. Let $\psi_I \in \mathcal{H}_e$ be such that $\|\psi_I\|_{L^2} = 1$. The unique solution $\phi(t,x)$ in $C^0(\mathbb{R}_+, \mathcal{H}_e) \cap C^0(]0,+\infty[, D(H)) \cap C^1(]0,+\infty[, \mathcal{H}_e)$ of the evolution problem

$$\left\{ \begin{array}{l} \dfrac{\partial \phi}{\partial t} = -H\phi = \dfrac{1}{2}\Delta\phi - V\phi \\ \phi(0,x) = \psi_I(x) \end{array} \right. \tag{6}$$

reads $\phi(t,\cdot) = e^{-tH}\psi_I$ and is such that

$$\| \exp(E_0 t)\ \phi(t) - (\psi_0, \psi_I)_{L^2}\ \psi_0\|_{L^2} \leq \|\psi_I - (\psi_0, \psi_I)_{L^2}\ \psi_0\|_{L^2}\ \exp(-\gamma t),$$

where as above, ψ_0 denotes a ground state of H. If moreover $(\psi_0, \psi_I)_{L^2} \neq 0$, one also has

$$0 \leq E(t) - E_0 \leq \frac{(\langle H\psi_I, \psi_I \rangle - E_0)}{(\psi_0, \psi_I)_{L^2}^2} \exp(-\gamma t)$$

where

$$E(t) = \frac{\langle H\psi_I, \phi(t) \rangle}{(\psi_I, \phi(t))_{L^2}}. \tag{7}$$

As equation (6) is posed on $\mathbb{R}^{3N}$, and as in addition, V may have singularities, it seems difficult to numerically solve it with deterministic methods.

On the other hand, a stochastic representation of the solution of (6) is available, and could *a priori* be used to estimate E_0. It indeed follows from the Feynman-Kac formula that, under convenient assumptions on V,

$$\phi(t,x) = \mathbb{E}\left(\psi_I\left(x+W_t\right)\,\exp\left(-\int_0^t V\left(x+W_s\right)\,ds\right)\right) \tag{8}$$

where $(W_t)_{t\geq 0}$ denotes a $\mathbb{R}^{3N}$-valued Wiener process. The above expression can be used in a number of formulae that provide estimations of E_0, for instance [17]

$$-\frac{1}{t}\ln\left(\mathbb{E}\left(\psi_I\left(x+W_t\right)\,\exp\left(-\int_0^t V\left(x+W_s\right)\,ds\right)\right)\right)\underset{t\to+\infty}{\longrightarrow} E_0.$$

As such, expression (8) is however not adapted to numerical simulations; it has indeed been observed that the variance of the random variable

$$Y_t = \psi_I\left(x+W_t\right)\,\exp\left(-\int_0^t V\left(x+W_s\right)\,ds\right)$$

increases very quickly with time.

In practice, physicists and chemists rather make use of the following importance sampling technique, which allows them to compute ground state energies with a satisfactory accuracy (in most cases, 90% of the correlation energy can be recovered). Assume that the function ψ_I, which from now on plays the role of an importance sampling function, is such that the local fields

$$b(x) = \frac{\nabla\psi_I(x)}{\psi_I(x)} \qquad \text{and} \qquad E_L(x) = \frac{(H\psi_I)(x)}{\psi_I(x)} = -\frac{1}{2}\frac{\Delta\psi_I(x)}{\psi_I(x)} + V(x) \tag{9}$$

can be calculated with a reasonable computational complexity for almost every $x\in\mathbb{R}^{3N}$ (for instance, $b(x)$ and $E_L(x)$ can be computed in $O(N^4)$ operations if ψ_I is a Slater determinant). Let us now consider the function

$$f_1(t,x) = \psi_I(x)\,\phi(t,x),$$

where ϕ is the solution of (6) defined above. The energy $E(t)$ defined by (7) also reads

$$E(t) = \frac{\displaystyle\int_{\mathbb{R}^3} E_L(x)\,f_1(t,x)\,dx}{\displaystyle\int_{\mathbb{R}^3} f_1(t,x)\,dx}, \tag{10}$$

and an elementary calculation shows that f_1 is solution of the equation

$$\left\{\begin{array}{l}\dfrac{\partial f}{\partial t} = \dfrac{1}{2}\Delta f - \mathrm{div}\;(bf) - E_L f,\\ f(0,x) = \psi_I^2(x),\end{array}\right. \tag{11}$$

where the fields b and E_L are defined almost everywhere by (9).

In order to emphasize the advantages of this reformulation, let us assume for a while that we are dealing with bosons rather than fermions. In other words, let us consider the problem of computing the ground state of the operator $H_B = -\frac{1}{2}\Delta + V$ operating on the bosonic subspace of $L^2(\mathbb{R}^{3N})$ consisting of the functions ψ satisfying the symmetry property $\psi(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \psi(x_1, \cdots, x_N)$. For simplicity, we assume in addition that the potential V is regular. It is well known (see e.g. [22]) that the bosonic ground state ψ_B of H_B is then non-degenerate, regular, and positive on $\mathbb{R}^{3N}$ (up to replacing ψ_B by $-\psi_B$ if necessary). By performing a mean-field calculation, it is possible to build a function ψ_I close to ψ_B and sharing the same properties of regularity and positivity. The fields b and E_L are then regular and problem (11) admits a unique regular solution, namely $f_1(t,x) = \psi_I(x) \left(e^{-tH_B}\psi_I\right)(x)$; in addition,

$$d\mu_t = \frac{1}{\int_{\mathbf{R}^{3N}} f_1(t,y)\, dy}\, f_1(t,x)\, dx$$

defines for any $t \geq 0$ a probability measure on $\mathbb{R}^{3N}$ (for f_1 is non negative a.e.). In the case when $\psi_I = \psi_B$, the variance $\displaystyle\int_{\mathbf{R}^{3N}} E_L^2\, d\mu_t - \left(\int_{\mathbf{R}^{3N}} E_L\, d\mu_t\right)^2$ of E_L under the probability measure μ_t is zero, since $E_L(x)$ is constant on $\mathbb{R}^{3N}$. If one chooses ψ_I close enough to ψ_B so that the variance of E_L under the probability measure μ_t is small, one can expect that (10) will provide an efficient way for estimating $E(t)$. Indeed, μ_t can be simulated by interprating (11) as a Fokker-Planck equation with a source term associated with the diffusion process with generator $\frac{1}{2}\Delta + b.\nabla$.

Exploiting formula (10) and (11) is an "exact" very efficient strategy for simulating bosonic systems. On the other hand, this approach is "biased", and consequently less efficient, for fermionic systems. It has indeed been observed in numerical simulations that this approach introduces a systematic error, except when the nodal surfaces of ψ_I and ψ_0 coincide. The approximation arising from the fact that, in practice, the nodal surfaces of ψ_I differ from those of ψ_0, is refered to as the Fixed Node Approximation (FNA). It has been put forward in the Physics and Chemistry literature that the source of this systematic error lays on the fact that the sample paths of the diffusion process associated with (11) cannot cross the nodal surfaces of ψ_I. Our purpose in this article is to give a sound mathematical foundation to this statement and to provide a rigorous analysis of the FNA.

In Section 4, we state our main results. We first analyse in Proposition 7 existence and uniqueness for the diffusion process with generator $\frac{1}{2}\Delta + b.\nabla$ and show in particular that its sample paths actually behave as expected: they cannot cross the nodal surfaces of ψ_I. Then we show in Propositions 10 and 11 that problem (11) admits several weak solutions and that the one we are interested in, namely f_1, is not that built from the density of the stochastic process associated with (11). Next, we identify in Theorem 12 the energy calculated with the Diffusion Monte Carlo method, using ψ_I as an important sampling function. For the sake of clarity, the proofs are postponed until Section 5. Lastly, we provide in Section 6 a simple illustrative example of two non interacting fermions in an anisotropic harmonic potential, for which analytical results can be carried out.

4 Analysis of the fixed node approximation

We have been able to rigorously analyse the DMC method under some hypotheses on the importance sampling function ψ_I. Let us first list these hypotheses:

[$\mathcal{H}1$] Regularity, antisymmetry and exponential fall-off

$$\psi_I \in D(H) \cap C^2(\mathbb{R}^{3N}) \quad \text{with} \quad \|\psi_I\|_{L^2} = 1 \tag{12}$$

$$\exists c > 0,\ \forall y \in \mathbb{R}^{3N},\ |\psi_I(y)| \leq e^{-c|y|}/c \tag{13}$$

[$\mathcal{H}$2] Nodal surfaces and critical points

$$\forall y \in \mathbb{R}^{3N} \text{ such that } \psi_I(y) = 0,\ \nabla\psi_I(y) \neq 0 \tag{14}$$

$$U_I = \mathbb{R}^{3N} \setminus \psi_I^{-1}(0) \text{ has a finite number } N_c^I \text{ of connected components} \tag{15}$$

[$\mathcal{H}$3] Behaviour at infinity : we assume that either for each connected component $\mathcal{C}$ of U_I

$$\begin{aligned} &\exists (x_0, C, C') \in \mathbb{R}^{3N} \times (\mathbb{R}_+)^2, \qquad \text{such that} \qquad \forall y \in \mathcal{C}, \\ &|y - x_0| \geq C \quad \Rightarrow \quad (y - x_0).b(y) \leq C'(1 + |y - x_0|^2) \end{aligned} \tag{16}$$

or

$$\exists K > 0,\ \forall x \in \mathbb{R}^{3N},\ |x| \geq K \Rightarrow \psi_I(x)\Delta\psi_I(x) \geq 0 \tag{17}$$

[$\mathcal{H}$4] Finite lower bound of the local energy E_L

$$\inf_{y \in \mathbb{R}^{3N}} E_L(y) > -\infty \tag{18}$$

[$\mathcal{H}$5] Spectrum of H and energy of ψ_I

$$H \text{ is bounded from below} \tag{19}$$

$$\langle H\psi_I, \psi_I \rangle < \inf \sigma_{\text{ess}}(H) \tag{20}$$

where $\sigma_{\text{ess}}(H)$ denotes the essential spectrum of H.

Hypotheses [$\mathcal{H}$1] is not very restrictive. Neither is [$\mathcal{H}$4] for V_1 and V_2 given by (4) or by (5) with smeared nuclei. We have in particular the following result :

Proposition 6. *If the potentials V_1 and V_2 are given by (5) with $\rho_k \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ (electronic structure calculation with smeared nuclei), and if $N \leq Z = \sum_{k=1}^{N} z_k$, then the problem*

$$\begin{aligned} \inf \Bigg\{ &\sum_{i=1}^{N} \frac{1}{2} \int_{\mathbb{R}^3} |\nabla\phi_i|^2 + \int_{\mathbb{R}^3} V_1 \rho_\Phi + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \rho_\Phi(x)\, V_2(x-y)\, \rho_\Phi(y)\, dx\, dy, \\ &\Phi = \{\phi_i\}_{1 \leq i \leq N} \in \left(H^1(\mathbb{R}^3)\right)^N, \quad \int_{\mathbb{R}^3} \phi_i \phi_j = \delta_{ij}, \quad \rho_\Phi(x) = \sum_{i=1}^{N} |\phi_i(x)|^2 \Bigg\} \end{aligned} \tag{21}$$

has a minimizer $\left\{\phi_i^H\right\}_{1 \leq i \leq N}$. Besides the N-body wavefunction

$$\psi_I(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!}} \det\left(\phi_i^H(x_j)\right) \tag{22}$$

fulfills the hypotheses [$\mathcal{H}$1] and [$\mathcal{H}$4]. In addition, ψ_I satisfies the tiling property.

Problem (21) corresponds to the Kohn-Sham model with a null exchange-correlation functional. More generally, [$\mathcal{H}$1] and [$\mathcal{H}$4] are satisfied by the Slater determinant built with Kohn-Sham orbitals for local or gradient corrected exchange-correlation energy functionals [11]. Let us now examine the remaining three hypotheses. Hypothesis [$\mathcal{H}$2] does not seem restrictive either, since, on the one hand, for a generic function ψ_I of $C^1(\mathbb{R}^{3N})$, $\nabla\psi_I \neq 0$ is satisfied almost everywhere for the surface measure on $\psi_I^{-1}(0)$, and since, on the other hand, (15) is fulfilled by the commonly used importance sampling functions for the latter satisfy the tiling property. As for hypothesis (16), it is a standard assumption to prevent the sample paths of the stochastic process X_t^x solution of the SDE (23) below, from going to infinity in finite time. Because $b(x) = \nabla\psi_I(x)/\psi_I(x)$, (16) is rather restrictive near the nodal surfaces of ψ_I. The alternative hypothesis (17) holds for instance for ψ_I given by (22) when for some $\varepsilon > 0$, $\varepsilon|x|^2$ is added to V_1 in problem (21) (see equation (31) below). Lastly, hypothesis [$\mathcal{H}5$] is always satisfied for V_1 and V_2 given by (4) for in that case, H is bounded from below and has a purely discrete spectrum. For V_1 and V_2 given by (5), (19) always holds. For neutral systems and positive ions, even a simple one-body model (Hartree-Fock or Kohn-Sham) allows in practice to construct an importance sampling function ψ_I satisfying (20).

Let us finally mention that in the example of two non-interacting fermions in a harmonic trap presented in Section 6, the hypotheses [$\mathcal{H}1$]-[$\mathcal{H}4$] are satisfied for ψ_I given by (47) with $0 < \widetilde{\omega} \leq 1 < \omega$.

Proposition 7 (Sample paths of the stochastic process). *Let $(W_t)_{t\geq 0}$ be a $3N$-dimensional Brownian motion. Under hypotheses [$\mathcal{H}1$]-[$\mathcal{H}3$], for any $x \in U_I$, the stochastic differential equation*

$$\begin{cases} dX_t^x = b(X_t^x)\,dt + dW_t, \\ X_0^x = x, \end{cases} \tag{23}$$

admits a unique solution. This solution is such that a.s., $t \mapsto X_t^x \in C^0(\mathbb{R}_+, \mathcal{C}(x))$ where $\mathcal{C}(x)$ denotes the connected component of U_I which contains x. In addition, X_t^x admits a density $p(t,x,y)$ w.r.t. the Lebesgue measure such that $\psi_I^2(x)p(t,x,y)$ is symmetric in variables x and y.

Remark 8. For $x \in U_I$, let us denote by P^x the law of $(X_t^x)_{t\geq 0}$. Combining Yamada-Watanabe theorem and the approach given by [25] Theorem 6.2.2 p.146, one obtains that for any connected component $\mathcal{C}$ of U_I, the family $\{P^x,\ x \in \mathcal{C}\}$ is strong Markov.

Remark 9. A solution to the stochastic differential equation $dX_t = dW_t + (\nabla \ln(\psi_I))(X_t)dt$ is a so-called distorted Brownian motion. Existence of a weak solution can be obtained by Dirichlet form techniques : for instance according to [1], (23) can be solved for each $x \in U$ if $\psi_I \in H^2_{\text{loc}}(\mathbb{R}^{3N})$ and if for some $\varepsilon > 0$, $|\nabla\psi_I(x)|^{3N+\varepsilon}/|\psi_I(x)|^{3N-2+\varepsilon}$ is locally integrable on $\mathbb{R}^{3N}$. Under [$\mathcal{H}1$]-[$\mathcal{H}2$], the latter integrability condition cannot hold since $\nabla\psi_I$ does not vanish on $\psi_I^{-1}(0)$ and $\psi_I^{-1}(0)$ is a $3N-1$-dimensional manifold because of the antisymmetry of ψ_I (U_I has at least two connected components). Our approach based on stochastic calculus enables us to obtain strong existence and trajectorial uniqueness for (23) and heavily relies on hypothesis (14) which prevents the sample paths from crossing the nodal surfaces of ψ_I.

Proposition 10 (Fokker-Planck equation). *Let us define*

$$f_2(t,x) = \psi_I^2(x)\mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^x)ds\right)\right)$$

where $(X_t^x)_{t\geq 0}$ denotes the stochastic process defined by (23), with convention $f_2(t,x) = 0$ when $\psi_I(x) = 0$. Under hypotheses [$\mathcal{H}1$]-[$\mathcal{H}4$], the function f_2 is a weak solution of (11) *in the following sense:* $\forall \varphi \in C_0^\infty(\mathbb{R}_+ \times \mathbb{R}^{3N})$, $\forall t \geq 0$,

$$\int_{\mathbf{R}^{3N}} \varphi(t,x) f_2(t,x) dx = \int_{\mathbf{R}^{3N}} \varphi(t,x) \psi_I^2(x) dx + \int_0^t \int_{\mathbf{R}^{3N}} \left(\frac{\partial \varphi}{\partial s} + \frac{1}{2}\Delta\varphi + b.\nabla\varphi - E_L\varphi \right)(s,x) f_2(s,x)\, ds\, dx. \tag{24}$$

The issue is now to characterize the function f_2. For this purpose, we introduce, for any connected component $\mathcal{C}$ of U_I, the self-adjoint operator $H_\mathcal{C}$ on $L^2(\mathcal{C})$ defined on the domain

$$D(H_\mathcal{C}) = \left\{ u \in H_0^1(\mathcal{C}), \quad -\frac{1}{2}\Delta u + Vu \in L^2(\mathcal{C}) \right\}, \tag{25}$$

by

$$H_\mathcal{C} u = -\frac{1}{2}\Delta u + Vu. \tag{26}$$

Note that it results from [$\mathcal{H}$1]-[$\mathcal{H}$2] that the boundary of the domain $\mathcal{C}$ is of class C^2. Therefore, in particular, $D(H_\mathcal{C}) = H^2(\mathcal{C}) \cap H_0^1(\mathcal{C})$ for V_2 given by (5), with point-like or smeared nuclei.

Proposition 11 (Identification of f_2). *For V_1 and V_2 given either by (4) or by (5), with point-like or smeared nuclei, and under hypotheses [$\mathcal{H}$1]-[$\mathcal{H}$4], the function*

$$\chi(t,x) = \frac{f_2(t,x)}{\psi_I(x)} = \psi_I(x) \mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^x) ds \right) \right)$$

is characterized by the following property: for each connected component $\mathcal{C}$ of U_I, the restriction v of χ to $\mathbb{R}_+ \times \mathcal{C}$ is the unique solution in $C^0(\mathbb{R}_+, D(H_\mathcal{C})) \cap C^1(\mathbb{R}_+, L^2(\mathcal{C}))$ of the problem

$$\left\{ \begin{array}{ll} \dfrac{\partial v}{\partial t} = \dfrac{1}{2}\Delta v - Vv & \text{in } \mathcal{D}'(]0,+\infty[\times\mathcal{C}), \\ v(0,\cdot) = \psi_I|_\mathcal{C}\,. & \end{array} \right. \tag{27}$$

Note that if ψ_I satisfies the tiling property, the N_c^I problems (27) are identical up to renumbering of particles.

Theorem 12 (Convergence of the DMC energy). *Let*

$$E^{\mathrm{DMC}}(t) = \frac{\displaystyle\int_{\mathbf{R}^3} E_L(x)\, f_2(t,x)\, dx}{\displaystyle\int_{\mathbf{R}^3} f_2(t,x)\, dx}.$$

For V_1 and V_2 given either by (4) or by (5), with point-like or smeared nuclei, and under hypotheses [$\mathcal{H}$1]-[$\mathcal{H}$5], one has

$$E^{\mathrm{DMC}}(t) = \frac{\displaystyle\int_{\mathbf{R}^{3N}} \psi_I^2(x)\, \mathbb{E}\left(E_L(X_t^x)\, \exp\left(-\int_0^t E_L\left(X_s^x\right) ds \right) \right) dx}{\displaystyle\int_{\mathbf{R}^{3N}} \psi_I^2(x)\, \mathbb{E}\left(\exp\left(-\int_0^t E_L\left(X_s^x\right) ds \right) \right) dx} \tag{28}$$

where $(X_t^x)_{t\geq 0}$ denotes the stochastic process defined by (23). When t goes to $+\infty$, $E^{\rm DMC}(t)$ converges exponentially fast toward

$$E_0^{\rm DMC} = \inf \left\{ \frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla\psi|^2 + \int_{\mathbf{R}^{3N}} V\psi^2, \quad \psi \in D(q_H), \quad \|\psi\|_{L^2} = 1, \quad \psi = 0 \text{ on } \psi_I^{-1}(0) \right\}.$$

One has $E_0^{\rm DMC} \geq E_0$, and the equality holds if and only if the nodal surfaces of ψ_I coincide with those of a ground state ψ_0 of H.

The Diffusion Monte Carlo (DMC) method consists in estimating $E^{\rm DMC}(t)$ for t large enough by using (28), or a similar expression [14]. The DMC method therefore provides with an upper bound $E_0^{\rm DMC}$ of E_0 which only depends on the nodal surfaces of the importance sampling function ψ_I (and not of the function ψ_I itself). Almost all the QMC calculations performed at the present time are based on the importance sampling technique described above. Some methods aiming at going beyong the Fixed Node Appoximation have been developed, but their use is still limited to small systems consisting of a few electrons, or to the special case of the homogenous electron gas. Let us incidently mention that very accurate QMC calculations on homogenous electron gas are used to fit the parameters of the approximated exchange-correlation functionals used in Density Functional Theory.

Remark 13. Formula (28) also reads

$$E^{\rm DMC}(t) = \frac{\displaystyle\sum_{n=1}^{N_c^I} \int_{\mathcal{C}_n} \psi_I^2(x)\, \mathbb{E}\left(E_L(X_t^x)\ \exp\left(-\int_0^t E_L\left(X_s^x\right) ds \right)\right) dx}{\displaystyle\sum_{n=1}^{N_c^I} \int_{\mathcal{C}_n} \psi_I^2(x)\, \mathbb{E}\left(\exp\left(-\int_0^t E_L\left(X_s^x\right) ds \right)\right) dx},$$

where $\mathcal{C}_1$, $\mathcal{C}_2$, ... $\mathcal{C}_{N_c^I}$ are the connected components of U_I. From Proposition 7, the whole sample path $t \mapsto X_t^x$ is a.s. trapped in the connected component containing x. One can therefore consider that in the DMC method, N_c^I calculations are done independently (one in each connected component) and that the N_c^I results are then averaged. If ψ_I satisfies the tiling property, the N_c^I problems are identical up to renumbering of particles, and therefore, the final result will not be affected if the walkers are not equally distributed in the various connected components of U_I.

Remark 14. The equivalent of Corollary 5 for $E_0^{\rm DMC}$ is the following : in the case when V_1 and V_2 are given by (4), if one introduces the ground state energy E_n^0 of $H_{\mathcal{C}_n}$ (where $\mathcal{C}_1$, $\mathcal{C}_2$, ... $\mathcal{C}_{N_c^I}$ are the connected components of U_I), then $E_0^{\rm DMC} = \min_{1\leq n\leq N_c^I} E_n^0$. In the case when V_1 and V_2 are given by (5), we have again $E_0^{\rm DMC} = \min_{1\leq n\leq N_c^I} \inf \sigma(H_{\mathcal{C}_n}^S)$, where $H_{\mathcal{C}_n}^S$ is the operator $H_{\mathcal{C}_n}$ with domain restricted to symmetric functions on $\mathcal{C}_n$. In any cases, if ψ_I satisfies the tiling property, one can check that the $(E_n^0)_{1\leq n\leq N_c^I}$ (resp. the $(\inf \sigma(H_{\mathcal{C}_n}^S))_{1\leq n\leq N_c^I}$) are equal, since all the connected components of U_I can be obtained from any one by permutations.

5 Proofs of the main results

Proof of Theorem 4. Let $\mathcal{C}$ be a connected component[1] of the open set $U_0 = \mathbb{R}^{3N} \setminus \psi_0^{-1}(0)$ and $\Omega = \bigcup_{\sigma \in \mathfrak{S}_N} \mathcal{C}_\sigma$. Let $\mathcal{I}$ be a subset of $\mathfrak{S}_N$ such that

$$\left\{ \begin{array}{l} \Omega = \bigcup_{\sigma \in \mathcal{I}} \mathcal{C}_\sigma \\ \forall (\sigma, \sigma') \in \mathcal{I} \times \mathcal{I}, \quad (\sigma \neq \sigma') \ \Rightarrow \ (\mathcal{C}_\sigma \cap \mathcal{C}_{\sigma'} = \emptyset). \end{array} \right.$$

Let ϕ be the function defined by

$$\phi(x) = \left| \begin{array}{ll} \psi_0(x) & \text{if } x \in \Omega \\ 0 & \text{otherwise,} \end{array} \right.$$

and $\widetilde{\psi}_0 = \dfrac{\phi}{\|\phi\|_{L^2}}$. It is easy to check that $\widetilde{\psi}_0 \in D(q_H)$ and that $\|\widetilde{\psi}_0\|_{L^2} = 1$. Besides,

$$\begin{aligned} \langle \widetilde{\psi}_0, H \widetilde{\psi}_0 \rangle &= \frac{1}{2} \int_{\mathbb{R}^{3N}} |\nabla \widetilde{\psi}_0|^2 + \int_{\mathbb{R}^{3N}} V \widetilde{\psi}_0^2 \\ &= \frac{1}{\|\phi\|_{L^2}^2} \left(\frac{1}{2} \int_\Omega |\nabla \psi_0|^2 + \int_\Omega V \psi_0^2 \right) \\ &= \frac{1}{\|\phi\|_{L^2}^2} \sum_{\sigma \in \mathcal{I}} \left(\frac{1}{2} \int_{\mathcal{C}_\sigma} |\nabla \psi_0|^2 + \int_{\mathcal{C}_\sigma} V \psi_0^2 \right) \\ &= \frac{|\mathcal{I}|}{\|\phi\|_{L^2}^2} \left(\frac{1}{2} \int_{\mathcal{C}} |\nabla \psi_0|^2 + \int_{\mathcal{C}} V \psi_0^2 \right) \end{aligned}$$

and

$$\|\phi\|_{L^2}^2 = |\mathcal{I}| \int_{\mathcal{C}} \psi_0^2.$$

As in addition $\psi_0|_{\mathcal{C}} \in H^1_0(\mathcal{C})$ and $-\frac{1}{2}\Delta \psi_0 + V \psi_0 = E_0 \psi_0$ in $\mathcal{D}'(\mathcal{C})$, it follows from Green's formula that

$$\frac{1}{2} \int_{\mathcal{C}} |\nabla \psi_0|^2 + \int_{\mathcal{C}} V \psi_0^2 = \int_{\mathcal{C}} \left(-\frac{1}{2} \Delta \psi_0 + V \psi_0 \right) \psi_0 = E_0 \int_{\mathcal{C}} \psi_0^2. \tag{29}$$

Therefore $\langle \widetilde{\psi}_0, H \widetilde{\psi}_0 \rangle = E_0$. The function $\widetilde{\psi}_0$ then is a ground state of the operator H and thus satisfies equation

$$-\frac{1}{2} \Delta \widetilde{\psi}_0 + V \widetilde{\psi}_0 = E_0 \widetilde{\psi}_0.$$

Let Σ be the (empty or finite) set of the points at which V_1 is not C^∞ and

$$\begin{aligned} \gamma &= \left\{ (x_1, \cdots, x_N) \in \mathbb{R}^{3N}, \quad \exists i \in |[1,N]|, \quad x_i \in \Sigma \right\} \\ & \quad \cup \left\{ (x_1, \cdots, x_N) \in \mathbb{R}^{3N}, \quad \exists (i,j) \in |[1,N]| \times |[1,N]|, \quad i \neq j, \quad x_i = x_j \right\}. \end{aligned}$$

It can be easily checked that γ is a closed negligeable set, that the open set $\mathbb{R}^{3N} \setminus \gamma$ is connected, that V is bounded on any compact set of $\mathbb{R}^{3N} \setminus \gamma$ and that $\widetilde{\psi}_0 \in H^2(\mathbb{R}^{3N})$. One can thus apply a unique continuation principle (see e.g. Theorem XIII.57 and the

[1] Notice that since we are in $\mathbb{R}^{3N}$ and U_0 is an open set, $\mathcal{C}$ is an open arc connected set.

comment just below, page 226 of [22]) : if $u \in L^2(\mathbb{R}^{3N})$ satisfies $-\frac{1}{2}\Delta u + Vu = E_0 u$ and vanishes on an open set of $\mathbb{R}^{3N}$, then u is identically zero. It follows that $\widetilde{\psi}_0$ is not identically equal to zero on each open set of $\mathbb{R}^{3N}$, and therefore that $\Omega = U_0$. $\square$

Proof of corollary 5. Let $\mathcal{C}$ be a connected component of $U_0 = \mathbb{R}^{3N} \setminus \psi_0^{-1}(0)$ and

$$E_{\mathcal{C}} = \inf \left\{ \frac{1}{2} \int_{\mathcal{C}} |\nabla \psi|^2 + \int_{\mathcal{C}} V\psi^2, \quad \psi \in H_0^1(\mathcal{C}), \quad \int_{\mathcal{C}} \psi^2 = 1 \right\}. \tag{30}$$

The restriction of ψ_0 to $\mathcal{C}$ is in $H_0^1(\mathcal{C})$ and satisfies (29). Let us denote by $\psi_{\mathcal{C}}$ the function defined on $\mathcal{C}$ by

$$\psi_{\mathcal{C}}(x) = \frac{\psi_0(x)}{\left(\int_{\mathcal{C}} |\psi_0|^2 \right)^{1/2}}.$$

We have $\psi_{\mathcal{C}} \in H_0^1(\mathcal{C})$, $\int_{\mathcal{C}} \psi_{\mathcal{C}}^2 = 1$ and

$$\frac{1}{2} \int_{\mathcal{C}} |\nabla \psi_{\mathcal{C}}|^2 + V |\psi_{\mathcal{C}}|^2 = E_0.$$

Therefore $E_0 \geq E_{\mathcal{C}}$. When V_1 and V_2 are given by (4), the remaining of the proof is easy. In this case indeed, the operator $H_{\mathcal{C}}$ defined by (25)-(26) has a purely discrete spectrum and $\psi_{\mathcal{C}}$ is an eigenvector of $H_{\mathcal{C}}$ which is either positive or negative on $\mathcal{C}$. Therefore, by standard arguments, $\psi_{\mathcal{C}}$ is the ground state of $H_{\mathcal{C}}$ and $E_{\mathcal{C}} = E_0$. When V_1 and V_2 are given by (5), we reason as follows. We denote by

$$\mathcal{E}(\psi) = \frac{1}{2} \int_{\mathcal{C}} |\nabla \psi|^2 + \int_{\mathcal{C}} V\psi^2 = \langle H_{\mathcal{C}} \psi, \psi \rangle$$

the energy functional (defined on $H_0^1(\mathcal{C})$) and we consider a minimizing sequence $(\psi_n)_{n \in \mathbb{N}}$ of problem (30). As for any $\psi \in H_0^1(\mathcal{C})$, $|\psi| \in H_0^1(\mathcal{C})$ and $\mathcal{E}(|\psi|) = \mathcal{E}(\psi)$, we can assume that ψ_n is non-negative on $\mathcal{C}$ for any $n \in \mathbb{N}$. We then introduce $\mathcal{J}$ the subgroup of $\mathfrak{S}_N$ consisting of the permutations σ such that [2]

$$\forall (x_1, \cdots, x_N) \in \mathcal{C}, \qquad (x_{\sigma(1)}, \cdots, x_{\sigma(N)}) \in \mathcal{C}.$$

Notice that as ψ_0 is antisymmetric, for any $\sigma \in \mathfrak{S}_N$, $\mathcal{C}_\sigma$ is a connected component of U_0, which ensures that $\mathcal{J} = \{\sigma \in \mathfrak{S}_N,\ \mathcal{C}_\sigma \cap \mathcal{C} \neq \emptyset\}$. Let

$$\chi_n = \frac{\displaystyle\sum_{\sigma \in \mathcal{J}} \psi_n^\sigma}{\left\| \displaystyle\sum_{\sigma \in \mathcal{J}} \psi_n^\sigma \right\|_{L^2}}$$

where $\psi_n^\sigma(x_1, \cdots, x_N) = \psi_n(x_{\sigma(1)}, \cdots, x_{\sigma(N)})$. The function χ_n is well-defined for ψ_n is non-negative and non-identically equal to zero. We then have $\chi_n \in H_0^1(\mathcal{C})$, $\|\chi_n\|_{L^2} = 1$

[2] Notice that the permutations in $\mathcal{J}$ are even since odd permutations change the sign of ψ and therefore cannot let a connected component of U_0 invariant.

and

$$\begin{aligned}
0 \leq \mathcal{E}(\chi_n) - E_{\mathcal{C}} &= \langle (H - E_{\mathcal{C}})\, \chi_n, \chi_n \rangle \\
&= \frac{1}{\left\| \displaystyle\sum_{\sigma \in \mathcal{J}} \psi_n^\sigma \right\|_{L^2}^2} \sum_{\sigma, \sigma' \in \mathcal{J}} \langle (H - E_{\mathcal{C}})\, \psi_n^\sigma, \psi_n^{\sigma'} \rangle \\
&\leq \sum_{\sigma, \sigma' \in \mathcal{J}} \langle (H - E_{\mathcal{C}})\, \psi_n^\sigma, \psi_n^{\sigma'} \rangle \\
&= \sum_{\sigma, \sigma' \in \mathcal{J}} \langle (H - E_{\mathcal{C}})^{1/2}\, \psi_n^\sigma, (H - E_{\mathcal{C}})^{1/2}\, \psi_n^{\sigma'} \rangle \\
&\leq \sum_{\sigma, \sigma' \in \mathcal{J}} \langle (H - E_{\mathcal{C}})\, \psi_n^\sigma, \psi_n^\sigma \rangle^{1/2} \langle (H - E_{\mathcal{C}})\, \psi_n^{\sigma'}, \psi_n^{\sigma'} \rangle^{1/2} \\
&= |\mathcal{J}|^2 \left(\mathcal{E}(\psi_n) - E_{\mathcal{C}} \right),
\end{aligned}$$

the last equality arising from the symmetry of H with respect to renumbering of particles. Therefore, $(\chi_n)_{n \in \mathbb{N}}$ is a minimizing sequence for problem (30). As by construction, each χ_n satisfies the symmetry property

$$\forall (x_1, \cdots, x_N) \in \mathcal{C}, \quad \forall \sigma \in \mathcal{J}, \qquad \chi_n(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \chi_n(x_1, \cdots, x_N),$$

whith $\mathcal{J} = \{\sigma \in \mathfrak{S}_N,\ \mathcal{C}_\sigma \cap \mathcal{C} \neq \emptyset\}$, the formula

$$\forall (x_1, \cdots, x_N) \in \mathcal{C}, \quad \forall \sigma \in \mathfrak{S}_N, \qquad \phi_n(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \sqrt{\frac{|\mathcal{J}|}{N!}}\, \epsilon(\sigma) \chi_n(x_1, \cdots, x_N),$$

(where, by definition, $\chi_n = 0$ outside of $\mathcal{C}$) provides a function of $D(q_H)$ such that $\|\phi_n\|_{L^2} = 1$ and $\langle \phi_n, H\phi_n \rangle = \mathcal{E}(\chi_n)$. Therefore $E_0 \leq \lim_{n \to +\infty} \langle \phi_n, H\phi_n \rangle = E_{\mathcal{C}}$. Finally, $E_{\mathcal{C}} = E_0$, which concludes the proof. □

Proof of Proposition 6. The existence of a minimizer $\left\{\phi_i^H\right\}_{1 \leq i \leq N}$ to the Hartree problem (21) for neutral or positively charged systems is proved e.g. in [18]. In the same article, it is shown that the ϕ_i^H satisfy the Hartree equations

$$-\frac{1}{2}\Delta \phi_i^H + V_1 \phi_i^H + (\rho \star V_2)\, \phi_i^H = \epsilon_i \phi_i^H$$

with $\rho = \displaystyle\sum_{i=1}^N |\phi_i^H|^2$, and that the eigenvalues ϵ_i are negative. It is then easy to check that $\phi_i^H \in C^\infty(\mathbb{R}^3) \cap H^2(\mathbb{R}^3)$, that $\rho \star V_2$ vanishes at infinity, and then using the maximum principle, that ϕ_i enjoys an exponential fall-off of exponent $\sqrt{-\epsilon}$ for any ϵ such that $\epsilon_i < \epsilon < 0$. Properties (12) and (13) follow. Besides, a simple calculation shows that

$$-\frac{1}{2}\Delta \psi_I + \sum_{i=1}^N \left(V_1(x_i) + (\rho \star V_2)(x_i) \right) \psi_I = \left(\sum_{i=1}^N \epsilon_i \right) \psi_I. \tag{31}$$

Consequently

$$E_L = \frac{H\psi_I}{\psi_I} = -\frac{1}{2}\frac{\Delta \psi_I}{\psi_I} + V = \sum_{i=1}^N \epsilon_i + \sum_{1 \leq i < j \leq N} V_2(x_i - x_j) - \sum_{i=1}^N (\rho \star V_2)(x_i).$$

As $\rho \star V_2$ is bounded and V_2 non negative, hypothesis $[\mathcal{H}4]$ is fulfilled. Lastly, it is easy to check that ψ_I is the ground state of the N-body fermionic hamiltonian

$$-\frac{1}{2}\Delta + \sum_{i=1}^{N} \left(V_1(x_i) + (\rho \star V_2)(x_i)\right)$$

and that Theorem 4 also holds true for one-body and two-body potentials respectively given by $V_1 + \rho \star V_2$ and 0. Therefore, ψ_I satisfies the tiling property. $\square$

Proof of Proposition 7. Let us first prove trajectorial uniqueness. For $x \in U_I$, assume that X_t^x is a solution of (23) such that $t \to X_t^x \in C^0(\mathbb{R}_+, \mathcal{C}(x))$ and that $\tilde{X}_t^x$ is another solution. Let $\sigma_n = \inf\{t \geq 0 : |\psi_I(X_t^x)| \wedge |\psi_I(\tilde{X}_t^x)| \leq 1/n\}$ for $n \in \mathbb{N}^*$. One has for any $t \geq 0$,

$$|X_{t\wedge\sigma_n}^x - \tilde{X}_{t\wedge\sigma_n}^x| \leq \int_0^{t\wedge\sigma_n} \left|\frac{\nabla\psi_I(X_s^x) - \nabla\psi_I(\tilde{X}_s^x)}{\psi_I(X_s^x)}\right| + \left|\frac{(\psi_I(\tilde{X}_s^x) - \psi_I(X_s^x))\nabla\psi_I(\tilde{X}_s^x)}{\psi_I(X_s^x)\psi_I(\tilde{X}_s^x)}\right| ds.$$

Because of (13) there is a constant K_n such that $\forall s \leq \sigma_n$, $|X_s^x| + |\tilde{X}_s^x| \leq K_n$. Since ψ_I is a C^2 function and using the definition of σ_n, one deduces that there is a constant C_n only depending on n such that

$$\forall t \geq 0,\ |X_{t\wedge\sigma_n}^x - \tilde{X}_{t\wedge\sigma_n}^x| \leq C_n \int_0^{t\wedge\sigma_n} |X_s^x - \tilde{X}_s^x| ds \leq C_n \int_0^t |X_{s\wedge\sigma_n}^x - \tilde{X}_{s\wedge\sigma_n}^x| ds.$$

By Gronwall's lemma, one obtains that X_t^x and $\tilde{X}_t^x$ coincide up to time σ_n for any $n \in \mathbb{N}^*$. Therefore $\sigma_n = \inf\{t \geq 0 : |\psi_I(X_t^x)| \leq 1/n\}$. Because $t \mapsto X_t^x \in C^0(\mathbb{R}_+, \mathcal{C}(x))$ a.s., $\lim_{n\to+\infty} \sigma_n = +\infty$ a.s., which concludes the proof of uniqueness.

To prove existence, we are going to introduce suitable regularizations of the drift coefficient $b = \nabla\psi_I/\psi_I$. Let $\gamma : \mathbb{R}_+ \to \mathbb{R}_+$ be an increasing C^2 function such that

$$\begin{cases} \gamma(r) = r \text{ for } r \geq 1, \\ \gamma(r) = 1/2 \text{ for } r \leq 1/4, \\ \forall r \geq 0,\ 0 \leq \gamma'(r) \leq 1. \end{cases}$$

For $n \in \mathbb{N}^*$, we define

$$g_n : y \in \mathbb{R}^{3N} \mapsto \frac{\exp(-|y-x|/(2n))}{\sqrt{n^{3N} s_{3N-1}\Gamma(3N)}},$$

where Γ denotes Euler's gamma function and s_{3N-1} the surface of the unit sphere in $\mathbb{R}^{3N}$. Notice that g_n^2 is a probability density on $\mathbb{R}^{3N}$. For $n \in \mathbb{N}^*$, we set

$$\psi_{n,T}(y) = c_n \times g_n(y)\gamma\left(\frac{|\psi_I|(y)}{g_n(y)}\right) \tag{32}$$

with $c_n = \left(\int_{\mathbb{R}^{3N}} g_n^2\gamma^2(|\psi_I|/g_n)(y)dy\right)^{-1/2}$.
As, by definition of γ, $g_n\gamma(|\psi_I|/g_n) \leq |\psi_I| \vee g_n$, the previous integral is finite. The associated regularized drift coefficient is $b_n(y) = \nabla \ln \psi_{n,T}(y)$. One easily checks that

$$b_n(y) = \begin{cases} b(y) & \text{if } |\psi_I|(y) \geq g_n(y), \\ -\dfrac{(y-x)}{2n|y-x|} & \text{if } |\psi_I|(y) \leq g_n(y)/4. \end{cases}$$

¿From now on we suppose that n is bigger than n_0 such that $n_0 > 1/c$ where c denotes the constant given by (13) and that $|\psi_I|(x) > ({n_0}^{3N} s_{3N-1}\Gamma(3N))^{-1/2}$. This way, b_n is equal to $-(y-x)/(2n|y-x|)$ outside a compact set and equal to b on a neighbourhood of x. Since one easily checks, using (32), that for any $i,j \in \{1,\dots,3N\}$, function $\partial^2_{y_i y_j} \ln(\psi_{n,T})(y)$ is locally bounded in $\mathbb{R}^{3N} \setminus \{x\}$, the drift coefficient b_n is globally bounded and Lipschitz continuous on $\mathbb{R}^{3N}$. Therefore existence and trajectorial uniqueness hold for the stochastic differential equation

$$dX_t^{x,n} = dW_t + b_n(X_t^{x,n})dt,\ X_0^{x,n} = x.$$

Let

$$\tau_n^x = \inf\{t \geq 0 : |\psi_I|(X_t^{x,n}) \leq (n^{3N} s_{3N-1}\Gamma(3N))^{-1/2}\}.$$

Setting $X_t^x = X_t^{x,n}, \forall t \in [\tau_{n-1}^x, \tau_n^x)$ for $n \geq n_0$ (convention $\tau_{n_0-1}^x = 0$), using the fact that when $n_0 \leq k \leq l$, $X_t^{x,k} = X_t^{x,l}$ for $t \in [0, \tau_k^x)$, one obtains a solution of (23) on $[0, \tau_\infty^x)$ where $\tau_\infty^x = \lim_{n\to+\infty} \tau_n^x$. Since $|\psi_I|(X_t^x)$ is positive for $t \in [0, \tau_\infty^x)$, X_t^x remains in $\mathcal{C}(x)$ on this time-interval. The next two lemmas are aimed at checking that for any $x \in U_I$, τ_∞^x is a.s. infinite, which also ensures that a.s., $t \mapsto X_t^x \in C^0(\mathbb{R}_+, \mathcal{C}(x))$. First, using especially (14), we will prove that if $|X_t^x|$ remains bounded on $[0, \tau_\infty^x)$, then $\tau_\infty^x = \infty$. When (17) holds, the same line of reasoning yields that τ_∞^x is a.s. infinite. We will next prove that when (16) holds, $|X_t^x|$ cannot go to infinity in finite time.

Lemma 15.

$$\forall x \in U_I,\ \mathbb{P}\left(\tau_\infty^x < +\infty,\ \sup_{t\in[0,\tau_\infty^x)} |X_t^x| < +\infty\right) = 0.$$

In addition, under (17), $\mathbb{P}(\tau_\infty^x < +\infty) = 0$.

Proof : On $\{\tau_\infty^x < \infty\}$, by definition of τ_n^x, one has $|\psi_I|(X_{\tau_n^x}^x) \leq (n^{3N} s_{3N-1}\Gamma(3N))^{-1/2}$ and therefore $\lim_{n\to+\infty} |\psi_I|(X_{\tau_n^x}^x) = 0$.
Let $s(x) = 1_{\{\psi_I(x)>0\}} - 1_{\{\psi_I(x)<0\}}$. For $t < \tau_\infty^x$,

$$d|\psi_I|(X_t^x) = \frac{|\nabla\psi_I|^2}{|\psi_I|}(X_t^x)\,dt + s(x)\nabla\psi_I(X_t^x).dW_t + \frac{1}{2}s(x)\Delta\psi_I(X_t^x)dt. \quad (33)$$

The main idea of the proof of the first assertion consists in checking that because of (14), the first term of the r.h.s. prevents $|\psi_I|(X_t^x)$ from vanishing in finite time while X_t^x remains in a compact set. Let $K, S > 0$ and $\sigma_K = \inf\{t \geq 0, |X_t^x| > K\}$. We are going to check that

$$\mathbb{P}\left(\tau_\infty^x \leq S,\ \sup_{t\in[0,\tau_\infty^x)} |X_t^x| \leq K\right) = \mathbb{P}\left(\tau_\infty^x \leq S \wedge \sigma_K\right) = 0. \quad (34)$$

By (14), there exist positive constants α and M such that

$$\forall y \in \mathcal{C}(x) \cap \bar{B}(0,K),\ |\psi_I|(y) \leq \alpha \Rightarrow |\Delta\psi_I(y)| \leq M|\nabla\psi_I(y)|^2. \quad (35)$$

Let $\rho : \mathbb{R}_+^* \to \mathbb{R}_-$ be a C^2 non decreasing function such that

$$\rho(y) = \begin{cases} \displaystyle\int_\alpha^y \frac{e^{Mz}}{z^2}\,dz & \text{if } r \leq \alpha/2, \\ 0 & \text{if } r \geq \alpha. \end{cases}$$

Applying Itô's formula, remarking that the non-negative function ρ' vanishes together with ρ'' on $[\alpha, +\infty)$ and using (35), one obtains

$$\rho(|\psi_I|(X^x_{S\wedge\sigma_K\wedge\tau^x_n})) = \rho(|\psi_I|(x)) + s(x)\int_0^{S\wedge\sigma_K\wedge\tau^x_n} \rho'(|\psi_I|(X^x_s))\nabla\psi_I(X^x_s).dW_s$$
$$+\int_0^{S\wedge\sigma_K\wedge\tau^x_n}\left(\frac{|\nabla\psi_I|^2}{|\psi_I|}(X^x_s)+\frac{s(x)}{2}\Delta\psi_I(X^x_s)\right)\rho'(|\psi_I|(X^x_s))+\frac{1}{2}|\nabla\psi_I(X^x_s)|^2\rho''(|\psi_I|(X^x_s))ds$$
$$\geq \rho(|\psi_I|(x)) + s(x)\int_0^{S\wedge\sigma_K\wedge\tau^x_n} \rho'(|\psi_I|(X^x_s))\nabla\psi_I(X^x_s).dW_s$$
$$+\int_0^{S\wedge\sigma_K\wedge\tau^x_n}|\nabla\psi_I(X^x_s)|^2\left[\left(\frac{1}{|\psi_I|}(X^x_s)-\frac{M}{2}\right)\rho'(|\psi_I|(X^x_s))+\frac{1}{2}\rho''(|\psi_I|(X^x_s))\right]ds. \tag{36}$$

For $s < \tau^x_n$, $|\psi_I(X^x_s)| > (n^{3N}s_{3N-1}\Gamma(3N))^{-1/2}$, and by (13), $|X^x_s|$ and therefore $|\nabla\psi_I(X^x_s)|$ are bounded. As a consequence the expectation of the stochastic integral in the right-hand-side of (36) is zero. The function $y \mapsto \left(\frac{1}{y}-\frac{M}{2}\right)\rho'(y)+\frac{1}{2}\rho''(y)$ vanishes on $]0,\alpha/2]\cup[\alpha,+\infty[$ and is bounded from below on $[\alpha/2,\alpha]$. Since because of (13), when $|\psi_I(X^x_s)|$ belongs to $[\alpha/2,\alpha]$, $|\nabla\psi_I(X^x_s)|$ remains bounded, taking expectations in (36), one obtains

$$\mathbb{E}\left(\rho(|\psi_I|(X^x_{S\wedge\tau^x_n\wedge\sigma}))\right) \geq -C(1+S),$$

where the positive constant C does not depend on n. As the left-hand-side is smaller than $\rho((n^{3N}s_{3N-1}\Gamma(3N))^{-1/2})\mathbb{P}(\tau^x_n \leq S\wedge\sigma_K)$ and $\rho((n^{3N}s_{3N-1}\Gamma(3N))^{-1/2})$ goes to $-\infty$ as n tends to $+\infty$, one deduces that (34) holds. As S and K are arbitrary, the first assertion follows.

Let us now assume (17). For K such that $\forall y \in \mathcal{C}(x)$, $|y| \geq K \Rightarrow s(x)\Delta\psi_I(y) \geq 0$, let α and M be such that (35) holds. Then

$$\forall y \in \mathcal{C}(x),\ |\psi_I(y)| \leq \alpha \Rightarrow s(x)\Delta\psi_I(y) \geq -M|\nabla\psi_I(y)|^2.$$

As a consequence (36) holds with $S\wedge\sigma_K$ replaced by S. As above, one concludes that $\mathbb{P}(\tau^x_\infty < +\infty) = 0$. □

Lemma 16. *When (16) holds,*

$$\forall x \in U_I,\ \mathbb{P}\left(\tau^x_\infty < +\infty,\ \sup_{t\in[0,\tau^x_\infty)}|X^x_t| = +\infty\right) = 0.$$

Proof : Let $(x_0, C, C') \in \mathbb{R}^{3N}\times(\mathbb{R}^*_+)^2$ be a triple associated to $\mathcal{C}(x)$ by (16).
Let $\rho : \mathbb{R}_+ \to \mathbb{R}_+$ be an increasing C^2 function constant on $[0, C]$ and such that $\rho(r) = r$ on $[C+1,+\infty)$ and $\rho(r) \geq r$ on $\mathbb{R}_+$. By Itô's formula and (16), for $t < \tau^x_\infty$,

$$\begin{aligned}\rho(|X^x_t-x_0|^2) =&\rho(|x-x_0|^2)+\int_0^t\rho'(|X^x_s-x_0|^2)\,(2(X^x_s-x_0).(b(X^x_s)ds+dW_s)+3Nds)\\&+2\int_0^t\rho''(|X^x_s-x_0|^2)|X^x_s-x_0|^2ds,\\ \leq&\rho(|x-x_0|^2)+((3N+2C')\|\rho'\|_\infty+2(C+1)^2\|\rho''\|_\infty)t\\&+2\int_0^t\rho'(|X^x_s-x_0|^2)(X^x_s-x_0).dW_s+2C'\|\rho'\|_\infty\int_0^t|X^x_s-x_0|^2\,ds.\end{aligned}$$

Therefore, we have:

$$|X^x_t - x_0|^2 \leq C''(1+t) + 2\int_0^t \rho'(|X^x_s - x_0|^2)(X^x_s - x_0).dW_s + 2C'\|\rho'\|_\infty \int_0^t |X^x_s - x_0|^2\, ds.$$

Introducing $\sigma_k = \inf\{t \geq 0 : |X^x_t - x_0| \geq k\}$ for $k \in \mathbb{N}^*$, one deduces that for $S > 0$, $\forall k \in \mathbb{N}^*$, $\forall n \geq n_0$, $\forall t \in [0, S)$,

$$\begin{aligned}\mathbb{E}(|X^x_{t\wedge\sigma_k\wedge\tau^x_n} - x_0|^2) \leq & C''(1+S) + 2C'\|\rho'\|_\infty \mathbb{E}\left(\int_0^{t\wedge\sigma_k\wedge\tau^x_n} |X^x_s - x_0|^2\, ds\right), \\ \leq & C''(1+S) + 2C'\|\rho'\|_\infty \int_0^t \mathbb{E}(|X^x_{s\wedge\sigma_k\wedge\tau^x_n} - x_0|^2)\, ds.\end{aligned}$$

Therefore, by Gronwall Lemma, $\forall k \in \mathbb{N}^*$, $\forall n \geq n_0$,

$$\mathbb{E}(|X^x_{S\wedge\sigma_k\wedge\tau^x_n} - x_0|^2) \leq K$$

where the constant K depends on S but neither on n nor on k. As

$$k^2\mathbb{P}(\sigma_k \leq S \wedge \tau^x_n) \leq \mathbb{E}(|X^x_{S\wedge\sigma_k\wedge\tau^x_n} - x_0|^2),$$

one obtains that $\mathbb{P}(\lim_{k\to+\infty} \sigma_k \leq S \wedge \tau^x_\infty) = 0$. Since

$$\left\{\tau^x_\infty \leq S,\ \sup_{t\in[0,\tau^x_\infty)} |X^x_t| = +\infty\right\} \subset \left\{\lim_{k\to+\infty} \sigma_k \leq S \wedge \tau^x_\infty\right\},$$

one concludes that $\mathbb{P}\left(\tau^x_\infty \leq S,\ \sup_{t\in[0,\tau^x_\infty)} |X^x_t| = +\infty\right) = 0$, where $S > 0$ is arbitrary. $\square$

To conclude the proof of Proposition 7, one still has to check that for any $t > 0$, X^x_t has a density $p(t, x, y)$ w.r.t. Lebesgue measure such that function $\psi_I^2(x)p(t, x, y)$ is symmetric in variables x and y. Let us briefly recall the argument given for instance in [24] which ensures that $X^{x,n}_t$ satisfies an analogous property.
According to Girsanov theorem, for $\phi : \mathbb{R}^{3N} \to \mathbb{R}$ measurable and bounded,

$$\mathbb{E}(\phi(X^{x,n}_t)) = \mathbb{E}\left(\phi(x + W_t)\exp\left(+\int_0^t b_n(x + W_s).dW_s - \frac{1}{2}\int_0^t |b_n|^2(x + W_s)ds\right)\right).$$

As $b_n = \nabla \ln \psi_{n,T}$ by Itô's formula,

$$\int_0^t b_n(x + W_s).dW_s = \ln\left(\frac{\psi_{n,T}(x + W_t)}{\psi_{n,T}(x)}\right) - \frac{1}{2}\int_0^t \Delta \ln \psi_{n,T}(x + W_s)ds.$$

Therefore conditioning by $x + W_t$ one obtains $\mathbb{E}(\phi(X^{x,n}_t)) = \int_{\mathbb{R}^{3N}} \phi(y)\frac{\psi_{n,T}(y)}{\psi_{n,T}(x)}\alpha(t, x, y)dy$, where

$$\alpha(t, x, y) = \mathbb{E}\left(\exp\left(-\frac{1}{2}\int_0^t \left(|b_n|^2 + \Delta \ln \psi_{n,T}\right)\left(x + W_s + \frac{s}{t}(y - x - W_t)\right) ds\right)\right)$$

is symmetric in variables x and y by time-reversal of the Brownian bridge. As a consequence, the density $p_n(t, x, y) = \psi_{n,T}(y)\alpha(t, x, y)/\psi_{n,T}(x)$ of $X^{x,n}_t$ is such that $\psi^2_{n,T}(x)p_n(t, x, y)/c_n^2$ is symmetric in variables x and y.
As $X^x_t = X^{x,n}_t$ on $\{\tau^x_n > t\}$ and $\lim_{n\to+\infty} \tau^x_n = +\infty$ a.s., the law of $X^{x,n}_t$ converges in

variation to the one of X_t^x. Therefore X_t^x has a density $p(t,x,y)$ which is the limit in $L^1(\mathbb{R}^{3N})$ of $p_n(t,x,y)$. Let $K>0$

$$\int_{B(0,K)\times\mathbf{R}^{3N}}\left|\frac{\psi^2_{n,T}(x)}{c_n^2}p_n(t,x,y)-\psi_I^2(x)p(t,x,y)\right|dxdy\le\int_{B(0,K)}\left|\frac{\psi^2_{n,T}(x)}{c_n^2}-\psi_I^2(x)\right|dx$$
$$+\int_{\mathbf{R}^{3N}\times\mathbf{R}^{3N}}\psi_I^2(x)|p(t,x,y)-p_n(t,x,y)|dxdy.$$

Remarking that for any $x\in\mathbb{R}^{3N}$, $\psi_{n,T}(x)/c_n$ converges to $|\psi_I(x)|$ as $n\to+\infty$ and that for $n\ge n_0$, $\psi^2_{n,T}(x)/c_n^2\le(n_0^{3N}s_{3N-1}\Gamma(3N))^{-1}\vee\psi_I^2(x)$, one easily check that both terms of the r.h.s. converge to 0 as $n\to+\infty$ according to Lebesgue's theorem. Therefore $\psi_I^2(x)p(t,x,y)$ is symmetric in variables x and y on $B(0,K)\times B(0,K)$ for any $K>0$. $\square$

Proof of Proposition 10. The proof relies on the following Lemma:

Lemma 17. *Let $t\ge0$. For any function $\phi:\mathbb{R}^{3N}\to\mathbb{R}$ non-negative or such that $\int_{\mathbf{R}^{3N}}|\phi(x)|f_2(t,x)dx<+\infty$,*

$$\int_{\mathbf{R}^{3N}}\phi(x)f_2(t,x)dx=\int_{\mathbf{R}^{3N}}\psi_I^2(x)\mathbb{E}\left(\phi(X_t^x)\exp\left(-\int_0^tE_L(X_s^x)ds\right)\right)dx.$$

Proof of Lemma 17 : Let us first suppose that ϕ is positive and bounded. Using Lebesgue's theorem, then the Markov property given in Remark 8 and the symmetry of $\psi_I^2(x)p(s,x,y)$ in variables x and y (see Proposition 7), one obtains

$$\int_{\mathbf{R}^{3N}}\phi(x)f_2(t,x)dx=\lim_{n\to+\infty}\int_{\mathbf{R}^{3N}}\phi(x)\psi_I^2(x)\mathbb{E}\left(\prod_{k=1}^n\exp(-tE_L(X^x_{kt/n})/n)\right)dx$$
$$=\lim_{n\to+\infty}\int_{\mathbf{R}^{(n+1)\times3N}}\phi(x_1)\psi_I^2(x_1)\prod_{k=1}^n\left[p(t/n,x_k,x_{k+1})\exp(-tE_L(x_{k+1})/n)\right]dx_1\dots dx_{n+1}$$
$$=\lim_{n\to+\infty}\int_{\mathbf{R}^{(n+1)\times3N}}\phi(x_1)\psi_I^2(x_{n+1})\prod_{k=1}^n\left[p(t/n,x_{k+1},x_k)\exp(-tE_L(x_{k+1})/n)\right]dx_1\dots dx_{n+1}$$
$$=\lim_{n\to+\infty}\int_{\mathbf{R}^{3N}}\psi_I^2(x)\mathbb{E}\left(\phi(X_t^x)\prod_{k=0}^{n-1}\exp(-tE_L(X^x_{kt/n})/n)\right)dx$$
$$=\int_{\mathbf{R}^{3N}}\psi_I^2(x)\mathbb{E}\left(\phi(X_t^x)\exp\left(-\int_0^tE_L(X_s^x)ds\right)\right)dx$$

We obtain the equality for general non-negative functions ϕ by writing the above equality for $\phi\wedge n$ and letting $n\to+\infty$ by the monotone convergence theorem. The case $\int_{\mathbf{R}^{3N}}|\phi(x)|f_2(t,x)dx<+\infty$ follows from the equalities for the positive and the negative parts of ϕ. $\square$

Let $\varphi\in C_0^\infty(\mathbb{R}_+\times\mathbb{R}^{3N})$ and $x\in U_I$. By Itô's formula,

$$\begin{aligned}e^{-\int_0^tE_L(X_s^x)ds}\varphi(t,X_t^x)&=\varphi(0,x)+\int_0^te^{-\int_0^sE_L(X_r^x)dr}\nabla\varphi(s,X_s^x).dW_s\\&+\int_0^te^{-\int_0^sE_L(X_r^x)dr}\left(-E_L\varphi+\partial_s\varphi+\frac12\Delta\varphi+b.\nabla\varphi\right)(s,X_s^x)ds.\end{aligned}$$

Taking expectations, one deduces

$$\mathbb{E}\left(e^{-\int_0^t E_L(X_s^x)ds}\varphi(t,X_t^x)\right) = \varphi(0,x)$$
$$+\,\mathbb{E}\left(\int_0^t e^{-\int_0^s E_L(X_r^x)dr}\left(-E_L\varphi+\partial_s\varphi+\frac{1}{2}\Delta\varphi+b.\nabla\varphi\right)(s,X_s^x)ds\right).$$

Integrating this equality w.r.t. $x\in\mathbb{R}^{3N}$ against density $\psi_I^2(x)$ and using Lemma 17, one concludes formally that (24) holds. To make this argument rigourous, one has to justify the use of Fubini's theorem for the second term of the r.h.s. and more specifically for the contribution of $-E_L\varphi+b.\nabla\varphi$. Using Lemma 17, then the definitions of E_L and b and last (18), one has

$$\begin{aligned}\int_{\mathbf{R}^{3N}}&\psi_I^2(x)\mathbb{E}\left(\int_0^t e^{-\int_0^s E_L(X_r^x)dr}|E_L\varphi+b.\nabla\varphi|(s,X_s^x)ds\right)dx\\ &=\int_0^t\int_{\mathbf{R}^{3N}}\psi_I^2(x)|E_L\varphi+b.\nabla\varphi|(s,x)\mathbb{E}\left(e^{-\int_0^s E_L(X_r^x)dr}\right)dxds\\ &\le C\int_0^t\int_{\mathbf{R}^{3N}}\left(\frac{1}{2}|\psi_I\Delta\psi_I\varphi|+|\psi_I^2V\varphi|+|\psi_I\nabla\psi_I.\nabla\varphi|\right)(s,x)dxds.\end{aligned}$$

The last integral is finite since function ψ_I is C^2 and potential V is locally integrable. □

Remark 18. One has $f_2(t,x)=\psi_I^2(x)u(t,x)$ where

$$u(t,x)=1_{\{x\in U_I\}}\mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^x)ds\right)\right). \tag{37}$$

By (18), the function $t\to\|u(t,.)\|_{L^\infty(\mathbf{R}^{3N})}$ is locally bounded and for fixed $x\in\mathbb{R}^{3N}$, $t\mapsto u(t,x)$ is continuous according to Lebesgue's theorem. Since $\psi_I\in L^2(\mathbb{R}^{3N})$, one deduces again by Lebesgue's theorem that f_2 belongs to $C^0(\mathbb{R}_+,L^1(\mathbb{R}^{3N}))$. Notice that the function u formally solves (Feynman-Kac approach)

$$\begin{cases}\dfrac{\partial u}{\partial t}=\dfrac{1}{2}\Delta u+b.\nabla u-E_Lu\\ u(0,x)=1_{\{x\in U_I\}}.\end{cases}$$

Proof of Proposition 11. By definition of f_2, one has $v(t,x)=\psi_I(x)u(t,x)$, with u given by (37). Reasoning like in Remark 18, one obtains that v belongs to $C^0(\mathbb{R}_+,L^2(\mathcal{C}))$. Besides, $v(t,x)=f_2(t,x)/\psi_I(x)$ in $\mathbb{R}_+\times\mathcal{C}$, where f_2 satisfies (24). For $\phi\in C_0^\infty(]0,+\infty[\times\mathcal{C})$, since ψ_I is of class C^2 and is either everywhere positive or everywhere negative on $\mathcal{C}$, one may choose $\varphi(t,x)=\mathbb{1}_{\mathcal{C}}(x)\phi(t,x)/\psi_I(x)$ where $\mathbb{1}_{\mathcal{C}}$ denotes the characteristic function of $\mathcal{C}$ in (24) . Since one easily checks that

$$\frac{\partial\varphi}{\partial t}=\frac{\mathbb{1}_{\mathcal{C}}}{\psi_I}\frac{\partial\phi}{\partial t}\quad\text{and}\quad\frac{1}{2}\Delta\varphi+b.\nabla\varphi-E_L\varphi=\frac{\mathbb{1}_{\mathcal{C}}}{\psi_I}\left(\frac{1}{2}\Delta\phi-V\phi\right),$$

we deduce that

$$\forall\phi\in C_0^\infty(]0,+\infty[\times\mathcal{C}),\quad\int_0^{+\infty}\int_{\mathcal{C}}\frac{\partial\phi}{\partial t}v+\int_0^{+\infty}\int_{\mathcal{C}}\left(\frac{1}{2}\Delta\phi-V\phi\right)v=0.$$

Therefore, v is solution to (27).

Considering only the test functions ϕ of the form $\phi(t,x) = \zeta(t)\,\xi(x)$, one obtains in particular

$$\forall \xi \in C_0^\infty(\mathcal{C}), \quad \frac{d}{dt}\left(\xi, v(t)\right)_{L^2(\mathcal{C})} = \left(\frac{1}{2}\Delta\xi - V\xi, v(t)\right)_{L^2(\mathcal{C})} \qquad \text{in } \mathcal{D}'(]0,+\infty[). \tag{38}$$

Let us now prove that (38) still holds true for any $\xi \in D(H_{\mathcal{C}})$. As explained below, this will actually imply that $v \in C^0(\mathbb{R}_+, D(H_{\mathcal{C}})) \cap C^1(\mathbb{R}_+, L^2(\mathcal{C}))$.
For convenience, we denote by the same letter a function supported in some subset of $\mathbb{R}^{3N}$ and its extension by zero on the whole space $\mathbb{R}^{3N}$. Let us first consider the case of a compactly supported function $\xi \in D(H_{\mathcal{C}})$ and let us denote by R a real number such that $\mathrm{Supp}(\xi) \subset B(0,R)$. Let $g \in C_0^\infty(\mathbb{R}^{3N})$ such that $\mathrm{Supp}(g) \subset B(0,1)$, $g \geq 0$ on $\mathbb{R}^{3N}$, and $\displaystyle\int_{\mathbb{R}^{3N}} g = 1$. For $\epsilon > 0$, we denote by g_ϵ the function defined by

$$g_\epsilon(x) = \frac{1}{\epsilon^{3N}}\, g\left(\frac{x}{\epsilon}\right).$$

We also introduce

$$\mathcal{C}_\epsilon = \left\{x \in \mathcal{C}, \quad d(x, \partial\mathcal{C}) > \epsilon\right\},$$

$\mathbb{1}_{\mathcal{C}_\epsilon}$ the characteristic function of $\mathcal{C}_\epsilon$,

$$h_\epsilon = \mathbb{1}_{\mathcal{C}_{3\epsilon}} \star g_\epsilon,$$

$$\xi_\epsilon = (\xi h_\epsilon) \star g_\epsilon,$$

and

$$K_\alpha^\beta = \left(\overline{\mathcal{C}}_\alpha \setminus \mathcal{C}_\beta\right) \cap \overline{B(0,R+1)}, \qquad \text{for } 0 \leq \alpha < \beta < +\infty.$$

For any $\epsilon > 0$ small enough, the C^∞ function ξ_ϵ is supported in the compact set $\overline{\mathcal{C}_\epsilon} \cap \overline{B(0,R+1)}$. Therefore,

$$\forall \epsilon > 0, \qquad \frac{d}{dt}\left(\xi_\epsilon, v(t)\right)_{L^2(\mathcal{C})} = \left(\frac{1}{2}\Delta\xi_\epsilon - V\xi_\epsilon, v(t)\right)_{L^2(\mathcal{C})} \qquad \text{in } \mathcal{D}'(]0,+\infty[). \tag{39}$$

We then split $\frac{1}{2}\Delta\xi_\epsilon - V\xi_\epsilon$ into four terms

$$\begin{aligned}\frac{1}{2}\Delta\xi_\epsilon - V\xi_\epsilon \;&=\; \left[\left(h_\epsilon\left(\frac{1}{2}\Delta\xi - V\xi\right)\right) \star g_\epsilon\right] + \left[(\nabla\xi \cdot \nabla h_\epsilon) \star g_\epsilon\right] \\ &\quad + \left[\frac{1}{2}\left(\xi \Delta h_\epsilon\right) \star g_\epsilon\right] - \left[V\left((\xi h_\epsilon) \star g_\epsilon\right) - (V\xi h_\epsilon) \star g_\epsilon\right].\end{aligned}$$

It is easy to check that if $u \in L^2(\mathcal{C})$, $u_\epsilon = (u h_\epsilon) \star g_\epsilon$ strongly converges toward u in $L^2(\mathcal{C})$ when ϵ goes to zero. Therefore, for any $t \geq 0$,

$$\left(\xi_\epsilon, v(t)\right)_{L^2(\mathcal{C})} \underset{\epsilon \to 0}{\longrightarrow} \left(\xi, v(t)\right)_{L^2(\mathcal{C})},$$

$$\left(\left(h_\epsilon\left(\frac{1}{2}\Delta\xi - V\xi\right)\right) \star g_\epsilon, v(t)\right)_{L^2(\mathcal{C})} \underset{\epsilon \to 0}{\longrightarrow} \left(\frac{1}{2}\Delta\xi - V\xi, v(t)\right)_{L^2(\mathcal{C})},$$

and

$$\left(V\left((\xi h_\epsilon) \star g_\epsilon\right) - (V\xi h_\epsilon) \star g_\epsilon, v(t)\right)_{L^2(\mathcal{C})} \underset{\epsilon \to 0}{\longrightarrow} 0.$$

To obtain the above inequality, we have used that $V\xi \in L^2(\mathcal{C})$. This is true when V_1 and V_2 are given by (4) since ξ is compactly supported. This is also true when V_1 and V_2 are given by (5), even in the case of point-like nuclei since by Hardy's inequality, $\|V\xi\|_{L^2} \leq 2\left(N + \sum_{k=1}^{M} z_k\right) \|\nabla\xi\|_{L^2}$.

Besides, one has $\|\nabla h_\epsilon\|_{L^\infty} \leq \dfrac{1}{\epsilon}\|\nabla g\|_{L^1}$ and $\|\Delta h_\epsilon\|_{L^\infty} \leq \dfrac{1}{\epsilon^2}\|\Delta g\|_{L^1}$, and both functions ∇h_ϵ and Δh_ϵ are supported in the compact set $K_{2\epsilon}^{4\epsilon}$. It follows that $(\nabla\xi \cdot \nabla h_\epsilon) \star g_\epsilon$ and $(\xi\Delta h_\epsilon) \star g_\epsilon$ are supported in $K_\epsilon^{5\epsilon}$. One thus has on the one hand,

$$\begin{aligned}
\left|((\nabla\xi \cdot \nabla h_\epsilon) \star g_\epsilon, v(t))_{L^2(\mathcal{C})}\right| &\leq \|(\nabla\xi \cdot \nabla h_\epsilon) \star g_\epsilon\|_{L^2(K_\epsilon^{5\epsilon})} \; \|v(t)\|_{L^2(K_\epsilon^{5\epsilon})} \\
&\leq \|\nabla\xi \cdot \nabla h_\epsilon\|_{L^2(K_{2\epsilon}^{4\epsilon})} \; \|g_\epsilon\|_{L^1} \; \|v(t)\|_{L^2(K_\epsilon^{5\epsilon})} \\
&\leq \frac{1}{\epsilon} \, \|\nabla g\|_{L^1} \; \|\nabla\xi\|_{L^2(K_0^{4\epsilon})} \; \|v(t)\|_{L^2(K_0^{5\epsilon})}, \qquad (40)
\end{aligned}$$

and on the other hand

$$\begin{aligned}
\left|((\xi\Delta h_\epsilon) \star g_\epsilon, v(t))_{L^2(\mathcal{C})}\right| &\leq \|(\xi\Delta h_\epsilon) \star g_\epsilon\|_{L^2(K_\epsilon^{5\epsilon})} \; \|v(t)\|_{L^2(K_\epsilon^{5\epsilon})} \\
&\leq \|\xi\Delta h_\epsilon\|_{L^2(K_{2\epsilon}^{4\epsilon})} \; \|g_\epsilon\|_{L^1} \; \|v(t)\|_{L^2(K_\epsilon^{5\epsilon})} \\
&\leq \frac{1}{\epsilon^2} \, \|\Delta g\|_{L^1} \; \|\xi\|_{L^2(K_0^{4\epsilon})} \; \|v(t)\|_{L^2(K_0^{5\epsilon})}. \qquad (41)
\end{aligned}$$

At that point, we make use of the inequality

$$|v(t,x)| = \left|\psi_I(x)\,\mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^x)ds\right)\right)\right| \leq \exp\left(-t\left(\inf_{\mathbf{R}^{3M}} E_L\right)\right) \; |\psi_I(x)|\,, \qquad (42)$$

which states that, in some sense, $v(t,\cdot)$ vanishes on the boundary $\partial\mathcal{C}$. As there exists a constant C_P depending only on ψ_I and on R such that, for ϵ small enough,

$$\forall u \in H_0^1(\mathcal{C}), \qquad \|u\|_{L^2(K_0^\epsilon)} \leq C_P\,\epsilon\,\|\nabla u\|_{L^2(K_0^\epsilon)}, \qquad (43)$$

we obtain, for ϵ small enough,

$$\|v(t)\|_{L^2(K_0^{5\epsilon})} \leq \epsilon\, C_P \exp\left(-t\left(\inf_{\mathbf{R}^{3M}} E_L\right)\right) \; \|\nabla\psi_I\|_{L^2(K_0^{5\epsilon})}, \qquad (44)$$

and

$$\|\xi\|_{L^2(K_0^{4\epsilon})} \leq \epsilon\, C_P \, \|\nabla\xi\|_{L^2(K_0^\epsilon)}. \qquad (45)$$

For the sake of brevity, we do not reproduce here the proof of the Poincaré-type inequality for narrow domains (43). This can be established by using hypotheses [$\mathcal{H}1$]-[$\mathcal{H}2$] which allow ones to work in local maps.

Putting all together, one obtains that for any $t \geq 0$,

$$(\xi_\epsilon, v(t))_{L^2(\mathcal{C})} \underset{\epsilon\to 0}{\longrightarrow} (\xi, v(t))_{L^2(\mathcal{C})}\,,$$

and

$$\left(\frac{1}{2}\Delta\xi_\epsilon - V\xi_\epsilon, v(t)\right)_{L^2(\mathcal{C})} \underset{\epsilon\to 0}{\longrightarrow} \left(\frac{1}{2}\Delta\xi - V\xi, v(t)\right)_{L^2(\mathcal{C})}.$$

In order to pass to the limit in (39), we need to check that, for instance, both $(\xi_\epsilon, v(t))_{L^2(\mathcal{C})}$ and $\left(\frac{1}{2}\Delta\xi_\epsilon - V\xi_\epsilon, v(t)\right)_{L^2(\mathcal{C})}$ are uniformly bounded on any compact time interval $[0,T]$, with bounds independent on ϵ. Clearly,

$$\begin{array}{rcl} \|\xi_\epsilon\|_{L^2(\mathcal{C})} & \leq & \|\,(\xi h_\epsilon)\star g_\epsilon\|_{L^2(\mathcal{C})} \\ & \leq & \|\xi h_\epsilon\|_{L^2(\mathcal{C})}\,\|g_\epsilon\|_{L^1} \\ & \leq & \|\xi\|_{L^2(\mathcal{C})}\,\|h_\epsilon\|_{L^\infty(\mathcal{C})}\,\|g_\epsilon\|_{L^1} \\ & \leq & \|\xi\|_{L^2(\mathcal{C})} \end{array}$$

since $0\leq h_\epsilon\leq 1$ and $\|g_\epsilon\|_{L^1}=1$. Thus,

$$\forall t\in[0,T],\qquad \left|(\xi_\epsilon, v(t))_{L^2(\mathcal{C})}\right| \leq \|\xi\|_{L^2(\mathcal{C})}\,\|v\|_{C^0([0,T],L^2(\mathcal{C}))}.$$

Besides, using (40), (41), (44), (45), together with the three inequalities

$$\left\|\left(\left(-\frac{1}{2}\Delta\xi + V\xi\right)h_\epsilon\right)\star g_\epsilon\right\|_{L^2(\mathcal{C})} \leq \left\|-\frac{1}{2}\Delta\xi + V\xi\right\|_{L^2(\mathcal{C})},$$

$$\|(V\xi h_\epsilon)\star g_\epsilon\|_{L^2(\mathcal{C})} \leq \|V\xi\|_{L^2(\mathcal{C})},$$

and

$$\|V\,((\xi h_\epsilon)\star g_\epsilon)\|_{L^2(\mathcal{C})} \leq \left| \begin{array}{ll} \left(\max\omega_i^2\right)\,(1+R)^2\,\|\xi\|_{L^2(\mathcal{C})} & (V_1,\,V_2 \text{ given by (4)}), \\ 2\left(N+\displaystyle\sum_{k=1}^M z_k\right)\,(1+C_P\|\nabla g\|_{L^1})\,\|\nabla\xi\|_{L^2(\mathcal{C})} & (V_1,\,V_2 \text{ given by (5)}), \end{array}\right.$$

we obtain that for ϵ small enough

$$\forall t\in[0,T],\qquad \left|\left(\frac{1}{2}\Delta\xi_\epsilon - V\xi_\epsilon, v(t)\right)_{L^2(\mathcal{C})}\right| \leq C$$

where the constant C is independent of ϵ.

Let us now consider the case of a function $\xi\in D(H_{\mathcal{C}})$ non necessarily compactly supported. For $R\geq 1$, we introduce the radial function k_R defined by

$$\left\{\begin{array}{lll} k_R(x)=1 & \text{if} & |x|<R \\ k_R(x)=(|x|-(R+1))^2\,(2(|x|-R)+1) & \text{if} & R<|x|<R+1 \\ k_R(x)=0 & \text{if} & |x|>R+1 \end{array}\right.$$

which is such that $0\leq k_R\leq 1$, $\|\nabla k_R\|_{L^\infty}\leq 3/2$, $\|\Delta k_R\|_{L^\infty}\leq 6+\frac{3}{2}(3N-1)$. Then $\xi_R=k_R\xi$ is a compactly supported function of $D(H_{\mathcal{C}})$ and thus

$$\forall R\geq 1,\qquad \frac{d}{dt}\,(\xi_R, v(t))_{L^2(\mathcal{C})} = \left(\frac{1}{2}\Delta\xi_R - V\xi_R, v(t)\right)_{L^2(\mathcal{C})} \qquad \text{in } \mathcal{D}'(]0,+\infty[).$$

Letting R goes to infinity, one obtains

$$\frac{d}{dt}\,(\xi, v(t))_{L^2(\mathcal{C})} = \left(\frac{1}{2}\Delta\xi - V\xi, v(t)\right)_{L^2(\mathcal{C})} \qquad \text{in } \mathcal{D}'(]0,+\infty[). \tag{46}$$

Using the fact that (46) holds for $\xi \in D(H_{\mathcal{C}})$, we can now prove that $v \in C^0(\mathbb{R}_+, D(H_{\mathcal{C}})) \cap C^1(\mathbb{R}_+, L^2(\mathcal{C}))$. Let us denote by $(P_\lambda)_{\lambda\in\mathbf{R}}$ the spectral family associated with the self-adjoint operator $H_{\mathcal{C}}$. For any $w \in L^2(\mathcal{C})$ and any $-\infty < \alpha < \beta < +\infty$, $P_{]\alpha,\beta]}w := (P_\beta - P_\alpha)\, w$ belongs to $D(H_{\mathcal{C}})$. Using (46) with $\xi = P_{]\alpha,\beta]}w$, one obtains

$$\begin{aligned} \frac{d}{dt}\left(w, P_{]\alpha,\beta]}v(t)\right)_{L^2(\mathcal{C})} &= \frac{d}{dt}\left(P_{]\alpha,\beta]}w, v(t)\right)_{L^2(\mathcal{C})} \\ &= \left(H_{\mathcal{C}}P_{]\alpha,\beta]}w, v(t)\right)_{L^2(\mathcal{C})} \\ &= \left(w, H_{\mathcal{C}}P_{]\alpha,\beta]}v(t)\right)_{L^2(\mathcal{C})}. \end{aligned}$$

Therefore

$$\frac{d}{dt}P_{]\alpha,\beta]}v(t) = H_{\mathcal{C}}P_{]\alpha,\beta]}v(t).$$

As $P_{]\alpha,\beta]}v \in C^0([0,+\infty[, L^2)$ and $v(0) = \psi_I|_{\mathcal{C}}$, and as $H_{\mathcal{C}}$ is bounded on $\mathrm{Ran}(P_{]\alpha,\beta]})$,

$$P_{]\alpha,\beta]}v(t) = e^{-tH_{\mathcal{C}}}P_{]\alpha,\beta]}\;\psi_I|_{\mathcal{C}}\,.$$

Passing to the limits $\alpha \to -\infty$ and $\beta \to +\infty$, one gets

$$v(t) = e^{-tH_{\mathcal{C}}}\;\psi_I|_{\mathcal{C}}\,.$$

As ψ_I is in $D(H) \cap C^2(\mathbb{R}^3)$ and satisfies $\psi_I = 0$ on $\psi_I^{-1}(0)$, one has $\psi_I|_{\mathcal{C}} \in D(H_{\mathcal{C}})$. Therefore $v \in C^0(\mathbb{R}_+, D(H_{\mathcal{C}})) \cap C^1(\mathbb{R}_+, L^2(\mathcal{C}))$. The solution of (27) in $C^0(\mathbb{R}_+, D(H_{\mathcal{C}})) \cap C^1(\mathbb{R}_+, L^2(\mathcal{C}))$ being unique (see [6]), the proof is completed. $\square$

Remark 19. We have shown that there exists a unique solution of class $C^0(\mathbb{R}_+, L^2(\mathcal{C}))$ to (38), if ξ can be chosen in $D(H_{\mathcal{C}})$. The fact that uniqueness holds for this kind of very weak solutions can be compared to uniqueness results for "generalized solutions" such as ones defined for example in [12], page 85. Let us sketch another proof of this uniqueness result inspired by [12], and which does not require $v(0)$ to be in $D(H_{\mathcal{C}})$, and does not use the notion of spectral family. Let $w = H_{\mathcal{C}}^{-1}(v)$ (one can suppose that $0 \notin \sigma(H_{\mathcal{C}})$ since H is bounded from below and V is defined up to a constant). Since $v \in C^0(\mathbb{R}_+, L^2)$, then $w \in C^0(\mathbb{R}_+, D(H_{\mathcal{C}}))$ (where $D(H_{\mathcal{C}})$ is equiped with the graph norm). For any $\zeta \in L^2(\mathcal{C})$, it is then easy to check that $\frac{d}{dt}(w,\zeta) = -(H_{\mathcal{C}}w, \zeta)$. Therefore, w is the unique solution to $w' = -H_{\mathcal{C}}w$ in $C^0(\mathbb{R}_+, D(H_{\mathcal{C}})) \cap C^1(\mathbb{R}_+, L^2(\mathcal{C}))$. As H is self adjoint, w is actually much more regular on $\mathbb{R}_+^*$: $\forall k, l \in \mathbb{N}$, $w \in C^k(\mathbb{R}_+^*, D(H_{\mathcal{C}}^l))$. As $v(0) \in L^2$, this shows that v is in $C^0(\mathbb{R}_+, L^2(\mathcal{C})) \cap C^1(\mathbb{R}_+^*, L^2(\mathcal{C})) \cap C^0(\mathbb{R}_+^*, D(H_{\mathcal{C}}))$ and the Hille-Yosida theorem for self-adjoint operators (see [6]) allows to complete the proof.

Proof of Theorem 12. Let us denote by $\mathcal{C}_1$, $\mathcal{C}_2$, ... $\mathcal{C}_{N_c^I}$ the connected components of

U_I. It follows from Proposition 11 that

$$
\begin{aligned}
E^{\mathrm{DMC}}(t) &= \frac{\displaystyle\int_{\mathbf{R}^3} E_L(x)\, f_2(t,x)\, dx}{\displaystyle\int_{\mathbf{R}^3} f_2(t,x)\, dx} \\
&= \frac{\displaystyle\sum_{n=1}^{N_c^I} \int_{\mathcal{C}_n} \left(H_{\mathcal{C}_n}\, \psi_I|_{\mathcal{C}_n}\right)(x)\, \chi(t,x)\, dx}{\displaystyle\sum_{n=1}^{N_c^I} \int_{\mathcal{C}_n} \psi_I(x)\, \chi(t,x)\, dx} \\
&= \frac{\displaystyle\sum_{n=1}^{N_c^I} \left(H_{\mathcal{C}_n}\, \psi_I|_{\mathcal{C}_n}, e^{-tH_{\mathcal{C}_n}}\, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)}}{\displaystyle\sum_{n=1}^{N_c^I} \left(\psi_I|_{\mathcal{C}_n}, e^{-tH_{\mathcal{C}_n}}\, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)}}.
\end{aligned}
$$

For V_1 and V_2 given by (4), the remaining of the proof is easy. In this case indeed, $H_{\mathcal{C}_n}$ has a purely discrete spectrum and a unique positive ground state ψ_n^0. Let us denote by $E_n^0 < E_n^1 \leq E_n^2 \leq \cdots$ the eigenvalues of $H_{\mathcal{C}_n}$, counted with their multiplicities, and by $(\psi_n^k)_{k\in\mathbf{N}}$ a Hilbert basis of $L^2(\mathcal{C}_n)$ such that $H_{\mathcal{C}_n}\psi_n^k = E_n^k \psi_n^k$ for all $k \in \mathbb{N}$. One has

$$
\left(H_{\mathcal{C}_n}\, \psi_I|_{\mathcal{C}_n}, e^{-tH_{\mathcal{C}_n}}\, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)} = \sum_{k=0}^{+\infty} E_n^k\, e^{-E_n^k t} \left| \left(\psi_n^k, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)} \right|^2
$$

and

$$
\left(\psi_I|_{\mathcal{C}_n}, e^{-tH_{\mathcal{C}_n}}\, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)} = \sum_{k=0}^{+\infty} e^{-E_n^k t} \left| \left(\psi_n^k, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)} \right|^2 .
$$

As ψ_n^0 is positive on $\mathcal{C}_n$ and as $\psi_I|_{\mathcal{C}_n}$ is either positive or negative on $\mathcal{C}_n$, then $\left| \left(\psi_n^k, \psi_I|_{\mathcal{C}_n}\right)_{L^2(\mathcal{C}_n)} \right|^2 >$ 0 and therefore,

$$
E^{\mathrm{DMC}}(t) = \min_{1\leq n\leq N_c^I} E_n^0 + O\left(e^{-\alpha t}\right)
$$

where $\alpha = \min \left\{ E_n^k - \min_{1\leq n\leq N_c^I} E_n^0,\ E_n^k \neq \min_{1\leq n\leq N_c^I} E_n^0 \right\} > 0$. Let us now prove that

$$
\min_{1\leq n\leq N_c^I} E_n^0 = E_0^{\mathrm{DMC}}.
$$

Let n_0 be such that $E_{n_0}^0 = \min_{1\leq n\leq N_c^I} E_n^0$ and $\mathcal{J}$ the subgroup of even permutations of $\{1, \cdots, N\}$ such that

$$
\forall \sigma \in \mathcal{J}, \quad \forall (x_1, \cdots, x_N) \in \mathcal{C}_{n_0}, \qquad (x_{\sigma(1)}, \cdots, x_{\sigma(N)}) \in \mathcal{C}_{n_0}.
$$

Since ψ_I is antisymmetric, $\mathcal{J} = \{\sigma \in \mathfrak{S}_N,\ \mathcal{C}_\sigma \cap \mathcal{C} \neq \emptyset\}$. As $\psi_{n_0}^0$ is the unique positive ground state of $H_{\mathcal{C}_n}$ and V is invariant under permutations, one necessarily has

$$
\forall \sigma \in \mathcal{J}, \qquad \forall (x_1, \cdots, x_N) \in \mathcal{C}_{n_0}, \qquad \psi_{n_0}^0(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \psi_{n_0}^0(x_1, \cdots, x_N).
$$

Therefore the function ψ obtained like in the proof of Corollary 5 by antisymmetrization and normalization of the extension of $\psi^0_{n_0}$ by 0, satisfies $\psi \in D(q_H)$, $\|\psi\|_{L^2} = 1$, $\psi = 0$ on $\psi_I^{-1}(0)$ and

$$\frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla\psi|^2 + \int_{\mathbf{R}^{3N}} V\psi^2 = E^0_{n_0}.$$

Therefore $\min\limits_{1\le n\le N_c^I} E^0_n \ge E_0^{\mathrm{DMC}}$. On the other hand, let ψ_0^{DMC} be a minimizer of

$$\inf\left\{\frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla\psi|^2 + \int_{\mathbf{R}^{3N}} V\psi^2, \quad \psi \in D(q_H), \quad \|\psi\|_{L^2} = 1, \quad \psi = 0 \text{ on } \psi_I^{-1}(0)\right\}.$$

Notice that $(\psi_0^{\mathrm{DMC}})^{-1}(0) = \psi_I^{-1}(0)$. Indeed, on any connected component $\mathcal{C}$ of $\psi_I^{-1}(0)$, $\psi_0^{\mathrm{DMC}}|_{\mathcal{C}}/||\psi_0^{\mathrm{DMC}}|_{\mathcal{C}}||_{L^2(\mathcal{C})}$ is a minimizer of

$$\inf\left\{\frac{1}{2}\int_{\mathcal{C}} |\nabla\psi|^2 + \int_{\mathcal{C}} V\psi^2, \quad \psi \in H^1_0(\mathcal{C}), \quad \|\psi\|_{L^2(\mathcal{C})} = 1\right\}$$

since if it was not the case, one could build by antisymmetrisation and normalization (again by the procedure used in the proof of Corollary 5) an antisymmetric function which is null on $\psi_I^{-1}(0)$ with a lower energy than ψ_0^{DMC}. On the other hand, since we know that the ground state of $H_{\mathcal{C}}$ is non-degenerate positive, this shows that $\psi_0^{\mathrm{DMC}}|_{\mathcal{C}}$ is either positive or negative.

One then has

$$\begin{aligned}
E_0^{\mathrm{DMC}} &= \frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla\psi_0^{\mathrm{DMC}}|^2 + \int_{\mathbf{R}^{3N}} V|\psi_0^{\mathrm{DMC}}|^2 \\
&= \sum_{n=1}^{N_c^I} \langle H_{\mathcal{C}_n}\, \psi_0^{\mathrm{DMC}}|_{\mathcal{C}_n}, \psi_0^{\mathrm{DMC}}|_{\mathcal{C}_n}\rangle \\
&\ge \sum_{n=1}^{N_c^I} E_n^0 \left\|\psi_0^{\mathrm{DMC}}|_{\mathcal{C}_n}\right\|^2_{L^2} \\
&\ge \min_{1\le n\le N_c^I} E_n^0.
\end{aligned}$$

Let us now consider the case when V_1 and V_2 are given by (5). For $1 \le n \le N_c^I$, we denote by $H^S_{\mathcal{C}_n}$ the unbounded operator defined by

$$\left\{\begin{array}{l} D(H^S_{\mathcal{C}_n}) = \left\{\phi \in H^2(\mathcal{C}_n) \cap H^1_0(\mathcal{C}_n), \quad \forall \sigma \in \mathcal{J}_n, \quad \phi^\sigma = \phi\right\}, \\ \forall \phi \in D(H^S_{\mathcal{C}_n}), \quad H^S_{\mathcal{C}_n}\phi = -\frac{1}{2}\Delta\phi + V\phi, \end{array}\right.$$

where $\mathcal{J}_n$ is the subgroup of the even permutations of $\{1, \cdots, N\}$ such that

$$\forall \sigma \in \mathcal{J}_n, \quad \forall (x_1, \cdots, x_N) \in \mathcal{C}_n, \qquad (x_{\sigma(1)}, \cdots, x_{\sigma(N)}) \in \mathcal{C}_n,$$

and where, again, $\psi^\sigma(x_1, \cdots, x_N) = \psi(x_{\sigma(1)}, \cdots, x_{\sigma(N)})$. The operator $H^S_{\mathcal{C}_n}$ is self-adjoint on $\left\{\phi \in L^2(\mathcal{C}_n), \ \forall \sigma \in \mathcal{J}_n, \ \phi^\sigma = \phi\right\}$ and one can check that

$$E_0^{\mathrm{DMC}} = \min_{1\le n\le N_c^I} \ \inf \sigma\left(H^S_{\mathcal{C}_n}\right);$$

the inequality $E_0^{\mathrm{DMC}} \ge \min\limits_{1\le n\le N_c} \ \inf \sigma\left(H^S_{\mathcal{C}_n}\right)$ can be established as above, replacing the minimum ψ_0^{DMC} by a minimizing sequence, and the argument used at the end of the proof of Corollary 5 leads to the converse inequality.

Let n_0 such that $E_0^{\rm DMC} = \inf\, \sigma\left(H^S_{\mathcal{C}_{n_0}}\right)$ and assume that $E_0^{\rm DMC} \in \sigma_{\rm ess}\left(H^S_{\mathcal{C}_{n_0}}\right)$. Then for all $\epsilon > 0$, and for all $k \in \mathbb{N}^*$, there exists a subspace V_k of $\left\{\phi \in H^1_0(\mathcal{C}_{n_0}),\ \forall \sigma \in \mathcal{J}_n,\ \phi^\sigma = \phi\right\}$ with dimension k such that

$$\sup_{\phi \in V_k,\, \|\phi\|_{L^2}=1} \frac{1}{2}\int_{\mathcal{C}_{n_0}} |\nabla \phi|^2 + \int_{\mathcal{C}_{n_0}} V|\phi|^2 \leq E_0^{\rm DMC} + \epsilon.$$

We then associate with V_k the subspace

$$W_k = \left\{ \psi \in \mathcal{H}_e, \quad \exists \phi \subset V_k, \quad \psi = \sum_{\sigma \in \mathfrak{S}_N} \epsilon(\sigma)\widetilde{\phi}^\sigma \right\}$$

where $\widetilde{\phi}$ denotes the extension by 0 of ϕ on $\mathbb{R}^{3N}$. Clearly, W_k is a subset of $D(q_H)$ with dimension k and

$$\sup_{\psi \in W_k,\, \|\psi\|_{L^2}=1} \frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla \psi|^2 + \int_{\mathbf{R}^{3N}} V|\psi|^2 = \sup_{\phi \in V_k,\, \|\phi\|_{L^2}=1} \frac{1}{2}\int_{\mathcal{C}_{n_0}} |\nabla \phi|^2 + \int_{\mathcal{C}_{n_0}} V|\phi|^2.$$

Then, using the min-max principle

$$\inf \sigma_{\rm ess}(H) = \lim_{k \to +\infty} \inf_{W \subset D(q_H),\, \dim W = k} \sup_{\psi \in W,\, \|\psi\|_{L^2}=1} \frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla \psi|^2 + \int_{\mathbf{R}^{3N}} V|\psi|^2 \leq E_0^{\rm DMC}.$$

Therefore $\inf \sigma_{\rm ess}(H) \leq E_0^{\rm DMC} \leq \langle \psi_I, H\psi_I \rangle$ and this contradicts hypothesis [$\mathcal{H}5$]. Therefore the bottom of the spectrum of $H^S_{\mathcal{C}_{n_0}}$ is an isolated eigenvalue of finite multiplicity. By standard argument, $H^S_{\mathcal{C}_{n_0}}$ has a non-degenerate, positive, ground state ϕ_{n_0} and $\psi_0^{\rm DMC} = C \displaystyle\sum_{\sigma \in \mathfrak{S}_N} \epsilon(\sigma)\widetilde{\phi}^\sigma_{n_0}$, where C is a normalisation constant and $\widetilde{\phi}_{n_0}$ the extension by 0 of ϕ_{n_0} on $\mathbb{R}^{3N}$, is a minimizer of problem

$$\inf\left\{ \frac{1}{2}\int_{\mathbf{R}^{3N}} |\nabla \psi|^2 + \int_{\mathbf{R}^{3N}} V\psi^2, \quad \psi \in D(q_H), \quad \|\psi\|_{L^2} = 1, \quad \psi = 0 \text{ on } \psi_I^{-1}(0) \right\}.$$

Notice that, by definition of $\psi_0^{\rm DMC}$, we also have in this case $(\psi_0^{\rm DMC})^{-1}(0) = \psi_I^{-1}(0)$. The same arguments as in the case of a purely discrete spectrum detailed previously, allow to conclude that $E^{\rm DMC}(t)$ converges exponentially fast toward $E_0^{\rm DMC}$.

Lastly, in any case (V_1 and V_2 given by (4) or by (5)) one obviously has $E_0^{\rm DMC} \geq E_0$. Now, if $E_0^{\rm DMC} = E_0$, then $\psi_0^{\rm DMC}$ is a ground state of H, and as we have shown that $\psi_I^{-1}(0) = (\psi_0^{\rm DMC})^{-1}(0)$, this concludes the proof. Notice that we also proved here the results presented in Remark 14. □

6 Analytical calculations on a simple example

Let us consider the hamiltonian

$$H = h(\vec{x}_1) + h(\vec{x}_2)$$

where

$$h(\vec{x}) = -\frac{1}{2}\Delta_{\vec{x}} + V_1(\vec{x})$$

and

$$\forall \vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3, \qquad V_1(\vec{x}) = \frac{1}{2}x^2 + \frac{1}{2}\omega^2 \left(y^2 + z^2\right),$$

with $\omega > 1$. This hamiltonian describes a system with two non-interacting identical particles with mass 1 submitted to the harmonic anisotropic potential V_1.

Let us denote

$$\lambda_{n_x,n_y,n_z} = \left(n_x + \frac{1}{2}\right) + \omega\ (n_y + n_z + 1), \qquad (n_x, n_y, n_z) \in \mathbb{N}^3$$

the eigenvalues of h and

$$\phi_{n_x,n_y,n_z}(\vec{x}) = \omega^{1/2}\, \phi_{n_x}(x)\, \phi_{n_y}(\sqrt{\omega}\ y)\, \phi_{n_z}(\sqrt{\omega}\ z)$$

the corresponding eigenfunctions. Functions $(\phi_n)_{n\in\mathbb{N}}$ are the eigenfunctions of the 1D harmonic oscillator with hamiltonian $-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$ and are given by

$$\phi_n(t) = \mathcal{H}_n(t)\ \exp(-t^2/2)$$

where $\mathcal{H}_n(t)$ is the n-th Hermite polynomial. Polynomials $\mathcal{H}_n(t)$ are normalized in such a way as

$$\forall (m,n) \in \mathbb{N} \times \mathbb{N}, \qquad \int_{-\infty}^{+\infty} \mathcal{H}_m(t)\, \mathcal{H}_n(t)\, e^{-t^2}\, dt = \delta_{mn}.$$

In particular,

$$\phi_0(t) = \frac{e^{-t^2/2}}{\pi^{1/4}}, \qquad \text{et} \qquad \phi_1(t) = \sqrt{2}\, t \frac{e^{-t^2/2}}{\pi^{1/4}}.$$

When $\omega > 1$, the fermionic ground state energy of the hamiltonian H is $E_0 = 2(1+\omega)$ and is non-degenerate. The ground state is given by the Slater determinant

$$\begin{aligned} \psi_0(\vec{x}_1, \vec{x}_2) &= \frac{1}{\sqrt{2}} \left(\phi_{000}(\vec{x}_1)\phi_{100}(\vec{x}_2) - \phi_{100}(\vec{x}_1)\phi_{000}(\vec{x}_2)\right) \\ &= \frac{\omega}{\pi^{3/2}}\ (x_2 - x_1)\ \exp\left(-\frac{1}{2}\left(x_1^2 + x_2^2\right) - \frac{\omega}{2}\left(y_1^2 + y_2^2 + z_1^2 + z_2^2\right)\right). \end{aligned}$$

Let us consider the importance sampling functions

$$\begin{aligned} \psi_I(\vec{x}_1, \vec{x}_2) &= c\left((x_2 - x_1)\cos\theta + (y_2 - y_1)\sin\theta\right) \\ &\quad \exp\left(-\frac{1}{2}\left(x_1\cos\theta + y_1\sin\theta\right)^2 - \frac{1}{2}\left(x_2\cos\theta + y_2\sin\theta\right)^2\right) \\ &\quad \exp\left(-\frac{\widetilde{\omega}}{2}\left((-x_1\sin\theta + y_1\cos\theta)^2 + (-x_2\sin\theta + y_2\cos\theta)^2 + z_1^2 + z_2^2\right)\right) \end{aligned} \tag{47}$$

where $\widetilde{\omega} \in]0,1]$, $\theta \in [0, 2\pi[$ and the normalization constant c ensures that $\int_{\mathbf{R}^6} \psi_I^2 = 1$. In case $\theta = \pi/2$, one remarks that the function

$$\begin{aligned} &\frac{1}{\sqrt{2}} \left(\phi_{000}(\vec{x}_1)\phi_{010}(\vec{x}_2) - \phi_{010}(\vec{x}_1)\phi_{000}(\vec{x}_2)\right) \\ &= \left(\frac{\omega}{\pi}\right)^{3/2} (y_2 - y_1) \exp\left(-\frac{1}{2}\left(x_1^2 + x_2^2\right) - \frac{\omega}{2}\left(y_1^2 + y_2^2 + z_1^2 + z_2^2\right)\right) \end{aligned}$$

is an eigenfunction of H for the eigenvalue $1+3\omega$ and only vanishes on $\{(\vec{x}_1,\vec{x}_2) : y_1 = y_2\} = \psi_I^{-1}(0)$. Hence its restriction to each connected component $\mathcal{C}$ of U_I is a ground state of $H_{\mathcal{C}}$ and according to Remark 14, $E_0^{\mathrm{DMC}} = 1+3\omega > 2(1+\omega) = E_0$. In general (for $\theta \notin \{0,\pi/2,\pi,3\pi/2\}$) it does not seem easy to compute analytically E_0^{DMC}.

Nevertheless, for each $\theta \in [0,2\pi[$, the function ψ_I satisfies the tiling property and hypothesis $[\mathcal{H}1]$. We are now going to check that hypotheses $[\mathcal{H}2]-[\mathcal{H}4]$ also hold and to exhibit the transition density associated with the stochastic differential equation (23).
With the new variables

$$\begin{aligned}
\widetilde{x}_1 &= \frac{(x_2-x_1)\cos\theta+(y_2-y_1)\sin\theta}{\sqrt{2}}, \quad \widetilde{y}_1 = y_1\cos\theta - x_1\sin\theta, \quad \widetilde{z}_1 = z_1,\\
\widetilde{x}_2 &= \frac{(x_2+x_1)\cos\theta+(y_2+y_1)\sin\theta}{\sqrt{2}}, \quad \widetilde{y}_2 = y_2\cos\theta - x_2\sin\theta, \quad \widetilde{z}_2 = z_2,
\end{aligned}$$

one has

$$\psi_I(\widetilde{x}_1,\widetilde{y}_1,\widetilde{z}_1,\widetilde{x}_2,\widetilde{y}_2,\widetilde{z}_2) = \sqrt{2}\,c\widetilde{x}_1 \exp\left(-\frac{1}{2}(\widetilde{x}_1^2+\widetilde{x}_2^2) - \frac{\widetilde{\omega}}{2}(\widetilde{y}_1^2+\widetilde{y}_2^2+\widetilde{z}_1^2+\widetilde{z}_2^2)\right).$$

Since $\partial_{\widetilde{x}_1}\psi_I$ does not vanish on $\{\widetilde{x}_1 = 0\} = \psi_I^{-1}(0)$, (14) and therefore $[\mathcal{H}2]$ hold. In addition,

$$b(\widetilde{x}_1,\widetilde{y}_1,\widetilde{z}_1,\widetilde{x}_2,\widetilde{y}_2,\widetilde{z}_2) = \begin{pmatrix} \frac{1}{\widetilde{x}_1} - \widetilde{x}_1 \\ -\widetilde{\omega}\widetilde{y}_1 \\ -\widetilde{\omega}\widetilde{z}_1 \\ -\widetilde{x}_2 \\ -\widetilde{\omega}\widetilde{y}_2 \\ -\widetilde{\omega}\widetilde{z}_2 \end{pmatrix}.$$

and $[\mathcal{H}3]$ is satisfied since (16) holds with $x_0 = 0$, $C = 1/\sqrt{\widetilde{\omega}}$ and $C' = 0$. Notice that (17) also holds with $K = 2\sqrt{1+\widetilde{\omega}}/\widetilde{\omega}$ since

$$\frac{\Delta\psi_I}{\psi_I} = -4(1+\widetilde{\omega}) + \widetilde{x}_1^2 + \widetilde{x}_2^2 + \widetilde{\omega}^2(\widetilde{y}_1^2+\widetilde{y}_2^2+\widetilde{z}_1^2+\widetilde{z}_2^2).$$

Combining this equality with

$$\begin{aligned}
V(\widetilde{x}_1,\widetilde{y}_1,\widetilde{z}_1,\widetilde{x}_2,\widetilde{y}_2,\widetilde{z}_2) &= \frac{1}{2}\Big[(1+(\omega^2-1)\sin^2\theta)(\widetilde{x}_1^2+\widetilde{x}_2^2) + (1+(\omega^2-1)\cos^2\theta)(\widetilde{y}_1^2+\widetilde{y}_2^2)\\
&+ 2(\omega^2-1)\sin\theta\cos\theta\left(\widetilde{y}_1\frac{\widetilde{x}_2-\widetilde{x}_1}{\sqrt{2}} + \widetilde{y}_2\frac{\widetilde{x}_2+\widetilde{x}_1}{\sqrt{2}}\right) + \omega^2(\widetilde{z}_1^2+\widetilde{z}_2^2)\Big],
\end{aligned}$$

one obtains

$$\begin{aligned}
E_L(\widetilde{x}_1,\widetilde{y}_1,\widetilde{z}_1,\widetilde{x}_2,\widetilde{y}_2,\widetilde{z}_2) &= 2(1+\widetilde{\omega}) + \frac{1}{2}\Big[(1-\widetilde{\omega}^2)(\widetilde{y}_1^2+\widetilde{y}_2^2) + (\omega^2-\widetilde{\omega}^2)(\widetilde{z}_1^2+\widetilde{z}_2^2)\\
&+ (\omega^2-1)\left(\left(\cos\theta\widetilde{y}_1 + \sin\theta\frac{\widetilde{x}_2-\widetilde{x}_1}{\sqrt{2}}\right)^2 + \left(\cos\theta\widetilde{y}_2 + \sin\theta\frac{\widetilde{x}_1+\widetilde{x}_2}{\sqrt{2}}\right)^2\right)\Big].
\end{aligned}$$

As $\omega > 1$ and $\widetilde{\omega} \in]0,1]$, E_L is greater than $2(1+\widetilde{\omega})$ and $[\mathcal{H}4]$ holds. Notice that in addition,

$$\exists C > 0,\ \forall 1 \le i \le 6,\ |\partial_i E_L| \le C(1+E_L). \tag{48}$$

In the new coordinates, the stochastic differential equation (23) writes

$$\begin{cases} dX_{1,t} &= \left(\frac{1}{X_{1,t}} - X_{1,t}\right) dt + dW_t^1, \\ dY_{1,t} &= -\widetilde{\omega} Y_{1,t} dt + dW_t^2, \\ dZ_{1,t} &= -\widetilde{\omega} Z_{1,t} dt + dW_t^3, \\ dX_{2,t} &= -X_{2,t} dt + dW_t^4, \\ dY_{2,t} &= -\widetilde{\omega} Y_{2,t} dt + dW_t^5, \\ dZ_{2,t} &= -\widetilde{\omega} Z_{2,t} dt + dW_t^6. \end{cases} \tag{49}$$

The last five coordinates are Ornstein-Uhlenbeck processes and the first one is linked to the Cox-Ingersoll-Ross model of interest rates. Indeed, setting $R_t = (X_{1,t})^2$, one obtains

$$dR_t = 2X_{1,t} dX_{1,t} + dt = (3 - 2R_t)dt + 2\sqrt{R_t}\left(1_{\{X_{1,t} \geq 0\}} - 1_{\{X_{1,t} < 0\}}\right) dW_t^1.$$

According to [13] p.126, for any $r > 0$, the stochastic differential equation

$$R_t^r = r + 3t - 2\int_0^t R_s^r ds + 2\int_0^t \sqrt{R_s^r} dB_s$$

where B is a 1D-Brownian motion admits a $\mathbb{R}_+^*$-valued solution. For $\widetilde{x}_1 \in \mathbb{R}^*$, choosing $B_t = (1_{\{\widetilde{x}_1 > 0\}} - 1_{\{\widetilde{x}_1 < 0\}}) W_t^1$, one easily checks that $X_{1,t}^{\widetilde{x}_1} = (1_{\{\widetilde{x}_1 > 0\}} - 1_{\{\widetilde{x}_1 < 0\}})\sqrt{R_t^{\widetilde{x}_1^2}}$ solves the first equation in (49). As the function $\frac{1}{x} - x$ is decreasing on $\mathbb{R}_+^*$ and on $\mathbb{R}_-^*$, one may check that any solution of the first equation in (49) starting from $\widetilde{x}_1$ is equal to $X_{1,t}^{\widetilde{x}_1}$. From [13] p.128, one obtains that for $t > 0$, $X_{1,t}^{\widetilde{x}_1}$ admits as a density w.r.t. the Lebesgue measure, the function p_1 defined by

$$p_1(t, \widetilde{x}_1, \bar{x}_1) = 1_{\{\widetilde{x}_1 \bar{x}_1 > 0\}} 2\left(1 - e^{-2t}\right)^{-3/2} \bar{x}_1^2 \exp\left(-\frac{e^{2t}\bar{x}_1^2 + \widetilde{x}_1^2}{e^{2t} - 1}\right) \sum_{n=0}^{\infty} \frac{e^{2nt}}{n!\Gamma(n + 3/2)} \left(\frac{\widetilde{x}_1 \bar{x}_1}{e^{2t} - 1}\right)^{2n}$$

where Γ is Euler's gamma function. One checks that $\widetilde{x}_1^2 \exp(-\widetilde{x}_1^2) p_1(t, \widetilde{x}_1, \bar{x}_1)$ is symmetric in variables $\widetilde{x}_1$ and $\bar{x}_1$. Similar symmetry relations are easily obtained for the Ornstein-Uhlenbeck components in (49). Hence the transition density p associated with (49) which is, by independence of the stochastic processes, the product of the transitions densities associated with each component, is such that

$$\psi_I^2(\widetilde{x}_1, \widetilde{y}_1, \widetilde{z}_1, \widetilde{x}_2, \widetilde{y}_2, \widetilde{z}_2) p(t, \widetilde{x}_1, \widetilde{y}_1, \widetilde{z}_1, \widetilde{x}_2, \widetilde{y}_2, \widetilde{z}_2, \bar{x}_1, \bar{y}_1, \bar{z}_1, \bar{x}_2, \bar{y}_2, \bar{z}_2)$$

is symmetric in variables $(\widetilde{x}_1, \widetilde{y}_1, \widetilde{z}_1, \widetilde{x}_2, \widetilde{y}_2, \widetilde{z}_2)$ and $(\bar{x}_1, \bar{y}_1, \bar{z}_1, \bar{x}_2, \bar{y}_2, \bar{z}_2)$. As an easy consequence ψ_I^2 is an invariant density for (49). For $\tilde{x} = (\tilde{x}_1, \tilde{y}_1, \tilde{z}_1, \tilde{x}_2, \tilde{y}_2, \tilde{z}_2) \in \mathbb{R}^* \times \mathbb{R}^5$, let us denote $X_t^{\tilde{x}} = (X_{1,t}^{\tilde{x}_1}, Y_{1,t}^{\tilde{y}_1}, Z_{1,t}^{\tilde{z}_1}, X_{2,t}^{\tilde{x}_2}, Y_{2,t}^{\tilde{y}_2}, Z_{2,t}^{\tilde{z}_2})$ where each coordinate solves the corresponding stochastic differential equation in (49) with an initial condition given by the superscript ($X_0^{\tilde{x}} = \tilde{x}$). One has

$$\partial_{\tilde{x}_1} X_{1,t}^{\tilde{x}_1} = \exp\left(-t - \int_0^t \frac{1}{(X_{1,s}^{\tilde{x}_1})^2} ds\right), \ \partial_{\tilde{x}_2} X_{2,t}^{\tilde{x}_2} = e^{-t},$$
$$\partial_{\tilde{y}_1} Y_{1,t}^{\tilde{y}_1} = \partial_{\tilde{z}_1} Y_{1,t}^{\tilde{z}_1} = \partial_{\tilde{y}_2} Y_{2,t}^{\tilde{y}_2} = \partial_{\tilde{z}_2} Y_{2,t}^{\tilde{z}_2} = e^{-\widetilde{\omega} t}.$$

One easily checks using Lebesgue's theorem that for any $t \geq 0$, $\partial_{\tilde{x}_1} \mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^{\tilde{x}}) ds\right)\right)$ is equal to

$$\mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^{\tilde{x}}) ds\right) \int_0^t \exp\left[-s - \int_0^s \frac{1}{(X_{1,r}^{\tilde{x}_1})^2} dr\right] \partial_1 E_L(X_s^{\tilde{x}}) ds\right).$$

Notice that because of (48), the variable in the last expectation is bounded, uniformly in x and locally in t. Again by Lebesgue's theorem, for fixed $x \in \mathbb{R}^* \times \mathbb{R}^5$ the expectation is continuous w.r.t. variable t. More generally, one obtains that $\nabla_{\tilde{x}} \mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^{\tilde{x}})ds\right)\right)$ is bounded, uniformly in $x \in \mathbb{R}^* \times \mathbb{R}^5$ and locally in t and continuous w.r.t. t for fixed $x \in \mathbb{R}^* \times \mathbb{R}^5$. This ensures that the restriction of $\chi(t, \tilde{x}) = \psi_I(\tilde{x}) \mathbb{E}\left(\exp\left(-\int_0^t E_L(X_s^{\tilde{x}})ds\right)\right)$ to each connected component $\mathcal{C}$ of U_I belongs to $C^0(\mathbb{R}_+, H_0^1(\mathcal{C}))$ and Proposition 11 can be proved by standard energy arguments.

ACKNOWLEDGEMENTS: we warmly thank Michel Caffarel (Laboratoire de Chimie Théorique, University of Paris VI) for helpful discussions.

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