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Stochastic quantization for a system of *N* identical interacting Bose particles

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Abstract

We apply stochastic quantization to a system of N interacting identical bosons in an external potential Φ, by means of a general stationary-action principle. The collective motion is described in terms of a Markovian diffusion on $\mathbb{R}^{3N}$, with joint density $\hat{\rho}$ and entangled current velocity field $\hat{V}$, in principle of non-gradient form, related to one another by the continuity equation. Dynamical equations relax to those of canonical quantization, in some analogy with Parisi–Wu stochastic quantization. Thanks to the identity of particles, the one-particle marginal densities ρ, in the physical space $\mathbb{R}^3$, are all the same and it is possible to give, under mild conditions, a natural definition of the single-particle current velocity, which is related to ρ by the continuity equation in $\mathbb{R}^3$. The motion of single particles in the physical space comes to be described in terms of a non-Markovian three-dimensional diffusion with common density ρ and, at least at dynamical equilibrium, common current velocity v. The three-dimensional drift is perturbed by zero-mean terms depending on the whole configuration of the N-boson interacting system. Finally, we discuss in detail under which conditions the one-particle dynamical equations, which in their general form allow rotational perturbations, can be particularized, up to a change of variables, to the Gross–Pitaevskii equations.

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1. Introduction

Stochastic quantization methods based on variational principles (see [4, 22, 27] and references quoted therein) were introduced in the latest 1980s, as a natural development of the approach proposed by Nelson in his pioneering work on stochastic mechanics [26], based on a stochastic reformulation of Newton's second law. Since the basic starting object is the classical Lagrangian, stochastic quantization procedures based on action principles could be applied in general to any system with a finite number of degrees of freedom, but this fact seems not to have been yet exploited in the literature. In this paper, we use a stochastic variational principle to obtain the dynamical evolution of a system of N identical interacting bosons. This in particular means that we improve the usual description, based on a time-dependent wavefunction on $Ł^2_{\mathbb{C}}(\mathbb{R}^{3N})$, through a $3N$-dimensional Markov diffusion uniquely associated with it. As a consequence, by using some well-defined mathematical manipulations and simplifications, one-particle three-dimensional equations of motion in conditional mean (propositions 2 and 3) can be obtained. Moreover precise assumptions, under which such dynamical equations can be particularized, up to a change of variables, to the Gross–Pitaevskii equations [10, 29], will be described.

Among the various action principles proposed in the literature we have chosen to apply the Lagrangian stochastic variational principle formulated in [17, 20, 21]. A variant with the introduction of a free parameter is proposed in [11]. An extension to curved configuration space is provided in [2].

This approach allows on the one hand to work with smooth mathematical objects and, on the other hand, to obtain generalized equations of motion where non-gradient velocity fields are allowed. These generalized solutions approximate the canonical ones after a relaxation time, in some analogy with the Parisi–Wu approach [28]. In the three-dimensional case the vorticity can concentrate in the zeros of the density, originating the typical singular solutions of Madelung fluid equations which correspond to wavefunctions with nodes (see [6] for a numerical example with the formation of central vortex lines).

We also quote that in [24] and [25] the case of Gaussian and linear solution for the bidimensional harmonic oscillator was carefully worked out, proving the global existence of solutions, for which Schrödinger Gaussian solutions constitute a centre manifold. It was in particular also proved that convergence is in the sense of the relative entropy.

As far as the present work is concerned, smoothness properties will be useful to prove in a quite elementary way the main results of section 2, while the occurrence of non-gradient velocity fields leaves open, in principle, the possibility of describing rotational excitations in the one-particle dynamical equations. We make reference to the problems connected to the existence of rotational excitations in a Bose condensate described by the Gross–Pitaevskii equation [3].

The plan of the paper is the following: in section 2 we describe the quantization of the N-particles system by means of the stochastic Lagrangian variational principle, in section 3 we study the consequences of working with identical particles and symmetric wavefunctions. Finally, in section 4 we particularize the dynamics in order to get, for a smooth short-range interaction potential, the Gross–Pitaevskii equation. Possible developments are outlined in section 5.

2. Quantization of the interacting N-particles system

We consider a system of N identical interacting particles with quantum Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \left\{ -\frac{\hbar^2}{2m}\nabla_i^2 + \Phi(\mathbf{r}_i) \right\} + \Phi_{\text{int}}(\mathbf{r}_1, \ldots, \mathbf{r}_N, \alpha)$$

where Φ and Φ_{int} denote, respectively, the external and interaction potentials, $\mathbf{r}_i$ is the position of the ith particle in the physical space and α is a coupling parameter. We assume that $\mathcal{H}$

is bounded from below, so that $\mathcal{H}$ has a self-adjoint extension which is the generator of the unitary group which describes the evolution in time of the wavefunction $\hat{\Psi}$ in $L^2_{\mathbb{C}}(\mathbb{R}^{3N}, \mathrm{d}\hat{r})$. The $3N$-dimensional Schrödinger equation reads, in compact form,

$$\mathrm{i}\hbar\partial_t\hat{\Psi} = \left(-\frac{\hbar^2}{2m}\hat{\nabla}^2 + \Phi^{\alpha,N}_{\text{tot}}\right)\hat{\Psi} \tag{2.1}$$

where $\hat{\nabla} := (\nabla_1, \dots, \nabla_N)$ and $\Phi^{\alpha,N}_{\text{tot}} := \sum_{i=1}^{N}\Phi(\mathbf{r}_i) + \Phi_{\text{int}}(\mathbf{r}_1, \dots, \mathbf{r}_N, \alpha)$.

In stochastic quantization by the Lagrangian variational principle the basic object is the classical Lagrangian

$$\mathcal{L}[\hat{q}^{\text{cl}}] = \sum_{i=1}^{N}\left\{\frac{1}{2}m\big(\dot{\mathbf{q}}_i^{\text{cl}}\big)^2(t) - \Phi\big(\mathbf{q}_i^{\text{cl}}(t)\big)\right\} - \Phi_{\text{int}}\big(\mathbf{q}_1^{\text{cl}}(t), \dots, \mathbf{q}_N^{\text{cl}}(t), \alpha\big)$$

where $\hat{q}^{\text{cl}}$ denotes the classical N-body configuration.

Quantization comes from requiring that the configuration of the system is in fact a Markov diffusion $\hat{q}$ with time-dependent drift $\hat{b}$ and diffusion matrix equal to $\frac{\hbar}{m}I$, where I denoting the identity matrix in $\mathbb{R}^{3N}$.

The assumptions needed by the quantization procedure are as follows:

(i) The drift, denoted by $\hat{b}$, is smooth both as a function of $\hat{r}$ and $t \in [0, T]$, $T < \infty$.

(ii) $\hat{q} = (\mathbf{q}_1, \dots, \mathbf{q}_N)$ is a pathwise solution of the $3N$-dimensional stochastic differential equation

$$\mathrm{d}\hat{q}(t) = \hat{b}(\hat{q}(t), t) + \left(\frac{\hbar}{m}\right)^{1/2}\mathrm{d}\hat{W}(t) \tag{2.2}$$

where $\hat{W} := (\mathbf{W}_1, \dots, \mathbf{W}_N)$ and $\mathbf{W}_i$, $i = 1, \dots, N$, are three-dimensional independent standard Brownian motions which model quantum fluctuations acting on the ith particle. A finite energy condition [9] is also assumed.

Then one can prove in particular that, denoting by $\hat{\rho}$ the time-dependent probability density of the configuration, there exists a smooth time-dependent current velocity field $\hat{V}$ such that

$$\hat{b} = \hat{V} + \frac{\hbar}{2m}\nabla\log\hat{\rho}$$

and the continuity equation holds, i.e.,

$$\frac{\partial\hat{\rho}}{\partial t} = -\hat{\nabla}\cdot(\hat{\rho}\hat{V}).$$

The stochastic Lagrangian variational principle introduced in [17, 20] and [21] claims that the actual motion is described by a Markov diffusion which makes extremal the mean discretized classical action related to $\mathcal{L}$ among smooth diffusions which satisfy a $3N$-dimensional stochastic differential equation of type (2.2), with the same fixed Brownian motion and such that the initial current velocity and the final configuration are fixed as random variables.

In the limit of the discretization going to infinity the necessary and sufficient condition is that the drift of the actual diffusion is given by

$$\hat{b} = \hat{V} + \frac{\hbar}{2m}\nabla\ln\hat{\rho}$$

where, for $k = 1, \dots, 3N$,

$$\partial_t\hat{\rho} = -\hat{\nabla}\cdot(\hat{\rho}\hat{V}) \tag{2.3}$$

$$\left[\partial_t \hat{V} + (\hat{V}\cdot\hat{\nabla})\hat{V} - \frac{\hbar^2}{2m^2}\hat{\nabla}\left(\frac{\hat{\nabla}^2\sqrt{\hat{\rho}}}{\sqrt{\hat{\rho}}}\right)\right]_k + \frac{\hbar}{2m}\sum_{p=1}^{3N}(\partial_p \ln\hat{\rho} + \partial_p)(\partial_k \hat{V}_p - \partial_p \hat{V}_k)$$
$$= -\frac{1}{m}\partial_k \Phi_{\text{tot}}^{\alpha,N}. \tag{2.4}$$

So, in case $\hat{V}$ is a smooth gradient field we get the familiar Madelung equations for the N-particle system. Indeed, putting, for some differentiable scalar field $\hat{S}$,

$$\hat{V} = \frac{1}{m}\hat{\nabla}\hat{S}$$

and

$$\hat{\Psi} = \hat{\rho}^{\frac{1}{2}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{S}}$$

we get the $3N$-dimensional Schrödinger equation (2.1).

Otherwise for general initial data the rotational terms, of the first order in $\frac{\hbar}{m}$, induce dissipation.

Indeed if $(\hat{\rho}, \hat{V})$ is a smooth solution of (2.3) and (2.4) such that $\frac{\hat{\nabla}\hat{\rho}}{\hat{\rho}}$ is finite at infinity[3], we have

$$\frac{\mathrm{d}}{\mathrm{d}t}E[\hat{\rho}, \hat{V}] = -\frac{\hbar}{2}\mathcal{E}\left[\sum_{k=1}^{3N}\sum_{p=1}^{3N}\frac{(\partial_p \hat{V}_k - \partial_k \hat{V}_p)^2}{2}\right]$$

with

$$E[\hat{\rho}, \hat{V}] = \int_{\mathbb{R}^{3N}}\left(\frac{1}{2}m\hat{V}^2 + \frac{1}{2}m\hat{U}^2 + \Phi_{\text{tot}}^{\alpha,N}\right)\hat{\rho}\,\mathrm{d}\hat{r}$$

and $\hat{U} := \frac{\hbar}{2m}\hat{\nabla}\ln\hat{\rho}$ ($3N$-dimensional osmotic velocity).

This *energy theorem* was proved in [17] for $N = 1$ and $d = 3$. The present generalization to a configurational space with higher dimension is straightforward.

Therefore irrotational solutions conserve the energy, which turns to be the usual quantum mechanical expectation of the observable energy, that is

$$E = \langle\Psi, \mathcal{H}\Psi\rangle$$

where $\langle\,,\rangle$ denotes the $L^2_{\mathbb{C}}(\mathbb{R}^{3N}, \mathrm{d}\hat{r})$ scalar product. For generic initial data, with $\mathcal{H}$ being bounded from below, Schrödinger solutions act as an attracting set, which corresponds to dynamical equilibrium. In this case, the constructed quantization procedure reproduces the canonical one after a relaxation, in some analogy with the Parisi–Wu approach [28].

We refer the reader to [23] for a recent survey on probabilistic and numerical aspects of the stochastic quantization procedure.

3. One-particle description

In this section, we study the behaviour of a single particle in the system. For simplicity, we will assume that the particles remain confined in a bounded region, for a finite time interval $[0, T]$. Under some regularity assumptions we can prove that, if the particles are bosons and the system is at dynamical equilibrium, then they have a common probability density

[3] We stress that the above-mentioned condition at infinity is only sufficient. Actually, there is at least one example, namely the Gaussian solutions for the bidimensional harmonic oscillator [24], such that the condition is not satisfied and the energy theorem still holds.

for the position ρ and a common current velocity field $\mathbf{v}$, which are related by the continuity equation (propositions 1 and 4). The current velocity $\mathbf{v}$ is defined as a conditional mean given the position of the particle. The full stochastic description of the motion is given by a non-Markovian diffusion (proposition 2). Moreover, we are able to describe the time evolution for $(\rho, \mathbf{v})$ as a generalization of the Madelung fluid equations where the effect of interactions are represented as disturbances (3.7) and (3.8).

To be precise we will assume in the following that $\hat{\rho}$ has support in a compact set for $t = 0$, and that the support remains in a given bounded domain for all $t \in [0, T]$. Both $\hat{\rho}$ and $\hat{V}$ are smooth by assumption. Indeed we will need that $\hat{\rho}$ is of class C_o^1 as a function of t and C_o^2 as function of the configuration variable $\hat{r}$, while the current $\hat{V}\hat{\rho}$ is assumed of class C_o^1 as functions of $\hat{r}$.

The requirement of these assumptions is motivated by the necessity in the following of the exchange of some derivatives and integrals in proving propositions 1 and 2.

Actually, the assumptions just stated are not the weakest ones: alternatively one could work in an unbounded region requiring that there exists an integrable function g on $\mathbb{R}^{3N}$ such that $|\partial_t \hat{\rho}(\hat{r}, t)| \leqslant g(\hat{r})\,\mathrm{d}\hat{r}$ a.s., and analogously for $\hat{\rho}$ and $\hat{\rho}\hat{V}$ as functions of the configurational variable.

3.1. Identical particles and decomposition of the drift

We first introduce, taking the marginals of $\hat{\rho}$, the one-particle probability densities $\rho_i(\mathbf{r}_i, t)$, $i = 1, \ldots, N$:

$$\rho_i(\mathbf{r}_i, t) = \int_{\mathbb{R}^{3(N-1)}} \hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N, t)\, \overbrace{\mathrm{d}\mathbf{r}_1, \ldots, \mathrm{d}\mathbf{r}_N}^{\mathbf{dr}_i \text{excluded}}.$$

It is easy to see that if $\hat{\rho}$ is invariant under permutation of the positions of two generic particles then the one-particle probability density is the same for all $i = 1, 2, \ldots, N$. Indeed if, for all $i, j = 1, 2, \ldots, N$, one has

$$\hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N, t) = \hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N, t)$$

then, with $\mathbf{r}_i = \mathbf{r}$,

$$\begin{aligned}\rho_i(\mathbf{r}, t) &= \int_{\mathbb{R}^{3(N-1)}} \hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}, \ldots, \mathbf{r}_N, t)\, \overbrace{\mathrm{d}\mathbf{r}_1, \ldots, \mathrm{d}\mathbf{r}_N}^{\mathbf{dr} \text{ excluded}} \\ &= \int_{\mathbb{R}^{3(N-1)}} \hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N, t)\, \overbrace{\mathrm{d}\mathbf{r}_1, \ldots, \mathrm{d}\mathbf{r}_N}^{\mathbf{dr} \text{ excluded}} = \rho_j(\mathbf{r}, t).\end{aligned}$$

Therefore, in the case of identical particles we can write, for every Borel set $I \subset \mathbb{R}^3$ and for $\rho_i(\mathbf{r}, t) \equiv \rho(\mathbf{r}, t), \forall i$,

$$\mathbb{P}[\mathbf{q}_i(t) \in I] = \int_I \rho(\mathbf{r}, t)\,\mathrm{d}\mathbf{r}.$$

Using the notation

$$\hat{V} = (\mathbf{V_1}, \ldots, \mathbf{V_N}).$$

we define the 'one-particle current velocity field' for the ith particle by the equality

$$\mathbf{v}_i(\mathbf{r}, t) = \mathbb{E}_{\mathbf{q}_i(t)=\mathbf{r}} \mathbf{V}_i(\mathbf{q}_1(t), \ldots, \mathbf{q}_i(t), \ldots, \mathbf{q}_N(t), t) \tag{3.1}$$

where $\mathbb{E}_{\mathbf{q}_i(t)=\mathbf{r}}$ denotes the conditional expectation, given $\mathbf{q}_i(t) = \mathbf{r}$.

As a consequence, we can state the following:

Proposition 1. *One-particle continuity equation.*

Let us assume that the particles are identical. Let also assumptions (i), (ii) and those stated at the beginning of this section hold. Let $\hat{\rho}$ be of class C_o^1 as a function of time and let $\hat{\rho}\hat{V}$ be of class C_o^1 as a function of $\hat{r}$. Then, the one-particle probability density ρ and the one-particle current velocity $\mathbf{v_i}$, defined in (3.1), for all $i = 1, \ldots, N$, are related by the continuity equation

$$\partial_t \rho = -\nabla \cdot (\rho \mathbf{v_i}).$$

Proof. In our assumptions we can write, for $t \in [0, T]$,

$$\begin{aligned}
\partial_t \rho_1(\mathbf{r}, t) &= \partial_t \int_{\mathbb{R}^{3(N-1)}} \hat{\rho}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N \\
&= \int_{\mathbb{R}^{3(N-1)}} \partial_t \hat{\rho}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N \\
&= -\int_{\mathbb{R}^{3(N-1)}} \sum_{i=1}^{N} \nabla_i (\hat{\rho}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) \mathbf{V}_i(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N))\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N \\
&= -\int_{\mathbb{R}^{3(N-1)}} \nabla_1 (\hat{\rho}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) \mathbf{V}_1(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N))\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N \\
&= -\nabla_1 \left[\rho_1(\mathbf{r}, t) \int_{\mathbb{R}^{3(N-1)}} \frac{\hat{\rho}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) \mathbf{V}_1(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)}{\rho_1(\mathbf{r}, t)}\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N \right] \\
&= -\nabla_1 (\rho_1(\mathbf{r}, t) \mathbf{v}_1(\mathbf{r}, t))
\end{aligned}$$

where we have integrated by parts all the terms of the sum except the first one and used the definition of conditional density. □

We now make explicit the deviation of the actual drift of the ith particle from the part depending only on the ith configuration.

Let us introduce the two scalar fields $\hat{R}$ and R by putting $\hat{\rho} := \mathrm{e}^{2\hat{R}}$ and $\rho := \mathrm{e}^{2R}$. We define ξ_i and Ξ by the equalities

$$\xi_i(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N, t) := \mathbf{V}_i(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N, t) - \mathbf{v}_i(\mathbf{r}_i, t)) \tag{3.2}$$

and

$$\Xi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) := \hat{R}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) - \sum_{j=1}^{N} R(\mathbf{r_j}, t). \tag{3.3}$$

It is important to note that, $\forall\, i = 1, \ldots, N$,

$$\begin{aligned}
&\mathbb{E}_{\mathbf{q}_i(t)=\mathbf{r}} \xi_i(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), t) = 0 \\
&\mathbb{E}_{\mathbf{q}_i(t)=\mathbf{r}} \nabla_i \Xi(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), t) = 0
\end{aligned}$$

where the second equality follows from the definition of conditional density. Indeed, putting, $i = 1$, we have in our assumptions, for $t \in [0, T]$ and integrating componentwise,

$$\begin{aligned}
\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \nabla_1 \hat{R}(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), t) &= \int_{\mathbb{R}^{3(N-1)}} (\nabla_1 \hat{R}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)) \\
&\quad \times \frac{\hat{\rho}(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)}{\rho(\mathbf{r}, t)}\, \mathrm{d}\mathbf{r}_2, \mathrm{d}\mathbf{r}_3, \ldots, \mathrm{d}\mathbf{r}_N \\
&= \frac{1}{2\rho(\mathbf{r}, t)} \nabla \rho(\mathbf{r}, t) = \nabla R(\mathbf{r}, t).
\end{aligned}$$

We summarize the results in the following two non-trivial propositions.

Proposition 2. *Non-Markovian one-particle diffusion.*

In the case of identical particles, under assumptions (i) and (ii) and those stated at the beginning of this section, the motion of the 1st particle is described by a non-Markovian diffusion $\mathbf{q}_1$, with probability density $\rho := \mathrm{e}^{2R}$ and current velocity $\mathbf{v_1}$, which satisfies the equality

$$\mathrm{d}\mathbf{q}_1(t) = \left(\mathbf{v}_1(\mathbf{q}_1(t), t) + \frac{\hbar}{m}\nabla_1 R(\mathbf{q}_1(t), t)\right)\mathrm{d}t$$
$$+\,\zeta_1(\mathbf{q}_1(t), \mathbf{q}_2(t), \ldots, \mathbf{q}_N(t), t)\,\mathrm{d}t + \left(\frac{\hbar}{m}\right)^{1/2}\mathbf{dW}_1(t)$$

where

$$\zeta_1 := \xi_1 + \frac{\hbar}{m}\nabla_1\Xi$$

with $\xi_\mathbf{1}$ and Ξ being defined by (3.2), (3.3), respectively, so that

$$\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\zeta_1 = 0.$$

Proposition 3. *General one-particle dynamics.*

Let assumptions (i), (ii) and those stated at the beginning of this section hold. Then, the one-particle marginal density ρ and the one-particle current velocity $\mathbf{v}_1$ of the 1st particle in a system of N identical particles satisfy the couple of PDEs, for $k = 1, 2, 3$,

$$[\partial_t\rho + \nabla\cdot(\rho\mathbf{v}_1)](\mathbf{r}, t) = 0 \tag{3.4}$$

$$\left[\partial_t\mathbf{v}_1 + (\mathbf{v}_1\cdot\nabla)\,\mathbf{v}_1 - \frac{\hbar^2}{2m^2}\nabla\left(\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right) + \frac{\hbar}{2m}\,(\nabla\ln\rho + \nabla)\wedge(\nabla\wedge\mathbf{v}_1)\right]_k(\mathbf{r}, t)$$
$$= -\frac{1}{m}\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\left\{\partial_k\Phi_{\mathrm{tot}}^{\alpha,N}(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t))\right\} - \beta_k(\alpha, N, \mathbf{r}, t) \tag{3.5}$$

where

$$\beta_k(\alpha, N, \mathbf{r}, t) := \left[\beta^{\mathrm{time}} + \beta^{\mathrm{conv}} + \frac{\hbar}{2m}\beta^{\mathrm{rot}} - \frac{\hbar^2}{2m^2}\beta^{Q}\right]_k(\alpha, N, \mathbf{r}, t)$$

and

$$\beta^{\mathrm{time}}(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}[\partial_t\mathbf{V}_1 - \partial_t\mathbf{v}_1]$$
$$\beta^{\mathrm{conv}}(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\{(\hat{V}\cdot\hat{\nabla})\mathbf{V}_1 - (\mathbf{v}_1\cdot\nabla)\mathbf{v}_1\}$$
$$\beta_k^{\mathrm{rot}}(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\left\{\sum_{p=1}^{3N}(\partial_p\ln\hat{\rho} + \partial_p)(\partial_k\hat{V}_p - \partial_p\hat{V}_k) - [(\nabla\ln\rho + \nabla)\wedge(\nabla\wedge\mathbf{v}_1)]_k\right\}$$
$$\beta^{Q}(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\left\{\nabla_1\left(\frac{\hat{\nabla}^2\sqrt{\hat{\rho}}}{\sqrt{\hat{\rho}}}\right) - \nabla_1\left(\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right)\right\}.$$

3.2. Symmetric and antisymmetric wavefunctions

In this subsection, we fix, without loss of generality, $N = 2$ and $d = 1$. We also do not make explicit the dependence on time. For any solution $\hat{\Psi}$ to the Schrödinger equation we have, by construction, that $|\hat{\Psi}|^2 = \hat{\rho}$. Thus, being $\hat{\rho}$ symmetric with respect to permutation of positions of two generic particles, $\hat{\Psi}$ can only be symmetric or antisymmetric.

We can prove the following:

Proposition 4. *Bosons.*

If $\hat{\Psi}$ is symmetric and belongs to $C^1(\mathbb{R}^2 \to \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R}^2)$, then, putting

$$\hat{\Psi} = \sqrt{\hat{\rho}} \exp \frac{\mathrm{i}}{\hbar} \hat{S} \qquad \hat{V} = \frac{1}{m} \hat{\nabla} \hat{S},$$

we have, $\forall\, r, r' \in \mathbb{R}$,

$$\hat{V}_1(r, r') = \hat{V}_2(r', r)$$

and

$$\begin{aligned} \mathbf{v}_1(r) &= \mathbb{E}_{q_1(t)=r} \hat{V}_1(q_1(t), q_2(t)) \\ &= \mathbb{E}_{q_2(t)=r} \hat{V}_2(q_1(t), q_2(t)) = \mathbf{v}_2(r). \end{aligned} \tag{3.6}$$

Proof. By symmetry of the wavefunction $\hat{\Psi}$ we can write

$$\hat{S}(r, r') = \hat{S}(r', r), \qquad \forall\, r, r' \in \mathbb{R}.$$

Moreover, being $\hat{\Psi}$ differentiable,

$$\begin{aligned} m\hat{V}_1(r, r') &= \partial_1 \hat{S}(r, r') \\ &= \lim_{h\to 0} \frac{\hat{S}(r + h, r') - \hat{S}(r, r')}{h} = \lim_{h\to 0} \frac{\hat{S}(r', r + h) - \hat{S}(r', r)}{h} \\ &= \partial_2 \hat{S}(r', r) = m\hat{V}_2(r', r). \end{aligned}$$

Therefore, in our assumptions, by the definition of conditional density, we get

$$\begin{aligned} \mathbb{E}_{q_1(t)=r} \hat{V}_1(q_1(t), q_2(t)) &= \int \hat{V}_1(r, r') \frac{\hat{\rho}(r, r')}{\rho(r)} \,\mathrm{d}r' = \int \hat{V}_2(r', r) \frac{\hat{\rho}(r', r)}{\rho(r)} \,\mathrm{d}r' \\ &= \mathbb{E}_{q_2(t)=r} \hat{V}_2(q_1(t), q_2(t)) \end{aligned}$$

which proves the assertion. □

Remark. This cannot be proved for fermions. Indeed if $\hat{\Psi} : \mathbb{R}^2 \to \mathbb{C}$ is antisymmetric then proposition 3 does not apply: since we have

$$\hat{\Psi}(r, r') = -\hat{\Psi}(r', r)$$

then, for some $n = 0, 1, 2, \ldots,$

$$\hat{S}(r, r') = \hat{S}(r', r) + (2n + 1)\pi.$$

As a consequence, one has, with $\epsilon > 0$,

$$\lim_{\epsilon\to 0} (\hat{S}(r + \epsilon, r) - \hat{S}(r, r + \epsilon)) \geqslant \pi.$$

Thus $\hat{S}$ is not differentiable and, for a system of N identical fermions, no $3N$-dimensional gradient current velocity field exists as a function of the configuration $\hat{r}$.

Concluding we can claim that, in the gradient case and in general at the dynamical equilibrium, up to mild regularity conditions, all bosons in the (isolated) interacting system have the same one-particle current velocity field and that the fluid-dynamical equations are

$$[\partial_t \rho + \nabla \cdot (\rho \mathbf{v})](\mathbf{r}, t) = 0 \tag{3.7}$$

$$\left[\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\,\mathbf{v} - \frac{\hbar^2}{2m^2} \nabla \left(\frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right)\right]_k (\mathbf{r}, t)$$
$$= -\frac{1}{m} \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left\{ \partial_k \Phi^{\alpha,N}_{\mathrm{tot}} (\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)) \right\} - \beta_k(\alpha, N, \mathbf{r}, t) \tag{3.8}$$

where

$$\beta_k(\alpha, N, \mathbf{r}, t) := \left[\beta^{\mathrm{time}} + \beta^{\mathrm{conv}} - \frac{\hbar^2}{2m^2} \beta^Q \right]_k (\alpha, N, \mathbf{r}, t).$$

We stress that this is a quite general (orthodox) description, which is expected to hold for any N and any sufficiently smooth interaction potentials. The study of various kinds of interactions and proper limits as well as rescalings under which this general boson dynamics can be written in a closed form (deterministic or stochastic) will be the subject of future work. As a first test we will consider in the next section the case of a short-range smooth pair interaction. This is known to lead, starting from the N-bodies Schrödinger equation, to the correct Gross–Pitaevskii ground state [14, 15]. Very recently this result has been extended to solutions of the time-dependent Gross–Pitaevskii equation for factorized initial states and zero external potential [8]. This proof is based on a proper rescaling of the interaction potential for N going to infinity. Both the one-particle limit solutions correspond to exactly factorized N-bodies states.

In the next section, we will exploit our stochastic description in order to fix the proper scales and orders of approximations so that the Gross–Pitaevskii equation can be derived in general from the N-body problem for a given pair short-range interaction potential.

4. A particular case: the Gross–Pitaevskii equation

We first introduce some natural restrictions under which the one-particle boson dynamics can be rewritten, up to the interaction term, in a closed deterministic form (subsection 4.1). Then we model the interaction as a smooth pair potential with compact support and we rigorously derive the Gross–Pitaevskii equation (subsection 4.2). Detailed calculation of the nonlinear term is given in the appendix.

4.1. General restrictions

In what follows, we will assume that the initial N-body state is *not entangled*. As a consequence, in case the coupling parameter α is equal to zero, the solution $\hat{\Psi}$ to the N-body Schrödinger equation would be factorized. We also require that $\hat{\Psi}$, together with its first and second spatial derivatives, be close to the factorized solution for small values of α. We assume

(a) $\hat{\Psi}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) - \Pi_{i=1}^N \psi_i(\mathbf{r}_i, t) = O(\alpha)$,
(b) $\nabla_i^{(p)} \hat{\Psi}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) - \nabla_i^{(p)} \Pi_{j=1}^N \psi_i(\mathbf{r}_i, t) = O(\alpha), \forall\, i = 1, \ldots, N;\ p = 1, 2$

where $|\psi_i|^2 = \rho$ and $\mathrm{Im} \frac{\nabla \psi_i}{\psi_i} = \mathbf{v}, \forall\, i = 1, \ldots, N$.

Moreover, we consider the following restrictions:

(c1) $\beta^{\text{time}} = 0$: this is true for all stationary solutions. If the solution is not stationary then we must choose a time scale where $\partial_t\left[\mathbf{V}_1(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), t) - \mathbf{v}(\mathbf{q}_1(t), t)\right], i = 1, \ldots, N$, has negligible conditional expectation given the position of the considered particle.

(c2) $\beta^{\text{conv}} = 0$: this is true for the ground state. In general on a scale where $\nabla_1\left[\mathbf{V}_1(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), t) - \mathbf{v}(\mathbf{q}_1(t), t)\right]$ has negligible conditional expectation given the position of the considered particle, we have

$$\begin{aligned}\beta^{\text{conv}} &= \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\left\{(\mathbf{V}_1 \cdot \nabla_1)\mathbf{V}_1 + \sum_{i=2}^{N}(\mathbf{V}_i \cdot \nabla_i)\mathbf{V}_1\right\} - (\mathbf{v}_1 \cdot \nabla_1)\mathbf{v}_1(\mathbf{r}, t) \\ &= O(\alpha^2) + \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\nabla_1 \sum_{i=2}^{N} \frac{1}{2}|\mathbf{V}_i|^2. \end{aligned} \tag{4.1}$$

But in the case of a great number of particles, the total kinetic energy due to current velocity contribution is expected not to be sensitive to variations of the position of a single particle. Thus, we will assume N finite but sufficiently large to neglect the last term in (4.1).

(c3) $\left(\frac{\hbar^2}{m^2}\right)\beta^{Q} = 0$: in our assumptions β^{Q} goes to zero as $O(\alpha)$. Thus, the condition means that, estimating the approximations in terms of $\frac{\hbar}{m}$ and α, we are neglecting a term of order $O\left(\frac{\hbar^2}{m^2}\right)O(\alpha)$.

Therefore, in our assumptions, for the proper spacetime and size scales, β_k in (3.8) can be neglected to the orders $O(\alpha)O\left(\frac{\hbar^2}{m^2}\right)$ and $O(\alpha^2)$.

4.2. Short-range smooth pair interaction potential

We now calculate, to the order $O(\alpha^2)$, the one-particle interaction potential for a dilute system with short-range smooth interaction.

We define

$$\Phi_{\text{int}}(\mathbf{r}_1, \ldots, \mathbf{r}_N, \alpha) := \frac{K}{2}\sum_{i=1}^{N}\sum_{j=1, j\neq i}^{N} h_{B^\alpha(\mathbf{r}_i)}(\mathbf{r}_j)$$

where K is a constant which can be positive or negative, $B^\alpha(\mathbf{r})$ is the open sphere centred in $\mathbf{r}$, with volume α, and $h_{B^\alpha(\mathbf{r})}$ satisfies the following assumptions, which simply mean that $h_{B^\alpha(\mathbf{r}_i)}$ is a good smooth approximation of the indicator of the sphere $B^\alpha(\mathbf{r}_i)$:

(i) $0 \leqslant h_{B^\alpha(\mathbf{r}_i)}(\mathbf{r}_j) = h_{B^\alpha(\mathbf{r}_j)}(\mathbf{r}_i)$,

(ii) $h_{B^\alpha(\mathbf{r})} \in C^1_o$, $\operatorname{supp} h_{B^\alpha(\mathbf{r})} = B^\alpha(\mathbf{r})$,

(iii) $0 \leqslant \int_{\mathbb{R}^3}(I_{B^\alpha(\mathbf{r}_i)}(\mathbf{r}) - h_{B^\alpha(\mathbf{r}_i)}(\mathbf{r}))d^3\mathbf{r} = O(\alpha^2)$,

where $I_{B^\alpha(\mathbf{r})}$ denotes the function which takes value 1 in $B^\alpha(\mathbf{r})$ and 0 outside.

We can then show that the interaction term can be written in the following form:

$$\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1}[\nabla_1\Phi_{\text{int}}](\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), \alpha) = K(N-1)\{O(\alpha^2) + \nabla_1[\alpha\rho(\mathbf{r}_1, t) + O(\alpha^2)]\}. \tag{4.2}$$

The calculation is reported in detail in the appendix.

Let us now introduce the expected number of particles in any finite volume $\delta V \subset \mathbb{R}^3$. The number of particles in δV at time t is the random variable

$$N_{\delta V}(t) := \sum_{i=1}^{N} I_{\delta V}(\mathbf{q}_i(t)).$$

Its expectation is

$$\mathbb{E}N_{\delta V}(t) = \int_{\delta V} N\rho(\mathbf{r}, t)\,\mathrm{d}^3\mathbf{r}.$$

Thus $\bar{\rho}(\mathbf{r}, t) := N\rho(\mathbf{r}, t)$, $\mathbf{r} \in \mathbb{R}^3$, is the expected density of particles in the physical space.

It is not trivial that the couple $(\bar{\rho}, v)$ is a true state of a physical fluid with density $\bar{\rho}$ and velocity field $\mathbf{v} \equiv \mathbf{v}_i, \forall i = 1, \ldots, N$.

With conditions (c1)–(c3) the dynamical equations, independently of the choice of the particle, become

$$\partial_t \bar{\rho} + \nabla \cdot (\bar{\rho} v) = 0 \tag{4.3}$$

$$\begin{aligned} \partial_t v + (v \cdot \nabla) v - \frac{\hbar^2}{2m^2} \nabla \left(\frac{\nabla^2 \sqrt{\bar{\rho}}}{\sqrt{\bar{\rho}}} \right) \\ = -\frac{1}{m} \nabla \Phi - \frac{1}{m} K \frac{N-1}{N} \{ N O(\alpha^2) + \nabla [\alpha \bar{\rho} + N O(\alpha^2))] \}. \end{aligned} \tag{4.4}$$

We now approximate $\frac{N-1}{N}$ to 1 and neglect terms of order $O(\alpha^2)$.

As a consequence, introducing the 'fluid wavefunction' $\bar{\psi} := \bar{\rho}^{\frac{1}{2}} \exp \frac{\mathrm{i}}{\hbar} S$, where $\frac{1}{m} \nabla S := v$, we find the Gross–Pitaevskii equation

$$\mathrm{i}\hbar \partial_t \bar{\psi} = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + \Phi + K\alpha |\bar{\psi}|^2 \right\} \bar{\psi}.$$

Concluding, in our assumptions, after properly fixing the spacetime and size scales, we have derived the dynamical equation for the complex field $\bar{\psi}$, normalized to N, whose physical meaning is in agreement with the canonical interpretation, and $|\bar{\psi}|^2$ representing in fact the expected density of particles.

This has been done up to terms of orders $O(\alpha) O\left(\left(\frac{\hbar}{m}\right)^2\right)$ and $O(\alpha^2)$. Note that the nonlinear term is calculated (see the appendix) without exploiting, as usual, any effective interaction potential (see, for example, [30]).

5. Conclusions and remarks

We have studied the behaviour in finite time of a (isolated) system of N identical interacting bosons starting from the N-body quantum problem. We have exploited the stochastic Lagrangian variational principle and derived, under regularity conditions, the one-particle dynamics essentially by means of conditional expectations given the position at time t of a single particle, leading to the general boson dynamics (3.7) and (3.8). This description is expected to hold for any N and reasonably smooth interaction potentials.

For the particular case of a dilute gas with short-range interaction our work provides a derivation of the Gross–Pitaevskii equation which starts from the N-body problem and where no effective interaction potential is introduced. In particular no low energy condition is assumed, as in most part of the literature tracing back to the work by Bogolubov [5] and developed by Gross [10] and Pitaevskii [29], where the system is initially described within quantum field theory (see, for example, [16] and [30] for accurate reviews).

A derivation of the Gross–Pitaevskii equation from the N-body Hamiltonian, as far as the ground state is concerned, was done in [14, 15] and very recently extended to the free evolution from factorized states [8]. This is obtained by means of a rigorous rescaling with N of the coupling constant in the Schrödinger equation. These particular cases correspond to exactly factorized limit solutions of the rescaled N-body quantum problem for N going to infinity. In contrast, in our approach, after fixing the proper scales, N remains finite and the approximations are estimated as orders of both α, i.e. the volume of the support of the interaction potential, and $\frac{\hbar}{m}$. On the other hand, we do not lead to factorized states but to a fluid-dynamical description for the evolution of the expected density of particles and the common one-particle current velocity field. The full stochastic description of the motion of a generic boson is given in terms of a non-Markovian diffusion, where the common drift is in fact perturbed by a noise due to the configuration of the whole N-body system (proposition 2).

The reason by which we have chosen to exploit the Lagrangian variational principle in place of other variational principles proposed in the literature, or simply starting from the 3N-dimensional Schrödinger equation and then associating its every solution with a Nelson diffusion in the standard way, is both mathematical and physical. We recall that, by Carlen's work [7], Nelson diffusions associated with any solution of a Schrödinger equation exist in weak sense, provided the finite energy condition is satisfied. But in the case of nodes of the wavefunction the current velocity is typically singular. As a consequence, the approach proposed in this work appears to be more convenient from the mathematical point of view: in fact one can assume in a quite natural way the regularity properties of $\hat{\rho}$ and $\hat{V}$ required to prove the results in section 3, since all time-dependent fields $(\hat{\rho}, \hat{V})$, related to diffusions which satisfy the Lagrangian variational principle, are smooth in finite time by construction. Singularities possibly arise asymptotically, as shown for example in [6].

From the physical point of view, it is not trivial that, if we relax the irrotationality condition, at least close to dynamical equilibrium, one can also take into account the interaction-dependent term $\frac{\hbar}{m}\beta^{\mathrm{rot}}$, which is of the order $O\left(\frac{\hbar}{m}\right)O(\alpha)$, in the general one-particle dynamics in proposition 3. This fact could represent a new insight to face the open problem of modelling rotonic excitations.

Moreover, the vorticity-induced dissipation, typical of a system described by the stochastic Lagrangian variational principle, would suggest an alternative to other solutions proposed in the literature [13] to simulate the relaxation towards vortex lattices of a rotating superfluid [1, 18, 19] and [31].

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Appendix

To prove equality (4.2) we first observe that, $\forall\, j \neq 1$, by (iii) of subsection 4.2, being $\hat{\rho}$ bounded as a consequence of the assumptions in section 3, and since the conditional expectation, given $\mathbf{q}_1(t) = \mathbf{r}_1$, is equal to zero if $\rho(\mathbf{r}_1, t)$ is equal to zero,

$$\begin{aligned}\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1} h_{B^\alpha(\mathbf{q}_1(t))}(\mathbf{q}_j(t)) &= \int_{\mathbb{R}^{3(N-1)}} h_{B^\alpha(\mathbf{r}_1)}(\mathbf{r}_j) \frac{\hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)}{\rho(\mathbf{r}_1, t)}\, \mathrm{d}^3\mathbf{r}_2 \cdots \mathrm{d}^3\mathbf{r}_j \cdots \mathrm{d}^3\mathbf{r}_N \\ &= 0(\alpha^2) + \frac{1}{\rho(\mathbf{r}_1, t)} \int_{\mathbb{R}^{3(N-1)}} I_{B^\alpha(\mathbf{r}_1)}(\mathbf{r}_j)\hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)\, \mathrm{d}^3\mathbf{r}_2 \cdots \mathrm{d}^3\mathbf{r}_j \cdots \mathrm{d}^3\mathbf{r}_N.\end{aligned}$$

By assumption (a) we get

$$\begin{aligned}\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1} h_{B^\alpha(\mathbf{q}_1(t))}(\mathbf{q}_j(t)) &= O(\alpha^2) + \int_{\mathbb{R}^{3(N-1)}} I_{B^\alpha(\mathbf{r}_1)}(\mathbf{r}_j)\Pi_{i=2}^N \rho(\mathbf{r}_i, t)\, \mathrm{d}^3\mathbf{r}_2 \cdots \mathrm{d}^3\mathbf{r}_j \cdots \mathrm{d}^3\mathbf{r}_N \\ &= O(\alpha^2) + \alpha\rho(\mathbf{r}_1, t). \qquad \text{(A.1)}\end{aligned}$$

The interacting force in one-particle dynamics reads, recalling in particular (i),

$$\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1}[\nabla_1\Phi_{\text{int}}](\mathbf{q}_1(t),\ldots,\mathbf{q}_N(t),\alpha) = K\sum_{j\neq 1}\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1}\left[\nabla_1 h_{B^\alpha(\mathbf{q}_j(t))}\right](\mathbf{q}_1(t)). \tag{A.2}$$

With the convention that the integral symbol is understood to be applied componentwise, we get, in our assumptions,

$$\begin{aligned}
\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1}&\left[\nabla_1 h_{B^\alpha(\mathbf{q}_j(t))}\right](\mathbf{q}_1(t)) \\
&= \int_{\mathbb{R}^{3(N-1)}}\nabla_1\left[h_{B^\alpha(\mathbf{r}_j)}(\mathbf{r}_1)\frac{\hat\rho(\mathbf{r}_1,\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_N,t)}{\rho(\mathbf{r}_1,t)}\right]\mathrm{d}^3\mathbf{r}_2\cdots\mathrm{d}^3\mathbf{r}_j\cdots\mathrm{d}^3\mathbf{r}_N \\
&\quad - \int_{\mathbb{R}^{3(N-1)}} h_{B^\alpha(\mathbf{r}_j)}(\mathbf{r}_1)\nabla_1\left[\frac{\hat\rho(\mathbf{r}_1,\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_N,t)}{\rho(\mathbf{r}_1,t)}\right]\mathrm{d}^3\mathbf{r}_2\cdots\mathrm{d}^3\mathbf{r}_j\cdots\mathrm{d}^3\mathbf{r}_N.
\end{aligned} \tag{A.3}$$

But recalling assumption (b) we have

$$\nabla_1\left(\frac{\hat\rho(\mathbf{r}_1,\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_N,t)}{\rho(\mathbf{r}_1,t)}\right) = \Pi_{j=2}^N\rho(\mathbf{r}_j,t)\nabla_1\exp[2\Xi(\mathbf{r}_1,\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_N,t)] = O(\alpha).$$

As a consequence, the second term in the equality above is $O(\alpha^2)$. Moreover, recalling again regularity assumptions introduced in section 3, we can obtain

$$\begin{aligned}
\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1}&\left[\nabla_1 h_{B^\alpha(\mathbf{q}_j(t))}\right](\mathbf{q}_1(t)) \\
&= \nabla_1\int_{\mathbb{R}^{3(N-1)}} h_{B^\alpha(\mathbf{r}_j)}(\mathbf{r}_1)\frac{\hat\rho(\mathbf{r}_1,\ldots,\mathbf{r}_j,\ldots,\mathbf{r}_N,t)}{\rho(\mathbf{r}_1(t))}\,\mathrm{d}^3\mathbf{r}_2\cdots\mathrm{d}^3\mathbf{r}_j\cdots\mathrm{d}^3\mathbf{r}_N + O(\alpha^2) \\
&= \nabla_1\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1}\left[h_{B^\alpha(\mathbf{q}_j(t))}\right](\mathbf{q}_1(t)) + O(\alpha^2)
\end{aligned} \tag{A.4}$$

and finally, by (A.2), (A.4) and (A.1), we get the equality (4.2).

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