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Mesoscopic scales in Stochastic Quantization of a Bose gas

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Abstract

In this technical report we describe some mesoscopic scales one can introduce in order to investigate the phenomenon of Bose-Einstein condensation with rigorous mathematical methods. We do this within the approach of stochastic quantization.

Keywords: Stochastic Quantization, Scaling limits, Bose-Einstein condensation

1 Introduction

The interest in classical stochastic methods for investigating systems of interacting Bosons from a theoretical point of view has been increasing in the last years : see for example [2] where, for large systems in a trap, a model based on path repelled brownian motions is proposed, and [31][3] , where interacting spatial permutations are considered for a weakly interacting homogeneous case. Moreover it was recently shown in [20] that an exact stochastic description is possible in terms of interacting diffusions, following the quantization procedure via stochastic variational principles (see also [7] for applications). The most challenging problem is of course to give a stochastic characterization of the condensation phenomenon. To this purpose it could be useful to get an exact stochastic description of the condensate at $T = 0$ in a realistic situation.

In this report we study some different scaling procedures which can be introduced within the stochastic quantization approach [20].

2 Stochastic quantization

2.1 Canonical Quantization and basic notations

Let us consider a system of N identical interacting particles. We denote the configuration of the system by $\hat{\mathbf{r}} = (r_1, \ldots, r_{3N}) = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$. $\mathbf{r}_i$ denotes the position of the i-th particle. We make use of the notation

$$r_{j_i}, \quad j_i \in \{3(i-1)+1, 3(i-1)+2, 3(i-1)+3\}$$

for the corresponding components in the configuration space $\mathbb{R}^{3N}$. Let also ∂_j denote the partial derivative with respect to $\hat{r}_j$, $j = 1, \ldots 3N$ and put

$$\hat{\nabla} := (\partial_1, \ldots, \partial_{3N}) = (\nabla_1, \ldots, \nabla_N)$$

where

$$\nabla_i := (\partial_{3(i-1)+1}, \partial_{3(i-1)+2}, \partial_{3(i-1)+3})$$

Quantum Mechanics claims that, neglecting spin variables, the system is completely described at time t by a wave function $\Psi \in L^2_{\mathbb{C}}(\mathbb{R}^{3N}, d\hat{r})$. The time evolution of the wave function is uniquely determined by the classical Hamiltonian, which in fact defines the Hamiltonian operator by canonical quantization rules.

The classical conserved Hamiltonian is, m denoting the mass of the particles and $\mathbf{q}_i^{cl} \in C^1$ the classical lagrangian path of the i-th particle,

$$H = \sum_{i=1}^{N} \left\{ \frac{1}{2m} (\dot{\mathbf{q}}_i^{cl})^2(t) + \Phi(\mathbf{q}_i^{cl}(t)) \right\} + \Phi_{int}(\mathbf{q}_1^{cl}(t), ..., \mathbf{q}_N^{cl}(t), \alpha)$$

Φ and Φ_{int}, which are assumed to be sufficiently regular to insure the assumption $\mathbf{q}_i^{cl} \in C^1$ is consistent, denote the external potential and the interaction potential respectively. The parameter $\alpha > 0$ is a coupling constant such that

$$\Phi_{int} := O(\alpha).$$

Quantum Hamiltonian operator reads

$$\mathcal{H} = \sum_{i=1}^{N} \left\{ -\frac{\hbar^2}{2m} \nabla_i^2 + \Phi(\mathbf{r}_i) \right\} + \Phi_{int}(\mathbf{r}_1, ..., \mathbf{r}_N, \alpha) \tag{2.1}$$

We will assume that Φ and Φ_{int} are such that $\mathcal{H}$ is bounded from below, so that $\mathcal{H}$ has a selfadjoint extension, still denoted by $\mathcal{H}$, which is the generator of the unitary group which describes the evolution in time of the wave function through the equality

$$\Psi_t = \exp^{\imath\hbar\mathcal{H}} \Psi_o$$

In differential form we have the $3N$-dimensional Schrödinger equation

$$\imath\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_1, .., \mathbf{r}_i, .., \mathbf{r}_N, t) = \mathcal{H}\, \Psi(\mathbf{r}_1, .., \mathbf{r}_i, ..., \mathbf{r}_N, t) \tag{2.2}$$

2.2 Stochastic Quantization by Lagrangian Variational Principle

In this approach the configuration of the system is assumed to perform a Markov diffusion $\hat{q}$ with time dependent drift $\hat{b}$ and diffusion matrix equal to $\frac{\hbar}{m} I$, I denoting the identity matrix in $\mathbb{R}^{3N}$.
We will also assume:

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

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

$$
\begin{aligned}
&d\mathbf{q}_1(t) = \mathbf{b}_1(\hat{q}(t), t) + \left(\tfrac{\hbar}{m}\right)^{1/2} d\mathbf{W}_1(t) \\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
&d\mathbf{q}_N(t) = \mathbf{b}_N(\hat{q}(t), t) + \left(\tfrac{\hbar}{m}\right)^{1/2} d\mathbf{W}_N(t)
\end{aligned}
\tag{2.3}
$$

where $\mathbf{W}_i$, $i = 1, \ldots, N$ are three-dimensional independent standard Wiener processes and, for any time $t \in \mathbb{R}^+$,we put

$$
\begin{aligned}
\hat{q}(t) &= (q_1(t), \ldots, q_{3N}(t)) = (\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)) \\
\hat{b}(\hat{q}(t), t) &= (b_1(\hat{q}(t), t), \ldots, b_{3N}(\hat{q}(t), t) = \\
&= (\mathbf{b}_1(\hat{q}(t), t), \ldots, \mathbf{b}_N(\hat{q}(t), t)
\end{aligned}
$$

iii) The finite energy condition [9] is satisfied.

Under the above stated assumptions 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.:

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

The quantization procedure needs the classical Lagrangian. Still denoting by $\hat{q}^{cl}$ the classical lagrangian path, we have

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

The discretized mean classical action, as a functional of a smooth $3N$-dimensional diffusion, $\hat{q}$, is, denoting by $\mathcal{E}$ the mathematical expectation,

$$A^N_{[t_a,t_b]}[\hat{q}] := \mathcal{E}\sum_{s=1}^{M}\left[\frac{1}{2}m\frac{\Delta^+\hat{q}(t_s)\cdot\Delta^+\hat{q}(t_s)}{\Delta^2} - \Phi^{\alpha,N}_{tot}\left(\hat{q}(t_s)\right)\right]\Delta \tag{2.4}$$

where

$$\Phi^{\alpha,N}_{tot}(\hat{q},t) := \sum_{i=1}^{N}\Phi\left(\mathbf{q}_i(t)\right) + \Phi_{int}(\mathbf{q}_1(t),.....,\mathbf{q}_N(t),\alpha)$$

and, for any finite time interval $[t_a,t_b]$ and positive integer M, we put

$$\Delta := \frac{t_b-t_a}{M} \qquad\qquad \Delta^+q(t_s) := q(t_{s+1}) - q(t_s)$$

The Stochastic Lagrangian Variational Principle introduced in [19], [21] and [22] claims that the actual motion is described by a Markov diffusion which makes extremal the mean discretized classical action among smooth diffusions which satisfy a system of stochastic differential equations of type (2.3) 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 $k = 1,\ldots,3N$,

$$\partial_t\hat{\rho} = -\hat{\nabla}\cdot\left(\hat{\rho}\,\hat{V}\right) \tag{2.5}$$

$$\left[\partial_t\hat{V} + \left(\hat{V}\cdot\hat{\nabla}\right)\hat{V} - \frac{\hbar^2}{2m^2}\hat{\nabla}\left(\frac{\hat{\nabla}^2\sqrt{\hat{\rho}}}{\sqrt{\hat{\rho}}}\right)\right]_k +$$

$$+\frac{\hbar}{2m}\sum_{p=1}^{3N}\left(\partial_p\ln\hat{\rho} + \partial_p\right)\left(\partial_k\hat{V}_p - \partial_p\hat{V}_k\right) = \tag{2.6}$$

$$= -\frac{1}{m}\partial_k\Phi^{\alpha,N}_{tot}$$

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

$$\hat{V} = \hat{\nabla}\hat{S}$$

and

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

we get the $3N$-dimensional Schrödinger equation

$$i\,\hbar\partial_t\hat{\Psi} = \left(-\frac{\hbar^2}{2m}\hat{\nabla}^2 + \Phi_{tot}^{\alpha,N}\right)\hat{\Psi}$$

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 (2.5) and (2.6) such that $\frac{\hat{\nabla}\hat{\rho}}{\hat{\rho}}$ is finite at infinity[1], we have

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

with

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

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

This **Energy Theorem** was proved in [19] for $N = 1$ and $d = 3$. The 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

$$E =< \Psi, \mathcal{H}\Psi >$$

where $<,>$ denotes the $L^2_{\mathbb{C}}(\mathbb{R}^{3N}, d\hat{r})$ scalar product.

For generic initial data, being $\mathcal{H}$ bounded from below, Schrödinger solutions act as an attracting set. In this case the constructed quantization procedure approaches the canonical one after a relaxation, in some analogy with Parisi-Wu approach [29].

3 Interacting diffusions

In the following we will assume that $\hat{\rho}$ has support in a compact set for $t = 0$, and that the support remains in a given bounded domain for all $t \in [0, T]$. We recall that, by i), both $\hat{\rho}$ and $\hat{V}$ are smooth.

[1] 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.

We will need in particular that $\hat{\rho}$ is of class C_o^1 as 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 $\hat{r}$.

We make use of the following notations

$$\hat{V} \equiv (V_1, V_2, ...V_{3N}) = (\mathbf{V_1}, ...\mathbf{V_N}) \ , \qquad \hat{\rho} = e^{2\hat{R}}$$

For the i-th particle we define the "one-particle current velocity field"

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

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

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

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

and

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

One can prove that [20] , in case of identical particles, under assumptions i) and ii) and those stated at the beginning of this section, the motion of the 1-th particle is described by a non-Markovian diffusion $\mathbf{q}_1$ with probability density $\rho := e^{2R}$ and current velocity $\mathbf{v_1}$, which satisfies the equality

$$d\mathbf{q}_1(t) = \left(\mathbf{v}_1\left(\mathbf{q}_1(t), t\right) + \frac{\hbar}{m}\nabla_1 R\left(\mathbf{q}_1(t), t\right)\right) dt +$$

$$+ \zeta_1\left(\mathbf{q}_1(t), \mathbf{q}_2(t), ..., \mathbf{q}_N(t), t\right) dt + \left(\frac{\hbar}{m}\right)^{1/2} \mathbf{dW}_1(t)$$

where

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

$\xi_\mathbf{1}$ and Ξ being defined by (3.2), (3.3) respectively, and $\mathcal{E}_{\mathbf{q}_1(t)=\mathbf{r}}\, \zeta_\mathbf{1} = \mathbf{0}$.[20]

Then one can prove the following

Proposition 1

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 1-th particle in a system of N identical bosons satisfy the couple of PDEs, for $k = 1, 2, 3$,

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

$$[\partial_t \mathbf{v}_1 + (\mathbf{v}_1 \cdot \nabla) \, \mathbf{v}_1 - \frac{\hbar^2}{2m^2} \nabla \left(\frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) + \frac{\hbar}{2m} \left(\nabla \ln \rho + \nabla \right) \wedge \left(\nabla \wedge \mathbf{v}_1 \right)]_k (\mathbf{r}, t) =$$

$$= -\frac{1}{m} \mathbb{E}_{\mathbf{q}_1(t)=r} \left\{ \partial_k \Phi^{\alpha,N}_{tot} \left(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t) \right) \right\} - \beta_k(\alpha, N, \mathbf{r}, t)$$

where

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

and

$$\beta^{time}(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left[\partial_t \mathbf{V}_1 - \partial_t \mathbf{v}_1 \right]$$

$$\beta^{conv}(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left\{ (\hat{V} \cdot \hat{\nabla}) \mathbf{V}_1 - (\mathbf{v}_1 \cdot \nabla) \mathbf{v}_1 \right\}$$

$$\beta^{rot}_k(\alpha, N, \mathbf{r}, t) :=$$

$$\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left\{ \sum_{p=1}^{3N} \left(\partial_p \ln \hat{\rho} + \partial_p \right) \left(\partial_k \hat{V}_p - \partial_p \hat{V}_k \right) - \left[(\nabla \ln \rho + \nabla) \wedge (\nabla \wedge \mathbf{v}_1) \right]_k \right\}$$

$$\beta^Q(\alpha, N, \mathbf{r}, t) := \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left\{ \nabla_1 \left(\frac{\hat{\nabla}^2 \sqrt{\hat{\rho}}}{\sqrt{\hat{\rho}}} \right) - \nabla_1 \left(\frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) \right\}$$

For any solution $\hat{\Psi}$ to Schrödinger equation we have, by construction, that $\hat{\rho}$ is symmetric w.r. to permutation of positions of two generic particles. One can also prove that in this case, at dynamical equilibrium, all particles have the same velocity field.

Moreover all the associated one-particle processes are equal in law.

Proposition 2 Let Ψ^N be any solution of the $3N$-dimensional equation (2.2) and assume it is of class C^1. Then the three-dimensional processes $\{X^N_i\}_{i=1,\ldots,N}$ are equal in law.

Proof

By the symmetry of Ψ^N the joint probability density $\rho^N := (\Psi^N)^2$ is also symmetric. This implies that all marginals are identical and symmetric. Moreover, for all $k = 2, \dots, N$ and $t \geq 0$, the permutations of $(X^N_{i_1}(t), \dots, X^N_{i_k}(t))$ are identically distributed random elements.

Let us also observe that, if Ψ^N is of class C^1, putting $\Psi^N := \exp R^N$ and $i < j$, we have (see for example proof of proposition 4 in [20])

$$\nabla_i R^N(\mathbf{r_1}, \dots, \mathbf{r_i}, \dots, \mathbf{r_j}, \dots, \mathbf{r_N}) = \nabla_{\mathbf{j}} \mathbf{R^N}(\mathbf{r_1}, \dots, \mathbf{r_j}, \dots, \mathbf{r_i}, \dots, \mathbf{r_N})$$

then

$$\begin{aligned} b^N_i(X^N_1, \dots, X^N_N) = \nabla_i R^N(X^N_1, \dots, X^N_i, \dots, X^N_j, \dots, X^N_N) = \\ = \nabla_j R^N(X^N_1, \dots, X^N_j, \dots, X^N_i, \dots, X^N_N) \approx \\ \approx \nabla_j R^N(X^N_1, \dots, X^N_i, \dots, X^N_j, \dots, X^N_N) = \\ = b^N_j(X^N_1, \dots, X^N_N) \end{aligned}$$

where $\approx$ denotes the equality in law and ∇_j denotes the gradient with respect to the variable in the j-th position.

Denoting by $(\hat{X}^N, \hat{W}^N)(\Omega^N, \mathcal{F}^N, \mathbb{P}^N)(\mathcal{F}^N_t)_{t\geq 0}$ a weak solution to the $3N-$*dimensional* SDE, we define, for any $i = 1, \dots, N$ the adapted process

$$\beta^N_i(t) := b^N_i(X^N_1(t), \dots, X^N_N(t))$$

Then, for any i, X^N_i satisfy the stochastic differential equation

$$X^N_i(t) = X^N(0) + \int_0^t \beta^N_i(s)ds + (\frac{\hbar}{m})^{\frac{1}{2}} W^N_i(t)$$

So, varying i from 1 to N, we get a family of three-dimensional non markovian diffusions on $(\Omega^N, \mathcal{F}^N, \mathbb{P}^N)$ with diffusion coefficient equal to 1 and identically distributed drifts. ◇

4 The ground state and the Yngvason-Lieb-Seiringer scaling

In this section we consider the important case of the limit for N going to infinity via the Lieb-Yngvason-Seiringer scaling [15] [18]. Such a rescaling is consistent with the Gross-Pitaevskii approximation [10][30] and allows a theoretical and rigorous proof from first principles of BEC for interacting trapped gases, in terms of factorization of the reduced density matrix [17] (see [13] and [1] for the study of the free evolution from the ground or factorized initial state and [16] for the extension to rotating condensates).

We consider the particular hamiltonian

$$H^N = \sum_{i=1}^{N}(-\frac{\hbar^2}{2m}\triangle_i + V(\mathbf{r_i})) + \sum_{\mathbf{1\leq i<j\leq N}} \mathbf{v}(\mathbf{r_i}-\mathbf{r_j})$$

where V is assumed locally bounded, positive and going to infinity when $|\mathbf{r_i}|$ goes to infinity. The interaction potential v is smooth, compactly supported, non negative, spherically symmetric, with fnite scattering length a.

The Lieb-Yngvason-Seiringer scaling [15], leaves N to go to infinity with the rule

$$v(r) = v_1(\frac{r}{a})/a^2$$

$$a \propto \frac{1}{N}$$

where v_1 has scattering length equal to 1.

A key tool in the proof of BEC given in [17] is a "localization of energy" lemma, which in synthesis claims the following: let Ψ^N denotes the ground state of H^N, that is the minimizer of the total energy functional

$$E^N[\Psi] = \int \Psi^*(H^N\Psi)d\mathbf{r}_1...d\mathbf{r}_N$$

(with $\mathbf{r}_i \in \mathbb{R}^3$, $i = 1\dots N$), and let ϕ^{GP} be the minimizer of the GP functional (which is unique up to a phase, which will be assumed equal to zero)

$$E^{GP}[\phi] = \int (\frac{\hbar^2}{2m}|\nabla\phi(r)|^2 + V(r)|\phi(r)|^2 + \frac{g}{2}|\phi(r)|^4)d\mathbf{r}$$

with $g = 4\pi\frac{\hbar^2}{m}Na$. Then if N goes to infinity and the interaction follows the Y-L-S scaling, then, with $X := (\mathbf{r}_2, ..., \mathbf{r}_N)$,

$$f_X(r) = \Psi^N(r, X)/\phi^{GP}(r)$$

has the property that, for great N, its gradient is almost zero outside small balls centered at the points of X.

Let Ψ^N be the ground state of H^N in $L^2(\mathbb{R}^{3N} \to \mathbb{C}, dx)$, $x \in \mathbb{R}^{3N}$. We assume that Ψ^N is real, and dx-a.s. positive. We denote by λ_o^N the corresponding eigenvalue.

The associated process $\hat{X}^N$ can be seen as the family of three-dimensional non Markovian diffusions $(X_1^N, \ldots X_N^N)$, which satisfy, with $i = 1, \ldots, N$, the equalities

$$X_i^N(t) = \int_0^t b_i^N(X_1^N(s), \ldots, X_N^N(s))ds + W_i(t)$$

where the drift is defined , with $(\mathbf{r}_i \in \mathbb{R}^3,\ i = 1, \ldots, N)$, as

$$b_i^N(\mathbf{r}_i, \ldots, \mathbf{r}_N) = (\frac{\nabla_{\mathbf{r}_i}\Psi^N}{\Psi^N})(\mathbf{r}_i, \ldots, \mathbf{r}_N)$$

and $\{W_i\}_{i=1,\ldots,N}$ are i.i.d. three-dimensional Brownian Motions, whose components have variance equal to $2t$ in the assumed unities.

We now study the behavior of X_1^N for N going to infinity via the Y-L-S scaling. To this purpose we introduce the ∞-product probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and the filtration $(\mathcal{F}_t)_{t\geq 0}$, naturally generated by $((\Omega^N, \mathcal{F}^N, \mathbb{P}^N), (\mathcal{F}_t^N)_{t\geq 0})_{N\in\mathbb{N}}$. Assume now there exists a process X^{GP} which, for some adapted brownian Motion W_1, satisfies the stochastic differential equation

$$X^{GP}(t) := X^{GP}(0) + \int_0^t u^{GP}(X^{GP}(s))ds + W_1(t)$$

$$u^{GP} := \frac{\nabla\phi^{GP}}{\phi^{GP}}$$

Let $X^{GP}(0)$ be distributed accordingly to the probability density $\rho^{GP} := (\phi^{GP})^2$: then $X^{GP}(t)$ has the probability density ρ^{GP} for all t. By the results in [15][17] we know that ρ^{GP} is in fact the L^1 limit of the one particle marginal of $(\Psi^N)^2$. So we expect there is some relationship between asymptotics of X_i^N and X^{GP}.

remark 1 We observe that

$$(\phi^{GP})^2(\nabla\frac{\Psi^N}{\phi^{GP}})^2 = (\Psi^N)^2(\frac{\nabla\Psi^N}{\Psi^N} - \frac{\nabla\phi^{GP}}{\phi^{GP}})^2$$

so that, being Ψ^N is of class C^1 by assumption, the distance of the two drifts b_i^N and u^{GP} in $L^2(\mathbb{R}^3 \to \mathbb{R}, (\Psi^N)^2 d\mathbf{r}_1, \ldots, d\mathbf{r}_N)$ is given by the following equality

$$\int_{\mathbb{R}^{3N}} \|b_1^N - u^{GP}\|^2(\Psi^N)^2 d\mathbf{r}_1, \ldots, d\mathbf{r}_N = \int_{\mathbb{R}^{3N}} (\nabla_1\frac{\Psi^N}{\phi^{GP}})^2(\phi^{GP})^2 d\mathbf{r}_1, \ldots, d\mathbf{r}_N$$

□

Following [17] we have

Lemma 1 Let Ψ^N be of class C^1 and let assumptions above stated on V and v hold. Then if N goes to infinity via the L-Y-S scaling with $g = 4\pi N a$ we have

a) There exists $s \in (0, 1]$ such that

$$lim_N \uparrow \infty \int_{\mathbb{R}^{3N}} \|b^N - u^{GP}\|^2 (\Psi^N)^2 d\mathbf{r}_1, \ldots, d\mathbf{r}_N = gs \int_{\mathbb{R}^3} (\phi^{GP})^4 d\mathbf{r}$$

b) Defining

$$F^N(\mathbf{r}_2, \ldots, \mathbf{r}_N) := (\bigcup_{i=2}^{N} B^N(\mathbf{r}_i))^c$$

where $B^N(\mathbf{r})$ denotes the open ball centered in $\mathbf{r}$ with radius $N^{-\frac{7}{17}}$,

$$lim_N \uparrow \infty \int_{\mathbb{R}^{3(N-1)}} \int_{F^N(\mathbf{r}_2, \ldots, \mathbf{r}_N)} \|b^N - u^{GP}\|^2 (\Psi^N)^2 d\mathbf{r}_1, \ldots, d\mathbf{r}_N = 0$$

Proof

The proof is an immediate consequence of remark 1 and of results given in [17]: see (7) for a) and Lemma 1 for b). ◇

In the following we simply denote $X_1^N(t)$, $\beta_1^N(t)$, $X^{GP}(t)$, $W_1(t)$ and $u^{GP}(X^{GP}(t))$ by X_t^N, β_t^N, X_t^{GP}, W_t and u_t^{GP} respectively. Moreover we augment $(\mathcal{F}_t)_{t\geq 0}$ so that it satisfies the usual conditions and X_o^{GP} is $\mathcal{F}_o$-measurable. Then, on the filtered probability space $(\Omega, \mathcal{F}, \mathbb{P})$, $(\mathcal{F}_t)_{t\geq 0}$, we consider the two S.D.E. (with $\hbar = m = 1$)

$$X_t^N - X_o^N = \int_0^t \beta_s^N ds + W_t \tag{4.1}$$

and

$$X_t^{GP} - X_o^{GP} = \int_0^t u_s^{GP} ds + W_t \tag{4.2}$$

where X_o^{GP} has probability density equal to $(\phi^{GP})^2$ and the solution of the second equation is assumed to hold in strong sense. This means that we can choose in the second equation the same Brownian Motion giving a solution to the first.

remark 2 Both β^N and u^{GP} satisfy the finite energy condition, that is, for all $t \in \mathbb{R}$

$$E_{\mathbb{P}} \int_0^t \|\beta_s^N\|^2 ds < \infty$$

and

$$E_{\mathbb{P}} \int_0^t \| u_s^{GP}\|^2 ds < \infty$$

which follows from the fact that Ψ^N is the minimizer of $E^N[\Psi]$ and ϕ^{GP} of $E^{GP}[\phi]$.

Then, by Girsanov Theorem [14] , there exist two measures Q^N and Q^{GP} on $(\Omega, \mathcal{F})$, absolutely continous with respect to $\mathbb{P}$, such that $X_t^N - X_o^N$ and $X_t^{GP} - X_o^{GP}$ are, respectively, two Brownian Motions on the considered filtered measurable space.□

remark 3 We have, $\mathbb{P}$ and Q^{GP} a.s.,

$$X_t^N - X_o^N = \int_0^t (\beta_s^N - u_s^{GP}) ds + X_t^{GP} - X_o^{GP}$$

so that, again by Girsanov Theorem, given any stopping time τ

$$\frac{dQ^N}{dQ^{GP}}|_{\mathcal{F}_{t\wedge\tau}} = \exp\{-\int_0^{t\wedge\tau} (\beta_s^N - u_s^{GP}) \cdot dX_s^N + \frac{1}{2}\int_0^{t\wedge\tau} \|\beta_s^N - u_s^{GP}\|^2 ds\}$$

We denote by $\mathcal{H}(Q^N, Q^{GP})$ the relative entropy between Q^N and Q^{GP}, that is, for any sub σ-algebra $\mathcal{G}$

$$\mathcal{H}(Q^N, Q^{GP})|_{\mathcal{G}} := \int_{\Omega} log \frac{dQ^N}{dQ^{GP}}|_{\mathcal{G}} dQ^N$$

Then, if the right side is finite, we can write, for any stopping time τ,

$$\mathcal{H}(Q^N, Q^{GP})|_{\mathcal{F}_{t \wedge \tau}} = \frac{1}{2} E_{Q^N} \int_0^{t \wedge \tau} \|\beta_s^N - u_s^{GP}\|^2 ds \tag{4.3}$$

□

To exploit lemma 1 we introduce the following time dependent random subset of R^3

$$D_N(t) := \bigcup_{i=2}^{N} B^N(X_i^N(t)) \tag{4.4}$$

where $B^N(\mathbf{r})$ is again the ball with radius $N^{-\frac{7}{17}}$ centered in $\mathbf{r}$, and the stopping time

$$\tau^N := inf\{t : X_t^N \in D_N(t)\} \tag{4.5}$$

Then we can prove the following partial result

Proposition 3 Let the same assumptions of lemma 1 hold and let the solution of (4.2) be in strong sense.

Defined

$$G_{N,s} := \|\beta_s^N - u_s^{GP}\|^2 I_{\{X_s^N \in D_N^c(s)\}}$$

assume that, for any $t > 0$, $\int_0^t G_{N,s} ds$ is bounded by a positive integrable functions and $lim_{N\to\infty} \int_0^t G_{N,s} ds$ is equal to some time dependent random variable g_t, $\mathbb{P}$-a.s..

Then, if τ^N is defined by (4.5) and (4.4), we have

$$lim_{\bar{N}\to\infty} lim_{N\to\infty} \frac{1}{2} E_{Q^{\bar{N}}} \int_0^{t \wedge \tau} \|\beta_s^N - u_s^{GP}\|^2 ds = 0$$

Proof

By remark 2 we have

$$E_{\mathbb{P}}\int_0^t \|\beta_s^N - u_s^{GP}\|^2 ds \leq E_{\mathbb{P}}[\int_0^t \|\beta_s^N\|^2 ds + \int_0^t \|u_s^{GP}\|^2 ds] < \infty$$

Recalling the definitions of $D_N(s)$ and of $G_{N,s}$ we get

$$E_{\mathbb{P}}\int_0^t G_{N,s} ds \leq E_{\mathbb{P}}\int_0^t \|\beta_s^N - u_s^{GP}\|^2 ds < \infty$$

so that by Fubini theorem and Lemma 1,

$$lim_{N\uparrow\infty} E_{\mathbb{P}}\int_0^t G_{N,s} ds = lim_{N\uparrow\infty}\int_0^t E_{\mathbb{P}}[G_{N,s}] ds =$$

$$= lim_{N\uparrow\infty}\{t\int_{\mathbb{R}^{3(N-1)}}\int_{F^N(\mathbf{r}_2,\ldots,\mathbf{r}_N)} \|b_1^N - u^{GP}\|^2 (\Psi^N)^2 d\mathbf{r}_1,\ldots,d\mathbf{r}_N\} = 0$$

As a consequence, in our assumptions on $G_{N,s}$, we get

$$E_{\mathbb{P}}[lim_{N\uparrow\infty}\int_0^t G_{N,s} ds] = 0$$

so that

$$\mathbb{P}\{lim_{N\uparrow\infty}\int_0^t G_{N,s} ds = 0\} = 1$$

Moreover, for any $\bar{N}\in\mathbb{N}$, being $\mathbb{Q}^{\bar{N}}$ absolutely continous with respect to $\mathbb{P}$, we also have

$$\mathbb{Q}^{\bar{N}}\{lim_{N\uparrow\infty}\int_0^t G_{N,s} ds = 0\} = 1$$

Thus we can write, for all $\bar{N}\in\mathbb{N}$,

$$0 = E_{\mathbb{Q}^{\bar{N}}}[lim_{N\uparrow\infty}\int_0^t G_{N,s} ds] = lim_{N\uparrow\infty}\mathbb{E}_{Q^{\bar{N}}}\int_0^t G_{N,s} ds$$

and

$$lim_{\bar{N}\uparrow\infty} lim_{N\uparrow\infty}\mathbb{E}_{Q^{\bar{N}}}\int_0^t G_{N,s} ds = 0$$

Concluding we have

$$\lim_{\bar{N}\uparrow\infty}\lim_{N\uparrow\infty}\frac{1}{2}E_{Q^{\bar{N}}}\int_0^{t\wedge\tau^N} |\beta_s^N - u_s^{GP}\|^2 ds =$$

$$= \lim_{\bar{N}\uparrow\infty} \lim_{N\uparrow\infty} \frac{1}{2} E_{Q^{\bar{N}}} \int_0^t \|\beta_s^N - u_s^{GP}\|^2 I_{\{\tau^N > t\}} ds \leq$$

$$\leq \lim_{\bar{N}\uparrow\infty} \lim_{N\uparrow\infty} \frac{1}{2} E_{Q^{\bar{N}}} \int_0^t G_{N,s} ds = 0$$

◇

For $d = 3$ the Lebesgue measure of D^N goes to zero in the limit of N going to infinity. Moreover, since the radius of each ball constituting D^N is $O(N^{-\frac{7}{17}})$ and the mean distance between two particles is $O(N^{-\frac{1}{3}})$, for great N the gas behaves as diluite on the scale of the small balls, so that the mean field contribution to the random motion is the relevant one on this scale.

5 Mesoscopic scales

For the Hamiltonian already considered in the preceding section, the general setting introduced in [20] allows in principle to study more general situations and in particular to formulate a novel set of assumptions, in particular concerning the initial state, the number of particles, the time scale and so on, which are necessary in order the Gross-Pitaevskii approximation to hold in the stochastic approach.

1) Irrotationality: this gets rid of the rotational terms $\frac{\hbar}{2m}\beta^{rot}$. Notice that this is equivalent to coming back to the **canonical quantization** or to the considering the system, when described within the Lagrangian Variational Principle, only at dynamical equilibrium. It is important to stress that in this case we have $\mathbf{v}_1 = \mathbf{v}_2 = \cdots = \mathbf{v}_N := \mathbf{v}$.

2) N is finite but sufficiently large to approximate $\frac{N-1}{N}$ with 1 in equation (5.2) and to neglect β^{conv} (cf 4).

3) $\beta^{time} = 0$: this is approximately true if we choose a time scale where $\partial_t \left[\mathbf{V}_i(\mathbf{r}_1, ..., \mathbf{r}_N, t) - \mathbf{v}(\mathbf{r}, t)\right]$, $i = 1, \ldots, N$ is negligible.

4) $\beta^{conv} = 0$: starting from the definition of β^{conv} we can see that, using the properties of conditional expectation

$$\beta^{conv} = \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left\{ (\mathbf{V}_1 \cdot \nabla_1)\mathbf{V}_1 + \sum_{i=2}^{N} (\mathbf{V}_i \cdot \nabla_i)\mathbf{V}_1 \right\} - (\mathbf{v}_1 \cdot \nabla_1)\mathbf{v}_1(\mathbf{r}, t) =$$

$$= O(\alpha^2) + \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \sum_{i=2}^{N} (\mathbf{V}_i \cdot \nabla_i)\mathbf{V}_1.$$

Using standard vector calculus and assumption 1), we get

$$\beta^{conv} = O(\alpha^2) + \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \nabla_i \sum_{i=2}^{N} \frac{1}{2}|\mathbf{V}_i|^2.$$

As a consequence, under assumption c_1), the condition $\beta^{conv} = 0$ is equivalent to assume, up to $O(\alpha^2)$ terms,

$$\lim_{N\to\infty} \mathbb{E}_{\mathbf{q}_i(t)=\mathbf{r}} \nabla_i \sum_{j\neq i} \frac{1}{2}|\mathbf{V}_j|^2 = 0$$

This looks reasonable in general from a physical point of view. In fact we expect that, in case of a great number of particles, the total kinetic energy due to current velocity contribution is not sensitive to variations of the position of a single particle.

5) $(\frac{\hbar^2}{m^2})\beta^Q = 0$: this is meaningful only if the initial state is not entangled when α goes to zero. Indeed only in this case β^Q goes to zero when the coupling parameter α goes to zero. If this is the case, the condition means that we neglect a term of order $O(\frac{\hbar^2}{m^2})O(\alpha)$.

In particular one can consider the interaction potential

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

where K is a constant which can be positive or negative, $B^\alpha(\mathbf{r})$ is the open sphere centered in $\mathbf{r}$, with volume α, and $h_{B^\alpha(\mathbf{r})}$ satisfies the following assumptions

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

ii) $h_{B^\alpha(\mathbf{r})} \in C_o^1, \qquad supp \quad h_{B^\alpha(\mathbf{r})} = B^\alpha(\mathbf{r})$

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

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

Further assumptions are, $\forall t \in [0,T]$,

a) $\lim_{\alpha\to 0} \hat{\rho}(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \Pi_{i=1}^N \rho(\mathbf{r}_i, t)$,

b) $\lim_{\alpha\to 0} \nabla_i \hat{\rho}(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \nabla_i \Pi_{j=1}^N \rho(\mathbf{r}_i, t), \quad \forall i = 1, \dots, N$

Introducing the expected number of particles in any finite volume $\delta V \subset \mathbb{R}^3$, that is the random variable

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

with expectation

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

we can see that $\bar{\rho}(\mathbf{r}, t) := N\rho(\mathbf{r}, t), \mathbf{r} \in \mathbb{R}^3$, 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 $\mathbf{v} \equiv \mathbf{v}_i$, $\forall i = 1, \cdots, N$.

One can show [20] that the dynamical equations, independently of the choice of the particle, become

$$[\partial_t \bar{\rho} + \nabla \cdot (\bar{\rho} v)] = 0 \tag{5.1}$$

$$\partial_t v + (v \cdot \nabla)\, v - \frac{\hbar^2}{2m^2} \nabla \left(\frac{\nabla^2 \sqrt{\bar{\rho}}}{\sqrt{\bar{\rho}}} \right) =$$

$$= -\frac{1}{m} \nabla \Phi - \frac{1}{m} K \frac{N-1}{N} \left\{ N O(\alpha^2) + \nabla \left[\alpha \bar{\rho} + N\, O(\alpha^2)) \right] \right\} \tag{5.2}$$

Then, approximating $\frac{N-1}{N}$ to 1 and neglecting terms of order $O(\alpha^2)$. the "fluid wave function" $\bar{\psi} := \bar{\rho}^{\frac{1}{2}} \exp \frac{i}{m} S$, where $\frac{1}{m} \nabla S := v$, satisfies the Gross-Pitaevskii equation:

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

This is the equation for the coherent part of one-particle dynamics. The main interest of this result comes from introducing approximations as function of both α and $\frac{\hbar}{m}$, for finite N.

In the following appendix 1 and appendix 2 we report some preliminary results concerning the structure of the dynamical perturbation for the ground state and some analysis for the weakly interacting case.

6 Appendix 1

Dynamical perturbation of the ground-state

The quantum dynamical perturbation can be written as

$$\beta^Q = E_{q_1(t)=r_1} \nabla_1 \{ \sum_1^N \nabla_i^2 \Xi + 2\nabla R(q_i(t), t) \cdot \nabla_i \Xi + (\nabla_i \Xi)^2 \}$$

Exploilting regularities we can write:

$$\nabla_1 \{ \sum_1^N [E_{q_1(t)=r_1} [\nabla_i{}^2 \Xi + 2\nabla R(q_i(t), t) \cdot \nabla_i \Xi + \nabla_i \Xi^2]\}$$

We can prove that all terms are identical.Putting $N = 3$ for simplicity we must prove that:

$$E_{q_1(t)=r_1} [\nabla_2^2 \Xi + 2\nabla R(q_2(t), t) \cdot \nabla_2 \Xi + (\nabla_2 \Xi)^2]$$
$$= E_{q_1(t)=r_1} [\nabla_3{}^2 \Xi + 2\nabla R(q_3(t), t) \cdot \nabla_3 \Xi + (\nabla_3 \Xi)^2] \qquad (1)$$

We know that :

$$\nabla_2 \Xi(r_1, r_2, r_3, t) = \nabla_2 \hat{R}(r_1, r_2, r_3, t) - \nabla R(r_2, t)$$

$$\nabla_3 \Xi(r_1, r_2, r_3, t) = \nabla_3 \hat{R}(r_1, r_2, r_3, t) - \nabla R(r_3, t)$$

We observe that:

$$\partial_2 \hat{R}(r_1, r_2, r_3, t) = lim_{h \to 0} \frac{\hat{R}(r_1, r_2 + h, r_3, t) - \hat{R}(r_1, r_2, r_3, t)}{h} =$$

$$lim_{h \to 0} \frac{\hat{R}(r_1, r_3, r_2 + h, t) - \hat{R}(r_1, r_3, r_2, t)}{h} = \partial_3 \hat{R}(r_1, r_3, r_2, t) \quad (2)$$

where the invariance of $\hat{R} = (1/2)log(\hat{\rho})$ with respect to permutations of r_2 and r_3 is exploited. By (2) we get:

$$\nabla_2 \Xi(r_1, r_2, r_3, t) = \nabla_2 \hat{R}(r_1, r_2, r_3, t) - \nabla R(r_2, t) =$$
$$= \nabla_3 \hat{R}(r_1, r_3, r_2, t) - \nabla R(r_2, t) = \nabla_3 \Xi(r_1, r_3, r_2, t) \qquad (3)$$

Moreover we have:

$$\partial_2(\partial_2 \hat{R}(r_1, r_2, r_3, t)) = lim_{h \to 0} \frac{\partial_2 \hat{R}(r_1, r_2 + h, r_3, t) - \partial_2 \hat{R}(r_1, r_2, r_3, t)}{h} =$$

$$lim_{h \to 0} \frac{\partial_3 \hat{R}(r_1, r_3, r_2 + h, t) - \partial_3 \hat{R}(r_1, r_3, r_2, t)}{h} = \partial_3 \partial_3 \hat{R}(r_1, r_3, r_2, t)(4)$$

where (2) is again exploited.Taking conditional expectations and recalling (4) we have

$$E_{q_1(t)=r_1}[\partial_2 \partial_2 \hat{R}] = \int \partial_2 \partial_2 \hat{R} \frac{\hat{\rho}(r_1, r_2, r_3)}{\rho(r_1)} = E_{q_1(t)=r_1}[\partial_3 \partial_3 \hat{R}]$$

We can write:

$$E_{q_1(t)=r_1}[\nabla^2 R] = \int \nabla^2 R(r_2, t) \frac{\hat{\rho}(r_1, r_2, r_3)}{\rho(r_1)} dr_2 dr_3 =$$

$$\int \nabla^2 R(r_3, t) \frac{\hat{\rho}(r_1, r_2, r_3)}{\rho(r_1)} dr_2 dr_3$$

and :

$$E_{q_1(t)=r_1}[\nabla_2^2 \Xi] = E_{q_1(t)=r_1}[\nabla_3^2 \Xi] \qquad (5)$$

By(3) we get:

$$E_{q_1(t)=r_1}[(\nabla_2 \Xi)^2] = \int (\nabla_2 \Xi)^2 \frac{\hat{\rho}(r_1, r_2, r_3)}{\rho(r_1)} dr_2 dr_3 =$$

$$\int (\nabla_3 \Xi)^2 \frac{\hat{\rho}(r_1, r_2, r_3)}{\rho(r_1)} dr_2 dr_3 = E_{q_1(t)=r_1}[(\nabla_3 \Xi)^2] \qquad (6)$$

Eventually we find:

$$E_{q_1(t)=r_1}[2 \nabla R(q_2(t), t)(\nabla_2 \Xi)] =$$

$$= \int \nabla R(r_2,t)(\nabla_2 \Xi)(r_1,r_2,r_3,t)\frac{\hat{\rho}(r_1,r_2,r_3)}{\rho(r_1)}dr_2 dr_3 =$$

$$= \int \nabla R(r_2,t)(\nabla_3 \Xi)(r_1,r_3,r_2,t)\frac{\hat{\rho}(r_1,r_3,r_2)}{\rho(r_1)}dr_2 dr_3 =$$

$$= E_{q_1(t)=r_1}[\nabla R(q_3(t),t)(\nabla_3 \Xi)] \qquad (7)$$

Concluding (5),(6) e (7) prove equality (1).

7 appendix 2

Weak interaction

We define

$$\Phi_{int}(r_1,...,r_N,K) \doteq K\sum_{i<j}^{N} V(r_i - r_j)$$

where K is a non negative constant, V is a smooth symmetric function. We assume:

$$a)\hat{\Psi}(r_1,...r_N,t) - \prod_{i=1}^{N}\Psi_i(r_i,t) = O(K)$$

$$b)\nabla_i^p\hat{\Psi}(r_1,...r_N,t) - \nabla_i^p\prod_{i=1}^{N}\Psi_i(r_i,t) = O(K)$$

for $i = 1,...,N$ and $p = 1,2$, where $|\Psi_i|^2 = \rho$.

We can prove that the interaction term can be calculated to give:

$$E_{q_1(t)=r_1}[\nabla_1\Phi_{int}](q_1(t),...,q_N(t),K) =$$

$$= K(N-1)\nabla_1[K\int_{R^3} V(r_1 - r_j)\rho(r_j)d^3r_j] + O(K^2) \quad (1)$$

Being V simmetric:

$$\Phi_{int}(r_1,...,r_N,K) \doteq \frac{K}{2}\sum_{i\neq j}^{N} V(r_i - r_j)$$

Because of ∇_1, only terms containing r_1 survive giving:

$$\nabla_1\Phi_{int}(r_1,...,r_N,K) = K\sum_{j\neq 1}^{N} V(r_1 - r_j)$$

Therefore:

$$E_{q_1(t)=r_1}[\nabla_1 \Phi_{int}](q_1(t), ..., q_N(t), K) =$$
$$= \sum_{j\neq 1} E_{q_1(t)=r_1}[K\nabla_1 V(q_1(t) - q_j(t))](q_1(t))$$
$$E_{q_1(t)=r_1}[K\nabla_1 V(q_1(t) - q_j(t))] =$$
$$= K \int_{R^{3(N-1)}} \nabla_1[V(r_1 - r_j)] \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)} d^3r_2 \cdot d^3r_j \cdot d^3r_N =$$
$$= K \int_{R^{3(N-1)}} \nabla_1[V(r_1 - r_j) \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)}] d^3r_2 \cdot d^3r_j \cdot d^3r_N -$$
$$- \int V(r_1 - r_j) \nabla_1[\frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)}] d^3r_2 \cdot d^3r_j \cdot d^3r_N$$

Now:

$$\nabla_1[\frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)}] = \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)} [\frac{\nabla_1 \hat{\rho}(r_1, ...r_N)}{\rho(r_1)} - \frac{\nabla_1 \rho(r_1)}{\rho(r_1)}] =$$
$$= 2 \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)} \nabla_1 \Xi$$

So we have:

$$E_{q_1(t)=r_1}[K\nabla_1 V(q_1(t) - q_j(t))] =$$
$$\nabla_1 E_{q_1(t)=r_1}[KV(q_1(t) - q_j(t))] -$$
$$-2K \int_{R^{3(N-1)}} V(r_1 - r_j) \nabla_1 \Xi \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)} d^3r_2 \cdot d^3r_j \cdot d^3r_N -$$

Now:

$$E_{q_1(t)=r_1}[KV(q_1(t) - q_j(t))] =$$
$$= K \int_{R^{3(N-1)}} V(r_1 - r_j) \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)} d^3r_2 \cdot d^3r_j \cdot d^3r_N$$
$$= K \int_{R^{3(N-1)}} V(r_1 - r_j) \prod_{k=2}^{N} \rho(r_k) d^3r_2 \cdot d^3r_j \cdot d^3r_N + O(K^2)$$
$$= K \int_{R^3} V(r_1 - r_j) \rho(r_j) d^3r_j \cdot d^3r_j + O(K^2)$$

using the factorization property (a). Finally (1) holds if:

$$\nabla_1 \{K \int_{R^{3(N-1)}} V(r_1 - r_j) \nabla_1 \Xi \frac{\hat{\rho}(r_1, ...r_N)}{\rho(r_1)} d^3r_2 \cdot d^3r_j \cdot d^3r_N\}$$

is an $O(K^2)$. But this is true if $\nabla_1 \nabla_1 \Xi$ is an $O(K)$, i.e. if (b) holds.

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