Cubic Nonlinear Schrödinger Equation with vorticity

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Abstract. In this paper we introduce a new class of Nonlinear Schrödinger Equations (NLSEs), with an electromagnetic potential $(\mathcal{A}, \Phi)$, both depending on the wave function Ψ. The scalar potential Φ depends on $|\Psi|^2$, while the vector potential $\mathcal{A}$ satisfies the equation of magnetohydrodynamics with coefficient depending on Ψ.

In Madelung variables the velocity field comes to be not irrotational in general and we prove that the vorticity induces dissipation, until the dynamical equilibrium is reached. The expression of the rate of dissipation is common to all NLSEs in the class.

We show that they are a particular case of the one-particle dynamics out of dynamical equilibrium for a system of N identical interacting Bose particles, as recently described within Stochastic Quantization by Lagrangian Variational Principle.

The cubic case is discussed in particular. Results of numerical experiments for rotational excitations of the ground state in a finite two-dimensional trap with harmonic potential are reported.

1. Introduction

Stochastic Quantization by Lagrangian Variational Principle [1, 2] allows to describe the behavior of a single particle in a system of N identical interacting Bosons in a particularly simple way, just exploiting conditional expectations given the position at time t of the considered particle [3]. Indeed in this setting the motion of a single particle in the physical space comes to be described by a non-Markovian three-dimensional diffusion with common density ρ and, at least at dynamical equilibrium, common current velocity $\boldsymbol{v}$. The three-dimensional drift is perturbed by zero-mean terms depending on the whole configuration of the N-Bosons interacting system. The evolution in time of the couple $(\rho, \boldsymbol{v})$ is governed by a system of two partial differential equations which, in the gradient case, have the structure of Madelung fluid equations with a dynamical perturbation. Such a description holds for very general interactions and for any N.

In case of smooth short-range pair interaction the stochastic description allows to derive rigorously the potential to which the single particle is subject, leading to the familiar term proportional to the density ρ. Moreover the formalism suggests a characterization of the mesoscopic scale where the general one-particle dynamics can be rewritten as a cubic Nonlinear Schrödinger Equation.

As is well known, this equation, usually called Gross–Pitaevskii (GP) Equation, plays a fundamental role in describing the hydrodynamics of a Bose–Einstein condensate [4] (see [5], [6] and [7] for accurate reviews). In our setting no condensation is a priori assumed and the cubic NLSE arises just as a tool for describing the one particle dynamics, for smooth short-range pair interaction, in terms of mathematical objects defined in conditional mean.

In this paper we consider the general one-particle Bose dynamics out of dynamical equilibrium. We observe that in the most simple sufficient conditions which allow to put the equations in closed form, one is reduced to consider a class of NLSEs with an electromagnetic potential $(\mathcal{A}, \Phi + G)$ such that G depends on the squared modulus of the wave function and $\mathcal{A}$ satisfies the equation of magnetohydrodynamics with coefficient depending on the wave function (see (7)). In agreement with the linear case [8], we can prove that the dynamics is dissipative until the dynamical equilibrium is reached. This corresponds to the case when $\nabla \wedge \mathcal{A}$ is equal to zero in all points where the wave function is different from zero. Quite surprisingly the rate of dissipation does not depend on G. The case with $G = g\rho$ for some constant g is the simplest one. The derivation of this term for the case of smooth short-range pair interaction is the same as in the dynamical equilibrium case.

The plan of the paper is the following: in Section 2 we recall the derivation of the one particle Bose dynamics within Stochastic Quantization by Lagrangian Variational Principle and introduce the class of NLSEs corresponding to the simplest closed form of evolution equations out of dynamical equilibrium. The particularization for the case of pair smooth short-range interaction is discussed in Section 2.1. Section 3 is a mathematical digression, where we study in general the Lagrangian and Hamiltonian structure of a class of Nonlinear Shrödinger Equations with time dependent external electromagnetic potentials. In Section 4 we apply results of Section 3 in order to show that all NLSEs with vorticity introduced in Section 2 are in fact dissipative, until vorticity goes to zero or concentrates in the zeros of the density, and we restrict our attention to the cubic case. Some not trivial numerical solutions for a Bose system in a finite two-dimensional trap with harmonic potential are presented.

2. One-particle dynamics for a system of N identical interacting Bosons

2.1. General one-particle equations

Let us consider an isolated system of N identical interacting particles with Hamiltonian

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

where Φ and Φ_{int} denote respectively the external and the interaction potentials, $\boldsymbol{r}_i$ the position of the i-th 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 selfadjoint extension which is the generator of the unitary group which describes the evolution in time of the wave function $\hat{\Psi}$ in $L^2_{\mathbb{C}}(\mathbb{R}^{3N}, \mathrm{d}\hat{r})$.

The $3N$-dimensional Schrödinger equation reads, in compact form,

$$\mathrm{i}\,\hbar\partial_t\hat{\Psi} = \left(-\frac{\hbar^2}{2m}\hat{\nabla}^2 + \Phi^{\alpha,N}_{\mathrm{tot}} \right)\hat{\Psi} \tag{1}$$

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

In Stochastic Quantization by Lagrangian Variational Principle (see [1] and [2]) the role of state is played by a time dependent couple $(\hat{\rho}, \hat{V})$, where, for every time t, $\hat{\rho}$ is a smooth probability density in $\mathbb{R}^{3N}$ and $\hat{V} := (\boldsymbol{V}_1, \ldots, \boldsymbol{V}_N)$ a smooth $3N$-dimensional vector field on $\mathbb{R}^{3N}$.

Schrödinger equation is substituted by the couple of PDEs

$$\begin{cases} \partial_t\hat{\rho} = -\hat{\nabla}\cdot\left(\hat{\rho}\,\hat{V}\right) \\ \left[\partial_t\hat{V} + \left(\hat{V}\cdot\hat{\nabla}\right)\hat{V} - \dfrac{\hbar^2}{2m^2}\hat{\nabla}\left(\dfrac{\hat{\nabla}^2\sqrt{\hat{\rho}}}{\sqrt{\hat{\rho}}}\right)\right]_k + \\ +\dfrac{\hbar}{2m}\displaystyle\sum_{p=1}^{3N}\left(\partial_p \ln\hat{\rho} + \partial_p\right)\left(\partial_k\hat{V}_p - \partial_p\hat{V}_k\right) = -\dfrac{1}{m}\partial_k\Phi^{\alpha,N}_{\mathrm{tot}} \end{cases} \tag{2}$$

(A modified version of the principle, leading to the same equations, but with a free parameter, is proposed in [9]. The extension to finite dimensional systems on curved manifolds is given in [10]).

Equations (2) (which are derived rigorously from first principles), describe an evolution of hydrodynamical type for the couple $(\hat{\rho}, \hat{V})$. One can prove that they represent a smooth approximation of the canonical quantum description (where in fact

$\hat{V}$ can be very singular), in the sense that every rotational solution of (2) relaxes on an irrotational canonical one.

To be more precise, one can see that if $\hat{V}$ is a smooth gradient-field we have Madelung equations for the N-particle system: putting, for some differentiable scalar field $\hat{S}$,

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

and, if $\hat{\rho}$ is positive on an open set Q,

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

we get the $3N$-dimensional Schrödinger equation (1) on Q.

Otherwise, for general initial data the rotational terms, of the first order in $\frac{\hbar}{m}$, induce dissipation. Under mild conditions, introducing the N-body energy functional

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

where $\hat{U} := \frac{\hbar}{2m}\hat{\nabla}\ln\hat{\rho}$ and which, in the gradient case, reduces to $E_N =< \hat{\Psi}, \mathcal{H}\hat{\Psi} >$, we have

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

where $\mathcal{E}$ denotes the mathematical expectation. Therefore irrotational solutions conserve the energy, which turns to be the usual quantum mechanical expectation of the observable energy.

For generic initial data, Schrödinger solutions are expected to work 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 Parisi–Wu approach [11]. (Global existence of solutions to (2) was proved in [12] for the Gaussian two-dimensional case. In the same case one can prove that irrotational solutions constitute a center manifold and that the convergence is in the sense of the relative entropy [13]).

To each solution of (2) is associated a $3N$-dimensional diffusion process $\hat{q} := (\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N)$ which satisfies the stochastic differential equation on $\mathbb{R}^{3N}$

$$\mathrm{d}\hat{q}(t) = \hat{b}(\hat{q}(t),t) + \left(\frac{\hbar}{m}\right)^{1/2}\mathrm{d}\hat{W}(t) \tag{3}$$

where

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

and $\hat{W}$ is a standard $3N$-dimensional Brownian Motion.

In [3] this structure was exploited to give some rigorous results concerning the one-particle dynamics and to discuss the GP model from a new point of view.

These results hold under some sufficient conditions which, in the most simple formulation are

(i) $\hat{\rho}$ has support in a compact set for $t = 0$, and the support remains in a given bounded domain for all $t \in [0, T]$, $T > 0$.

(ii) $\hat{\rho}$ is of class C_0^1 as function of t and C_0^2 as function of the configuration variable $\hat{r}$, while the current $\hat{V}\hat{\rho}$ is assumed of class C_0^1 as functions of $\hat{r}$.

Remark. Assumptions (i) and (ii) 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 $|\partial_t \hat{\rho}(\hat{r}, t)| \leq g(\hat{r})$ d$\hat{r}$-a.s., and analogously for $\hat{\rho}$ and $\hat{\rho}\hat{V}$ as functions of the configuration.

One can then prove that the evolution in time of the position $\boldsymbol{q}_i$ of the i-th particle turns to be represented by a non-Markovian diffusion of equation

$$d\boldsymbol{q}_i(t) = \left(\boldsymbol{v}_i \left(\boldsymbol{q}_i(t), t \right) + \frac{\hbar}{2m} \nabla_i \ln \rho \left(\boldsymbol{q}_i(t), t \right) \right) \mathrm{d}t + \zeta_i \left(\boldsymbol{q}_1(t), \boldsymbol{q}_2(t), \ldots, \boldsymbol{q}_N(t), t \right) \mathrm{d}t + \left(\frac{\hbar}{m} \right)^{1/2} \mathrm{d}\boldsymbol{W}_i(t)$$

where ρ is the one-particle probability density (which is common to all the particles, by the symmetry of $\hat{\Psi}$), and $\boldsymbol{v}_i$ is defined by

$$\boldsymbol{v}_i(\boldsymbol{r}, t) = \mathcal{E}_{\boldsymbol{q}_i(t)=\boldsymbol{r}} \left[\boldsymbol{V}_i(\boldsymbol{q}_1(t), \ldots, \boldsymbol{q}_i(t), \ldots, \boldsymbol{q}_N(t), t) \right] \tag{4}$$

$\mathcal{E}_{\boldsymbol{q}_i(t)}$ denoting the conditional expectation given $\boldsymbol{q}_i(t)$.

The term ζ_i depends on the whole configuration of the N-particles system and one can easily prove that it has zero mean once fixed $\boldsymbol{q}_i(t) = \boldsymbol{r}$. This shows that the interaction with the other $N - 1$ particles produces a differentiable noise.

In addition, one has the following general one-particle dynamical equations (where for simplicity we put $i = 1$ and $k = 1, 2, 3$)

$$\begin{cases} [\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}_1)](\boldsymbol{r}, t) = 0 \\ \left[\partial_t \boldsymbol{v}_1 + (\boldsymbol{v}_1 \cdot \nabla) \boldsymbol{v}_1 - \dfrac{\hbar^2}{2m^2} \nabla \left(\dfrac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) + \dfrac{\hbar}{2m} (\nabla \ln \rho + \nabla) \wedge (\nabla \wedge \boldsymbol{v}_1) \right]_k (\boldsymbol{r}, t) = \\ = -\dfrac{1}{m} \mathcal{E}_{\boldsymbol{q}_1(t)=\boldsymbol{r}} \left[\partial_k \Phi_{\mathrm{tot}}^{\alpha,N}(\boldsymbol{q}_1(t), \ldots, \boldsymbol{q}_N(t)) \right] - \beta_k(\alpha, N, \boldsymbol{r}, t) \end{cases} \tag{5}$$

where β_k represents the dynamical perturbation, due to the interactions, to the evolution of the one particle velocity field $\boldsymbol{v}_1$. The main point here is that such a perturbation does not affect the one-particle continuity equation.

Notice that if the N-body system is at dynamical equilibrium, which corresponds to canonical quantization, then

$$\rho = \int_{\mathbb{R}^{3(N-1)}} |\hat{\Psi}|^2(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, t) \mathrm{d}\boldsymbol{r}_2 \cdots \mathrm{d}\boldsymbol{r}_N$$

and

$$\boldsymbol{v}_1(\boldsymbol{r}, t) = \mathcal{E}_{\boldsymbol{q}_1(t)=\boldsymbol{r}} \left[\nabla_1 \hat{S}(\boldsymbol{q}_1(t), \ldots, \boldsymbol{q}_N(t), t) \right] \tag{6}$$

where $\hat{S}$ is the phase of the N-body wave function $\hat{\Psi}$. In addition, we can prove that $\boldsymbol{v}_1 = \boldsymbol{v}_2 = \ldots = \boldsymbol{v}_N$.

We consider in this paper the particular case when β_k is negligible and there exists a smooth function G such that

$$\mathcal{E}_{\boldsymbol{q}_1(t)=\boldsymbol{r}}\left[\partial_k \Phi_{\mathrm{int}}(\boldsymbol{q}_1(t), \ldots, \boldsymbol{q}_N(t))\right] = \partial_k G[\rho](\boldsymbol{r}, t)$$

Then, recalling results given in [2], one can easily prove that there exists a smooth scalar field S such that, defining

$$\begin{aligned} &\mathcal{A} := \nabla S - m\boldsymbol{v}_1 \\ &\psi := \rho^{\frac{1}{2}} \exp\left(\frac{\mathrm{i}}{\hbar} S\right) \end{aligned}$$

one gets the Nonlinear Schrödinger Equation with vorticity

$$\begin{cases} \mathrm{i}\hbar\partial_t \psi = \dfrac{1}{2m}(\mathrm{i}\hbar\nabla + \mathcal{A})^2\psi + (\Phi + G(|\psi|^2))\psi \\ \partial_t \mathcal{A} = \boldsymbol{b}_- \wedge (\nabla \wedge \mathcal{A}) - \dfrac{\hbar}{2m}\nabla \wedge (\nabla \wedge \mathcal{A}) \end{cases} \tag{7}$$

where

$$\boldsymbol{b}_- := \frac{1}{m}(\nabla S - \mathcal{A}) - \frac{\hbar}{2m}\nabla \ln(|\psi|^2)$$

Neglecting β_k means that the effects the interactions on the one-particle dynamics, which affects only second equation, are taken explicitly into account only in the term containing the interaction potential.

As detailed in [3], β_k is essentially of kinematical origin and basically depends on time, space and size scales. As a consequence, properly neglecting β_k would correspond to fixing suitable mesoscopic scales.

Concluding, equation (7) represents the simplest closed form of one-particle dynamics out of equilibrium, for a system of identical interacting Bosons.

Notice that the second equation in (7) is the analogous of the equation of magnetohydrodynamics.

2.2. The cubic case

Let us consider the case when $G(\rho) = g\rho$ for some constant g and $\mathcal{A} = 0$ ($d = 3$). Then we have the cubic NLSE, usually called Gross–Pitaevskii Equation, which plays a fundamental role in describing the dynamics of a Bose–Einstein condensate in a number of experimental situations [4, 14, 5].

Unfortunately, as is well known, the problem of deriving rigorously the GP Equation from the N-body Hamiltonian $\mathcal{H}$ is still partially open, in the sense that a rigorous derivation of the general time dependent GP equation and a control of errors for finite N in the rescaling procedures are still lacking.

The most important results are given in [15] and [16] (see also [17] and references therein for recent results and an accurate review of mathematical aspects). It is proved that, if the interaction potential is of the type

$$\Phi_{\rm int} = \frac{1}{2}\sum_{i\neq j} V_N(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

where (Lieb–Seiringer–Yngvason scaling)

$$V_N(\boldsymbol{r}) := N^2 V(N\boldsymbol{r})$$

and V is a positive, spherically symmetric, compactly supported smooth potential with scattering length equal to a_0 (which implies that the scattering length of V_N is equal to $\frac{a_0}{N}$), then, for N going to infinity, the N-body ground state approaches in a precise sense $\Pi_{i=1}^N \phi_{\rm GP}(\boldsymbol{r}_i)$, where $\phi_{\rm GP}$ is the ground state of the cubic NLSE with $g = 4\pi\frac{\hbar^2}{m}a_0$.

Extensions to time-dependent situations are done in [18] for the free evolution from a class of factorized initial states. In this case the limit equation is the cubic NLSE with zero external potential. Moreover it is proved that the asymptotic solutions are still factorized.

In Stochastic Quantization approach proposed in [3], the considered interaction potential is of the type

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

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

(a) $0 \le h_{B^\alpha(\boldsymbol{r}_i)}(\boldsymbol{r}_j) = h_{B^\alpha(\boldsymbol{r}_j)}(\boldsymbol{r}_i)$

(b) $h_{B^\alpha(\boldsymbol{r})} \in C_0^1, \quad \mathrm{supp}(h_{B^\alpha(\boldsymbol{r})}) = B^\alpha(\boldsymbol{r})$

(c) $0 \le \int_{\mathbb{R}^3}\left(I_{B^\alpha(\boldsymbol{r}_i)}(\boldsymbol{r}) - h_{B^\alpha(\boldsymbol{r}_i)}(\boldsymbol{r})\right)\mathrm{d}^3\boldsymbol{r} = O(\alpha^2)$

It is also assumed that conditions (i) and (ii) in Section 2.1 are preserved in the limit of α going to zero and that $\hat\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N,t)$ and its spatial derivatives up to the order 2 have a good behavior in the same limit. Then, neglecting terms of order $o(\alpha)$, one gets

$$\mathcal{E}_{\boldsymbol{q}_1(t)=\boldsymbol{r}}\left[\partial_k \Phi_{\rm int}(\boldsymbol{q}_1(t),\ldots,\boldsymbol{q}_N(t))\right] = \partial_k G[\rho](\boldsymbol{r},t)$$

where

$$G(\rho) = K\alpha(N-1)\rho$$

Moreover, the new formalism suggests a characterization of the proper mesoscopic scales where the dynamical perturbation $\beta(\alpha,N,\boldsymbol{r},t)$ in (5) can be neglected.

3. Digression: Lagrangian and Hamiltonian densities for a class of Nonlinear Schrödinger Equations with external time dependent four-vector potentials

We plan now to study how the dissipative character of the general N-body dynamics out of dynamical equilibrium is preserved in the one particle description. We will see that all NLSEs with vorticity we are considering are in fact dissipative and we will give the expression of the rate of dissipation. To do this we need some general results given in this section.

Let $(\mathcal{A}, \Phi)$ denotes a smooth time dependent four-vector potential on $\mathbb{R}^3$ and consider the nonlinear Schrödinger equation

$$\mathrm{i}\hbar\partial_t\psi = \frac{1}{2m}(\mathrm{i}\hbar\nabla + \mathcal{A})^2\psi + (\Phi + G(|\psi|^2)\psi \tag{8}$$

where G is a continuous function from $\mathbb{R}^+$ to $\mathbb{R}$.

Assume now that ψ is a smooth solution of (8) such that $|\psi|^2$ is strictly positive on an open domain Q (possibly extended to the whole $\mathbb{R}^3$), for all $t \geq 0$. Putting

$$\begin{aligned} &|\psi|^2 = \rho \\ &\boldsymbol{v} = \frac{1}{m}(\nabla S - \mathcal{A}) \end{aligned} \tag{9}$$

we get the equivalent Madelung-like equations on Q

$$\begin{cases} \partial_t\rho = -\nabla\cdot\dfrac{1}{m}(\rho(\nabla S - \mathcal{A})) \\ \partial_t S + \dfrac{(\nabla S - \mathcal{A})^2}{2m} - \dfrac{\hbar^2}{2m}\dfrac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} + \Phi + G(\rho) = 0 \end{cases} \tag{10}$$

Let us now introduce the time dependent Hamiltonian density

$$\mathcal{H}[\rho, S, t] := \left[\frac{(\nabla S - \mathcal{A})^2}{2} + \frac{1}{2m}\left(\frac{\hbar}{2}\nabla\ln\rho\right)^2 + \Phi\right]\rho + F(\rho) \tag{11}$$

where F denotes a primitive of G.

The time dependent Lagrangian density is

$$\mathcal{L}[\rho, \partial_t\rho, S, t] := S\partial_t\rho - \mathcal{H}[\rho, S, t] \tag{12}$$

We can prove the following

Proposition 1. *Let us consider the action functional*

$$I_{[t_a,t_b]}[\rho, S] = \int_{t_a}^{t_b}\mathrm{d}t\int_Q \mathcal{L}[\rho_t, \partial_t\rho_t, S_t, t](x)\mathrm{d}x \tag{13}$$

Let $\delta\rho$ and δS be arbitrary smooth functions of x and t such that

$$\delta\rho_{t_a} = \delta\rho_{t_b} = 0 \tag{14}$$

$$\delta S|_{\partial Q} = 0 \tag{15}$$

$$\left.\frac{\nabla\rho}{\rho}\delta\rho\right|_{\partial Q} = 0 \tag{16}$$

Then a necessary and sufficient condition in order ρ and S to make stationary the action functional with respect to the above defined class of variations is that they satisfy equations (10).

Proof. We require that

$$\delta_\rho I_{[t_a,t_b]} := I_{[t_a,t_b]}[\rho+\delta\rho, S] - I_{[t_a,t_b]}[\rho, S] = o(\delta\rho) \tag{17}$$

and

$$\delta_S I_{[t_a,t_b]} := I_{[t_a,t_b]}[\rho, S+\delta S] - I_{[t_a,t_b]}[\rho, S] = o(\delta S) \tag{18}$$

with $\delta\rho$ and δS smooth functions satisfying the above described conditions.

Then

$$\delta_S I_{[t_a,t_b]} = \int_{t_a}^{t_b} \mathrm{d}t \int_Q \mathrm{d}x (\partial_t\rho\delta S - \delta_S\mathcal{H})(x,t) \tag{19}$$

$$\delta_\rho I_{[t_a,t_b]} = \int_{t_a}^{t_b} \mathrm{d}t \int_Q \mathrm{d}x (-\partial_t S\delta\rho - \delta_\rho\mathcal{H})(x,t) \tag{20}$$

where in (20) we have exploited (14), and

$$\delta_S\mathcal{H} := \frac{1}{m}\left\{\nabla\cdot[(\nabla S-\mathcal{A})\rho\delta S] - \nabla\cdot[(\nabla S-\mathcal{A})\rho]\delta S\right\} \tag{21}$$

$$\begin{aligned}\delta_\rho\mathcal{H} :=& \left[\frac{1}{2m}(\nabla S-\mathcal{A})^2 + \Phi + G(\rho)\right]\delta\rho+ \\ &+\frac{\hbar^2}{2m}\left[\nabla\cdot\left(\nabla\rho\frac{\delta\rho}{2\rho}\right) - \nabla\cdot\left(\frac{\nabla\rho}{2\rho}\right)\delta\rho - \left(\frac{\nabla\rho}{2\rho}\right)^2\delta\rho\right]\end{aligned} \tag{22}$$

Recalling the properties of δS and $\delta\rho$ at the border of Q ((15) and (16)) and integrating by parts one gets that sufficient and necessary conditions in order smooth functions S and ρ to make stationary the action functional are the two equations (10). □

Corollary (Energy-theorem). Let us assume

$$\rho|_{\partial Q} = 0 \tag{23}$$

$$\left.\frac{\nabla\rho}{\rho}\right|_{\partial Q} < \infty \tag{24}$$

Introducing the energy functional

$$E := \int_Q \mathcal{H}[\rho, S, t](x,t)\mathrm{d}x \tag{25}$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}t}E = -\int_Q \left[\frac{1}{m}(\nabla S-\mathcal{A})\cdot(\partial_t\mathcal{A})\rho\right](x,t)\mathrm{d}x + \int_Q \partial_t\Phi\rho\mathrm{d}x \tag{26}$$

Proof. The proof is an extension of results given in [2].

Following the traditional route in analytical mechanics, we consider the variations

$$\delta\rho = \partial_t\rho\delta t$$
$$\delta S = \partial_t S\delta t$$

Let now (ρ, S) be a smooth solution of (10). We then find

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E &= \frac{\mathrm{d}}{\mathrm{d}t}\int_Q \mathcal{H}(\rho, S, \mathcal{A})(x,t)\mathrm{d}x \\ &= \lim_{\delta t\to 0}\frac{1}{\delta t}\int_Q [\delta_{(S)}\mathcal{H} + \delta_{(\rho)}\mathcal{H}]\mathrm{d}x - \int_Q\left[\frac{1}{m}(\nabla S - \mathcal{A})\cdot(\partial_t\ \mathcal{A})\rho\right](x,t)\mathrm{d}x + \int_Q \partial_t\Phi\rho\mathrm{d}x\end{aligned} \tag{27}$$

We observe that, for any smooth δS, the expression of $\delta_{(S)}\mathcal{H}$ is given by (21). As a consequence, comparing with the first of (10), we see that $\delta_{(S)}\mathcal{H}$ is equal to $\partial_t\rho\delta S$ plus a boundary term which disappears in the integral by (23).

Analogously, for any smooth $\delta\rho$, the expression of $\delta_{(\rho)}\mathcal{H}$ is given by (22). Then, comparing with the second of (10), we can see that $\delta_{(\rho)}\mathcal{H}$ is equal to $-\partial_t S\delta\rho$ plus a boundary term which disappears in the integral by (24).

Concluding, substituting δS and $\delta\rho$ by $\partial_t S\delta t$ and $\partial_t\rho\delta t$ we find that the only contribution to the variation in time of the energy E comes from the time dependent fields $\mathcal{A}$ and Φ, giving

$$\frac{\mathrm{d}}{\mathrm{d}t}E = -\int_Q\left[\frac{1}{m}(\nabla S - \mathcal{A})\cdot\partial_t\mathcal{A}\rho\right](x,t)\mathrm{d}x + \int_Q \partial_t\Phi\rho\mathrm{d}x$$

□

Of course this result implies that all NLSEs of the type we have considered conserve the expected energy if the four vector potential $(\mathcal{A}, \Phi)$ is independent of time.

Notice also that the time derivative of the energy does not depend explicitly on the term $G(\rho)$.

Finally, we stress that condition (24) is only sufficient. Indeed, there exists at least one example, namely the Gaussian solutions of the two-dimensional harmonic oscillator, where (24) is not verified (with $Q = \mathbb{R}^2$) and the energy theorem still holds [12].

4. Cubic NLSE with vorticity: rotational excitations of the ground state

Let us now consider the cubic case of the general NLSE with vorticity (7) (with ψ normalized to 1)

$$\begin{cases}\mathrm{i}\hbar\partial_t\psi = \dfrac{1}{2m}(\mathrm{i}\hbar\nabla + \mathcal{A})^2\psi + (\Phi + g|\psi|^2)\psi \\ \partial_t\mathcal{A} = \boldsymbol{b}_- \wedge (\nabla\wedge\mathcal{A}) - \dfrac{\hbar}{2m}\nabla\wedge(\nabla\wedge\mathcal{A})\end{cases} \tag{28}$$

where

$$\boldsymbol{b}_- = \frac{1}{m}(\nabla S - \mathcal{A}) - \frac{\hbar}{2m}\nabla\ln(|\psi|^2)$$

Then the first in (28), for any given time dependent field $\mathcal{A}$, is a particular case in the class of conventional NLSEs we have studied in Section 2, with time independent Φ and $G(\rho) = g\rho$. Recalling that $\psi := \rho^{\frac{1}{2}} \exp \frac{\mathrm{i}}{\hbar} S$, the energy functional reads, in terms of ρ and S,

$$E = \int_Q \left[\frac{1}{2m}(\nabla S - \mathcal{A})^2 + \frac{1}{2}(\frac{\hbar}{2m}\nabla \ln \rho)^2 + \Phi + \frac{g}{2}\rho \right] \rho \mathrm{d}x$$

and the energy theorem, which holds for any time dependent vector field $\mathcal{A}$, gives

$$\frac{\mathrm{d}}{\mathrm{d}t}E = -\int_Q \left[\frac{1}{m}(\nabla S - \mathcal{A}) \cdot (\partial_t \mathcal{A})\rho \right] (x,t)\mathrm{d}x$$

Recalling the position $\frac{1}{m}(\nabla S - \mathcal{A}) := \boldsymbol{v}$ and the expression of $\partial_t \mathcal{A}$, a simple component-wise calculation and an integration by parts, with ρ equals to zero on ∂Q, gives

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}E &= -m \int_Q \left\{ \boldsymbol{v} \cdot \left[\left(\frac{\hbar}{2m}\nabla \ln \rho + \frac{\hbar}{2m}\nabla \right) \wedge \nabla \wedge \boldsymbol{v} \right] \right\} \rho \mathrm{d}x = \\ &= -\frac{\hbar}{2}\int_Q (\nabla \wedge \boldsymbol{v})^2 \rho \mathrm{d}x = -\frac{\hbar}{2}\int_Q (\nabla \wedge \mathcal{A})^2 \rho \mathrm{d}x \end{aligned} \tag{29}$$

Notice that the expression of the rate of dissipation is independent both of m and g, and it is the same as in the non-interacting case. Moreover, by the results of Section 3, system (7) has the same rate of dissipation if $g\rho$ is replaced by any continuous function of ρ itself‡.

We now come back to the equations in Madelung form and make use of standard adimensional variables, which are still denoted by r, t, ρ and $\boldsymbol{v}$ (see, for example, [8] for details).

We get the system of coupled PDEs

$$\begin{cases} \partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} - 2\nabla \left(\dfrac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) + (\nabla \ln \rho + \nabla) \wedge (\nabla \wedge \boldsymbol{v}) = -\nabla \Phi - c\nabla \rho \\ \partial_t \rho = -\nabla \cdot (\rho \boldsymbol{v}) \end{cases} \tag{30}$$

where c is a constant.

In the following, we consider the two-dimensional case with trap harmonic potential $\Phi := \frac{1}{2}r^2$ and an infinite barrier at $r = R$. The linear case, corresponding to $c = 0$, was firstly studied in [8], showing concentration of vorticity in the minima of the density during the dissipative transients. Asymptotically, the vorticity concentrates close to a central vortex line, suggesting the formation of a singularity in Madelung fluid.

In this work we present a comparison with the cubic NLSE with vorticity we have just introduced by solving numerically (30) for $c = 0, 10, 100$. The initial density is chosen to be the squared absolute value of the corresponding ground states and the initial velocity field is fixed with a uniform vorticity. The last plays the role of a "rotational excitation". The ground state in the finite trap is approximated by the

‡ We recall that Q is an open set which does not contain points where the wave function has nodes. As a consequence, the case when nodes are present and their position varies in time is not automatically described in this setting.

ground state in $\mathbb{R}^2$, truncated at $r = R$, where ρ is of order 10^{-10}. This value remains fixed during the simulation.

The code exploits FEM technique, with triangular finite elements in a circular domain D of radius $R = 6.5$, linear shape functions and standard Galerkin variational formulation. The system is reduced of one order by introducing the (adimensional) osmotic velocity $\boldsymbol{u} := \nabla \ln \rho$. In particular this allows to rewrite equivalently the system with a diffusive and stabilizing term in each equation. For the time discretization a θ-method is adopted, with a modified Newton nonlinear solver. The numerical calculation of the ground state, see Figure 1, was performed by directly minimizing the energy functional under the normalization constraint of ψ (see [19] for details).

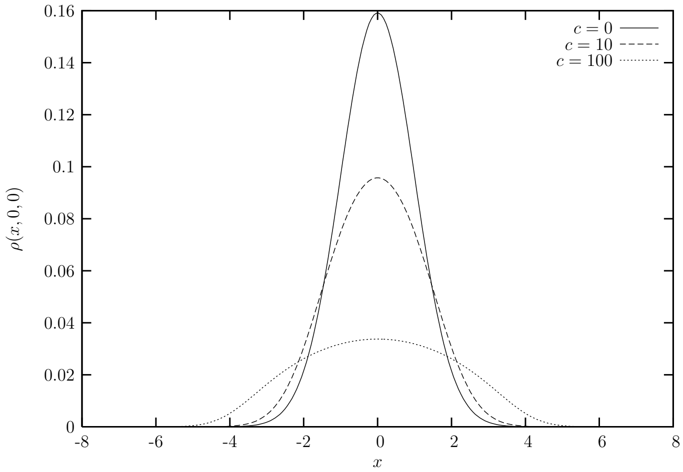

Figure 1. Profiles of the two-dimensional initial densities as a function of x for different values of c.

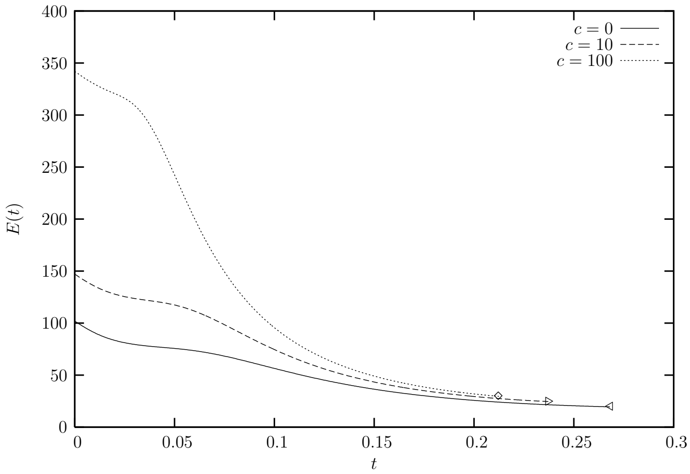

Figure 2. Energy as a function of time for different values of c.

The boundary conditions, ν denoting the unitary external normal vector, are

$$\begin{cases} -\nabla \cdot (\boldsymbol{u} - \boldsymbol{v})\Big|_{\partial D} \nu + \dfrac{\partial \boldsymbol{v}}{\partial \nu}\Big|_{\partial D} = 0 \\ \boldsymbol{u}\Big|_{\partial D} = \boldsymbol{u}_0\Big|_{\partial D} \\ \rho\Big|_{\partial D} = \rho_0\Big|_{\partial D} \approx 10^{-10} \end{cases} \tag{31}$$

Strong variations in time to the value at the border of the current velocity field $\boldsymbol{v}$ are allowed.

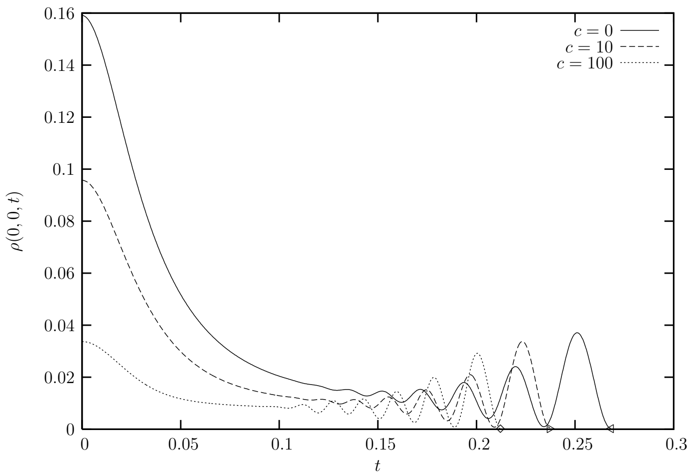

Figure 3. Density at the origin as a function of time for different values of c.

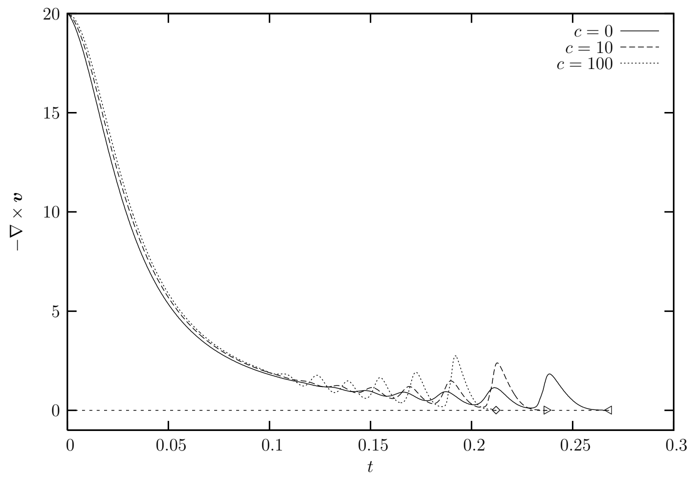

Figure 4. Vorticity $(-\nabla \times \boldsymbol{v})$ at the origin as a function of time for different values of c.

We have performed several numerical simulations up to a final time $\bar{t}$ defined as follows: $\bar{t}$ it is the first time at which the density ρ assumes a value less than 10^{-4}, which happens in a small neighborhood of the origin. We have observed that $\bar{t}$ strongly depends on the value of the nonlinearity constant c, the radius of the trap R and of the initial vorticity $\nabla \times \boldsymbol{v}_0$. The behavior of the simulation was satisfactory up to few steps before $\bar{t}$: the radial symmetry was naturally conserved on the mesh and the positivity of the density was preserved. Moreover, for each time step, only a reasonable (less than 10) number of nonlinear iterations was necessary. The profiles of the vorticity in Figure 5 are reconstructions of $\nabla \times \boldsymbol{v}$, computed a posteriori starting from the piecewise-linear velocity field.

In all the simulations, dissipative transients and concentration of vorticity in the minima of the density were observed.

This seems to be a general behavior which somehow occurs for any initial density. The effect is spectacular for the excitation of the ground state, as one can see from Figures 2–5 which illustrate the results of numerical experiments for $R = 6.5$, initial velocity $\boldsymbol{v} = -\Omega_0 r \boldsymbol{\theta}$, $\Omega_0 = 10$, and different values of c (namely $c = 0, 10, 100$). The values of the parameters were chosen in order $\bar{t}$ to be less than 0.3.

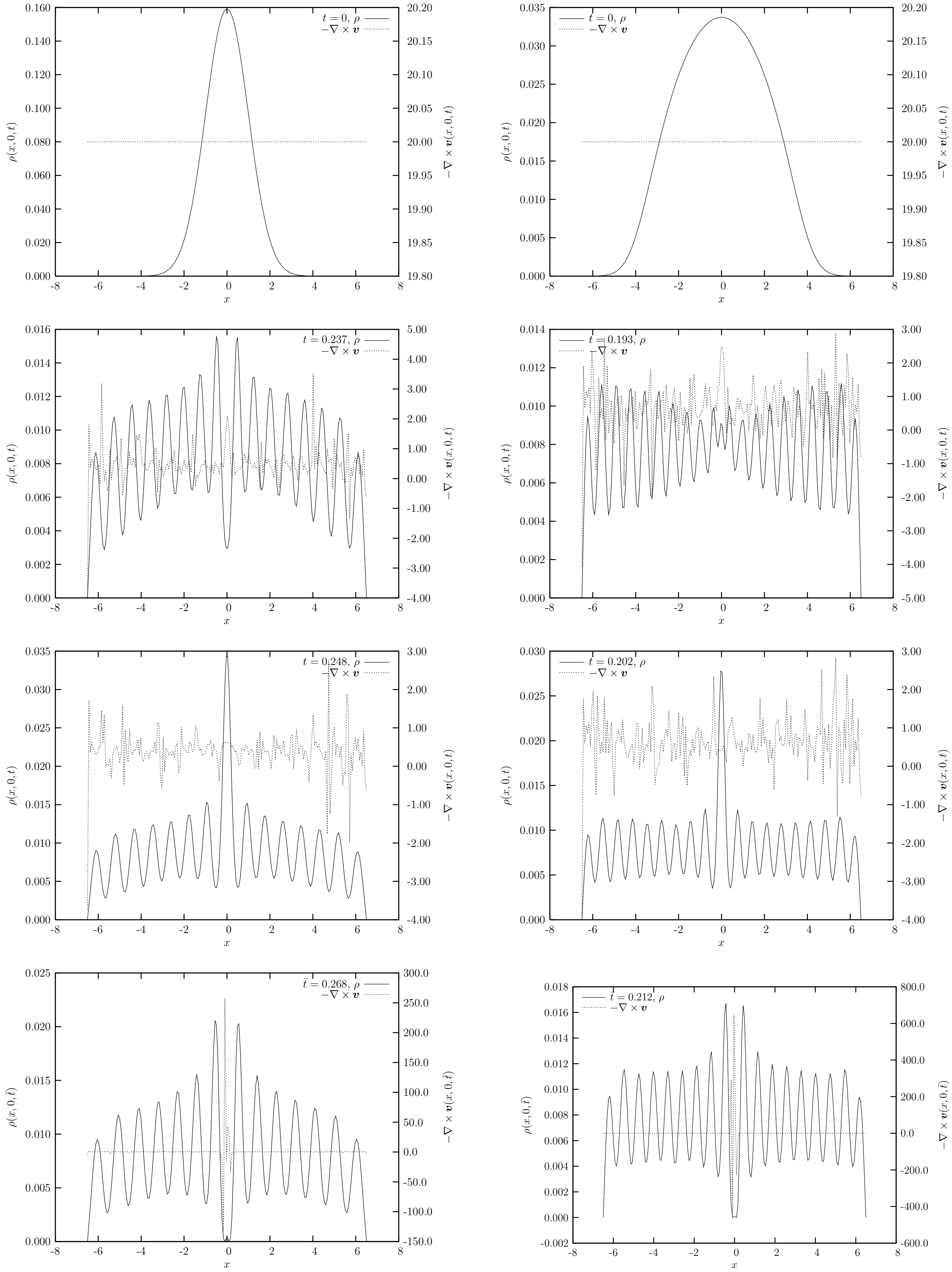

Figure 5. Profiles of density (solid line) and vorticity (dotted line) as a function of x for $c = 0$ and $c = 100$ at four values of t, respectively the initial time, the time at which the last maximum of vorticity at the origin occurs in $[0, \bar{t}]$, the time at which the last maximum of density occurs in $[0, \bar{t}]$, and the final time $\bar{t}$.

5. Conclusions

We have introduced from first principles a new class of NLSEs with electromagnetic potential depending on the wave function. The dynamics is dissipative until the vorticity of the magnetic potential goes to zero or eventually concentrates in nodes of the wave function itself. For the cubic case, this expected qualitative behavior is validated by numerical solutions where, for the case of a finite two-dimensional trap with harmonic potential, the ground state is initially excited by a field with uniform vorticity.

We have shown that such a class of NLSEs is related to the description of the one-particle dynamics for a system of N identical interacting Bose particles out of dynamical equilibrium: the cubic case corresponds to a pair short-range smooth interaction. This put the present work in the context of modeling the dynamics of a Bose–Einstein condensate, leading in fact to a new version of the Gross–Pitaevskii Equation, with dissipation induced by a vorticity field. This fact represents an alternative to other solutions proposed in the literature in order to simulate the relaxation towards vortex lattices of a rotating superfluid [21, 22, 23, 24, 25]. To this purpose GP equation is usually modified by adding a dissipative term, which is interpreted as a friction due to the non-condensed fraction (see for example [20]). In our approach the dissipation has a purely kinematical (and quantum) origin and it does not depend on the size of the non-condensed fraction.

It is worth mentioning that, as far as the rotating superfuids is concerned, equation (28) could be applied in modeling experiments where a diluite Bose gas with pair short range interaction is put into rotation and the condensation occurs only after the stirring procedure is completed. Indeed in this case the initial conditions for the superfluid velocity would exhibit a distributed vorticity: unlike the canonical description, the new equations allow such an initial condition and the (dissipative) evolution is expected to lead to a concentration of the vorticity in the nodes of the wave function (which correspond to a gradient-like and conservative superfluid motion). One could also observe that it would be interesting to check in the experiment whether the stirring of a condensate preserves quantum coherence or not.

As a final comment, we stress that the one-particle dynamics as derived by the Lagrangian stochastic variational principle for the N-body system, is not exactly the dynamics of the condensate, unless the dynamical perturbation β in (5) and the kinematic noise ζ in (3) are equal to zero in some sense. A situation which roughly corresponds to a factorized N body state and a complete condensation.

The deeper understanding of connections between one-particle dynamics, introduced in terms of objects defined in conditional mean, and Bose–Einstein condensation, as well as the study of dynamical excitations, are challenging subjects of further investigation.

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