Stochastic Quantization for a system of N identical interacting Bose particles

L. M. Morato

(in collaboration with M. I. Loffredo)

Pisa, july 16, 2007

CONTENTS

1. Quantization of the interacting N-particles system (Loffredo and M. J Phys. A Math.Theor. **40** 2007) http://stacks.iop.org/1751-8121/40/8709

   - One-particle description

   - One-particle boson dynamics at dynamical equilibrium

   - A particular case : diluite Bose gas with short range smooth interactions and Gross-Piteavskii equation.

2. Rotational dynamics ?

CANONICAL QUANTIZATION

Quantum Hamiltonian

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

($\mathcal{H}$ is bounded from below)

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

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

STOCHASTIC QUANTIZATION BY LAGRANGIAN VARIATIONAL PRINCIPLE

The basic object is the classical lagrangian

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

$\hat{q}^{cl} :=$ classical N- body configuration.

Quantization comes from requiring that the configuration of the system evolves in fact as a Markov diffusion $\hat{q}$ in $\mathbb{R}^{3N}$.

ASSUMPTIONS

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

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

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

iii) A finite energy condition is satistied.

$\hat{W} := (\mathbf{W}_1, \ldots, \mathbf{W}_N)$ and $\mathbf{W}_i$, $i = 1, \ldots, N$ are three-dimensional independent standard Brownian Motions which model quantum fluctuations acting on the i-th particle.

NOTICE:

$\hat{\rho}$:= time dependent joint probability density of the N-particles configuration

- there exists smooth 3-N dimensional current velocity field $\hat{V}$ such that

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

- the 3-N dimensional continuity equation holds

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

STOCHASTIC LAGRANGIAN VARIATIONAL PRINCIPLE

"The actual motion of a finite dimensions quantum system is described by a Markov diffusion which makes extremal the mean discretized classical action related to $\mathcal{L}$ among smooth diffusions which satisfy a stochastic differential equation in the configurations space, with the same fixed Brownian Motion and such that the initial current velocity and the final configuration are fixed as random variables" (M., Phys. Rev. D '85; Loffredo and M., JMP '88)

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

(in the limit of the discretization going to infinity)

$$\begin{cases} \partial_t \hat{\rho} = -\hat{\nabla}\cdot\left(\hat{\rho}\,\hat{V}\right) \\ \left[\partial_t \hat{V} + \left(\hat{V}\cdot\hat{\nabla}\right)\hat{V} - \frac{\hbar^2}{2m^2}\hat{\nabla}\left(\frac{\hat{\nabla}^2\sqrt{\hat{\rho}}}{\sqrt{\hat{\rho}}}\right)\right]_k + \\ \quad + \frac{\hbar}{2m}\sum_{p=1}^{3N}\left(\partial_p \ln\hat{\rho} + \partial_p\right)\left(\partial_k \hat{V}_p - \partial_p \hat{V}_k\right) = -\frac{1}{m}\partial_k \Phi_{tot}^{\alpha,N} \qquad k = 1,\dots,3N \end{cases}$$

MADELUNG EQUATIONS WITH VORTICITY

Irrotational and rotational solutions

NOTE :

1) if $\hat{V} = \frac{1}{m}\hat{\nabla}\hat{S}$ (smooth gradient-field)

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

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

($3N$-dimensional Schrödinger equation)

2) For general initial data the rotational terms, of the first order in $\frac{\hbar}{m}$, induce dissipation !!

Relaxation to dynamical equilibrium

Energy Theorem (Loffredo and M., JMP '88; extended in 2007)

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

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

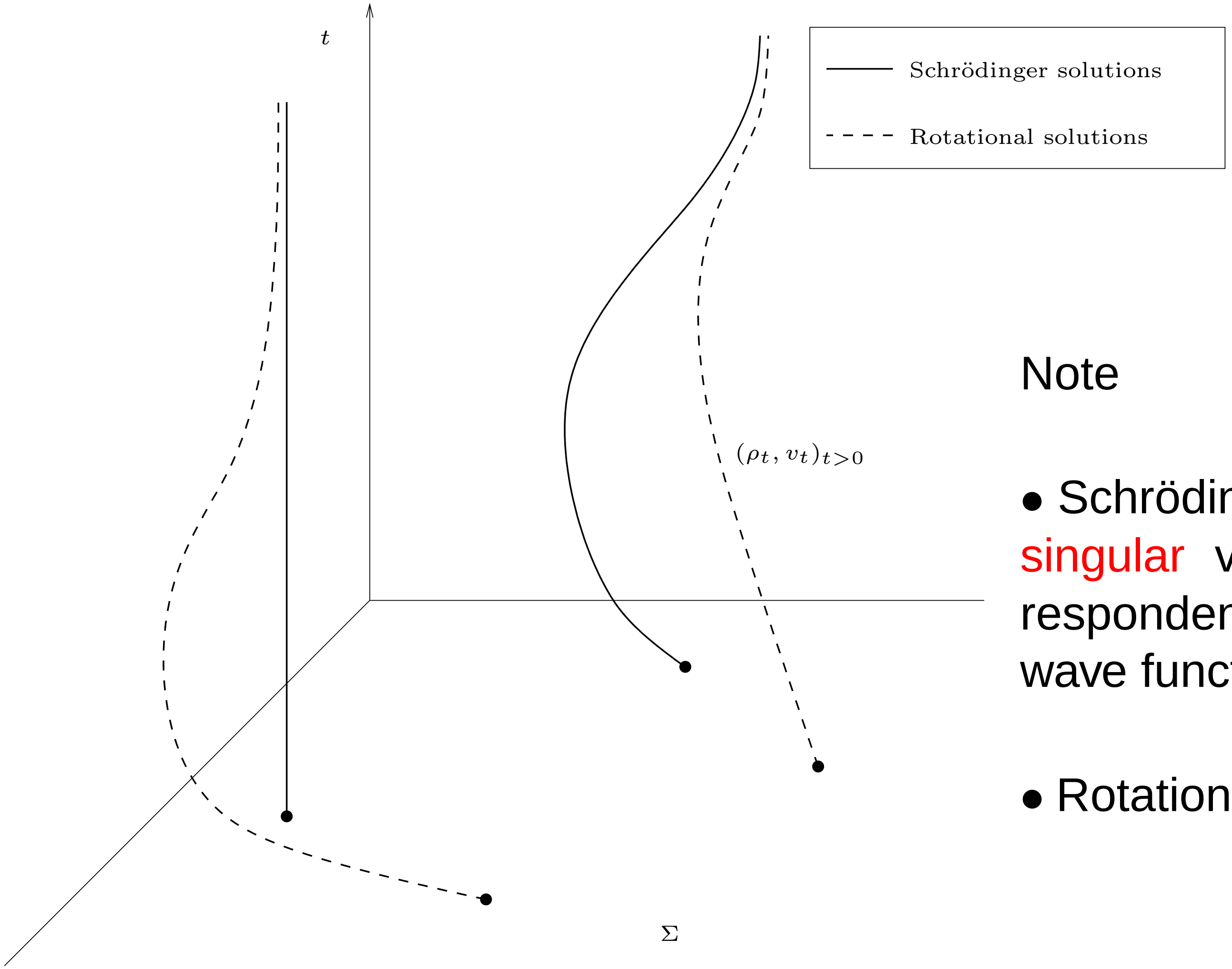
$$\frac{d}{dt} E[\hat{\rho}, \hat{V}] = -\frac{\hbar}{2} \mathcal{E} \left[\sum_{k=1}^{3N} \sum_{p=1}^{3N} \frac{(\partial_p \hat{V}_k - \partial_k \hat{V}_p)^2}{2} \right]$$

NOTE: Irrotational solutions conserve the energy and

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

For generic initial data Schrödinger solutions act as an attracting set, which corresponds to DYNAMICAL EQUILIBRIUM.

SCHRÖDINGER VERSUS ROTATIONAL SOLUTIONS



Note

- Schrödinger solutions : singular velocity field in correspondence of nodes of the wave function.

- Rotational solutions : smooth

ADVANTAGES OF STOCHASTIC QUANTIZATION FOR THE N-PARTICLE SYSTEM ?

- At dynamical equilibrium : ancillary stochastic description

- Out of dynamical equilibrium: non canonical rotational dynamics ?

ONE PARTICLE CURRENT VELOCITY

Define: $(i = 1)$

"1-th particle probability density" :

$$\rho_1(\mathbf{r}_1, t) = \int_{3(N-1)} \hat{\rho}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) d\mathbf{r}_2, \ldots, d\mathbf{r}_N$$

"1-th particle current velocity":

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

notations:

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

$\mathcal{E}_{\mathbf{q}_1(t)=\mathbf{r}}$:= expectation given $\mathbf{q}_1(t) = \mathbf{r}$

ONE PARTICLE CONTINUITY EQUATION

Proposition 1

Defining $\quad (i = 1)$

$$\mathbf{v}_1(\mathbf{r}, t) = \mathcal{E}_{\mathbf{q_1}(t)=\mathbf{r}} \mathbf{V}_1$$

Then under mild regularity assumptions, if $\hat{\rho}$ is invariant under permutation of positions of any two particles (IDENTICAL PARTICLES), then

$$\rho_1(\mathbf{r}) = \rho_2(\mathbf{r}) = \cdots = \rho_N(\mathbf{r}) := \rho(\mathbf{r})$$

and

$$\boxed{\partial_t \rho = -\nabla \cdot (\rho\, \mathbf{v_1})}$$

One-particle non Markovian diffusion

Proposition 2

Under mild regularity assumptions, if $\hat{\rho}$ is invariant under permutation of positions of any two particles (IDENTICAL PARTICLES), then, ($i = 1$)

$$d\mathbf{q}_1(t) = \left(\mathbf{v}_1\left(\mathbf{q}_1(t), t\right) + \frac{\hbar}{m}\nabla_1 \frac{1}{2}\ln\rho\left(\mathbf{q}_1(t), t\right)\right) dt + \\ + \zeta_1\left(\mathbf{q}_1(t), \mathbf{q}_2(t), ..., \mathbf{q}_N(t), t\right) dt + \left(\frac{\hbar}{m}\right)^{\frac{1}{2}} \mathbf{dW}_1(t)$$

where

$$\mathcal{E}_{\mathbf{q}_1(t)=\mathbf{r}}\, \zeta_{\mathbf{1}} = \mathbf{0}$$

$\zeta_{\mathbf{1}}$= differentiable noise due to interactions !!

One-particle Bose Dynamics

Theorem

If particles are identical BOSONS, then, in the GRADIENT-case (and in general at dynamical equilibrium), up to mild regularity conditions, we have

$$\mathbf{v} = \mathbf{v}_1, \ldots, \mathbf{v}_N$$

and the couple $(\rho, \mathbf{v})$ **evolves as**

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

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

$$= -\frac{1}{m} \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}} \left\{ \nabla_1 \Phi_{tot}^{\alpha,N}(\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)) \right\} - \beta(\alpha, N, \mathbf{r}, t)$$

This is a rigorous result which holds for any N

Decomposition of dynamical pertubation β

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

where

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

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

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

PROBLEM

“Find proper scales and orders of approximation so that dynamical equations for $(\rho, \mathbf{v})$ can be put in a (deterministic or stochastic) closed form “

DILUITE GAS WITH SMOOTH SHORT-RANGE INTERACTION

Gross-Pitaevskii equation ?

- Necessary condition :

$\hat{\Psi}(0)$ is not entangled and $\hat{\Psi}(t)$ has a regular dependence on α.

- Method :

1) Fix natural scales from the analysis of β.
2) Rigorously calculate the interation therm to $O(\alpha^2)$.

Analizing contributions to β - 1

c_1) $\beta^{time} = 0$: true for all stationary solutions.

In general: fix a time scale where

$$E_{\mathbf{q}_1(t)=\mathbf{r}} \partial_t [\mathbf{V}_1(\mathbf{q}_1(t), ..., \mathbf{q}_N(t), t) - \mathbf{v}(\mathbf{q}_1(t), t)] = 0$$

Analizing contributions to β - 2

c_2) $\beta^{conv} = 0$: true for the ground state.

In general: if we fix a space scale where

$$E_{\mathbf{q}_1(t)=\mathbf{r}}\nabla_1[\mathbf{V}_1(\mathbf{q}_1(t),...,\mathbf{q}_N(t),t) - \mathbf{v}(\mathbf{q}_1(t),t)] = 0$$

we have

$$\beta^{conv} = O(\alpha^2) + \mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}}\nabla_1\sum_{i=2}^{N}\frac{1}{2}|\mathbf{V}_i|^2$$

We will assume N finite but sufficiently large to neglect the last term (size scale)

Analizing contributions to β - 3

c_3) $(\frac{\hbar^2}{m^2})\beta^Q = 0$: we are neglecting a term of order $O(\frac{\hbar^2}{m^2})O(\alpha)$.

Therefore, in our assumptions, in general for the proper space-time and size scales, β can be neglected to the order $O(\alpha)O(\frac{\hbar^2}{m^2})$ and $O(\alpha^2)$.

Calculating interaction term

- $B^{\alpha}(\mathbf{r})$ sphere of volume α
- $h_{B^{\alpha}(\mathbf{r})}$ good smooth approximation of the indicator of $B^{\alpha}(\mathbf{r})$.

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

then we prove

$$\mathbb{E}_{\mathbf{q}_1(t)=\mathbf{r}_1} \left[\nabla_1 \Phi_{int}\right] (\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t), \alpha) =$$

$$= K(N-1) \left\{ O(\alpha^2) + \nabla_1 \left[\alpha \rho(\mathbf{r}_1, t) + O(\alpha^2)\right] \right\}$$

• N finite
• No low energy assumption !

G.P. EQUATION

We can prove

$$\bar{\rho} := N\rho = \text{expected density of particles}$$

Introducing

$$\bar{\psi} := \bar{\rho}^{\,\frac{1}{2}} \exp \frac{i}{\hbar} S$$

$$\frac{1}{m} \nabla S := \mathbf{v}$$

we get, up to terms of order $O(\alpha)O((\frac{\hbar}{m})^2)$ and $O(\alpha^2)$, in the proper scales,

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

"MEAN FIELD" description by conditional expectations !

Additional stochastic description

To every solution $\bar{\Psi}$ to G.P. equation one can associate N diffusion processes :
($\mathbf{v} = \frac{1}{m}\nabla S$, $\bar{\rho} = |\bar{\Psi}|^2$)

$$d\mathbf{q}_i(t) = \left(\mathbf{v}\left(\mathbf{q}_i(t), t\right) + \frac{\hbar}{2m}\nabla \ln \bar{\rho}\left(\mathbf{q}_i(t), t\right)\right) dt +$$

$$+ \ \zeta_i\left(\mathbf{q}_1(t), \mathbf{q}_2(t), ..., \mathbf{q}_N(t), t\right) dt + \left(\frac{\hbar}{m}\right)^{\frac{1}{2}} \mathbf{dW}_i(t) \ , \quad i = 1, \ldots, N$$

- common drift !

- interactions and quantum effects are represented as noises

MORE TO BE DONE

- The limit for N going to infinity under proper rescalings ($K\alpha N = $ const)
  (Lieb and Seiringer, PRL 2002 : exact factorization of the ground state)

- Estimates of space-time and size scales

- More general interactions.

NON CANONICAL ROTATIONAL DYNAMICS ?

Consider MADELUNG EQUATIONS WITH VORTICITY for $N = 1, \; d = 3$

- $$\begin{cases} \partial_t \rho = -\nabla \cdot (\rho v) \\ \partial_t v + (v \cdot \nabla) v - \frac{\hbar^2}{2m^2} \nabla \left(\frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) - \frac{\hbar}{m} (\nabla \ln \rho + \nabla) \wedge (\nabla \wedge v) = -\frac{1}{m} \nabla \Phi \end{cases}$$

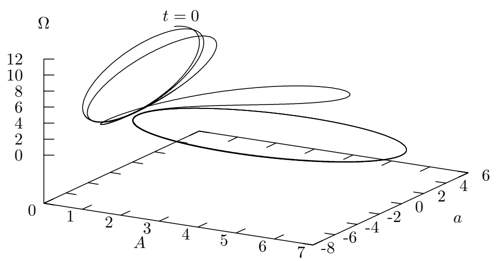
- $\exists \; S$ s.t. $\Psi := \rho^{\frac{1}{2}} \mathrm{e}^{\frac{\imath}{\hbar} S}, \qquad \mathcal{A} := mv - \nabla S$

$$\begin{cases} \imath \hbar \partial_t \Psi = \frac{1}{2m} (\imath \nabla + \mathcal{A})^2 \Psi + \Phi \Psi \\ \partial_t \mathcal{A} = b_* \wedge (\nabla \wedge \mathcal{A}) - \frac{\hbar}{2m} \nabla \wedge (\nabla \wedge \mathcal{A}) \end{cases}$$

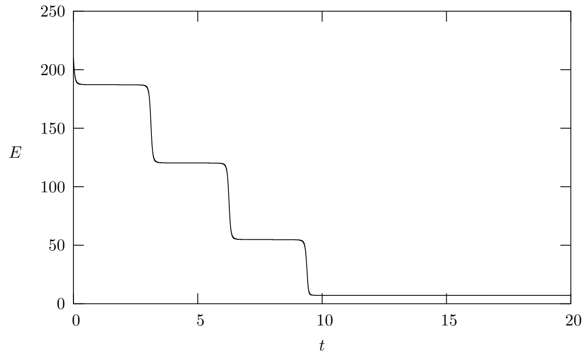
$$b_* := \frac{1}{m} [\nabla S - \mathcal{A} - \frac{\hbar}{2} \nabla \ln |\Psi|^2]$$ (Loffredo, M., JMP '88)

Non trivial behavior of vorticity

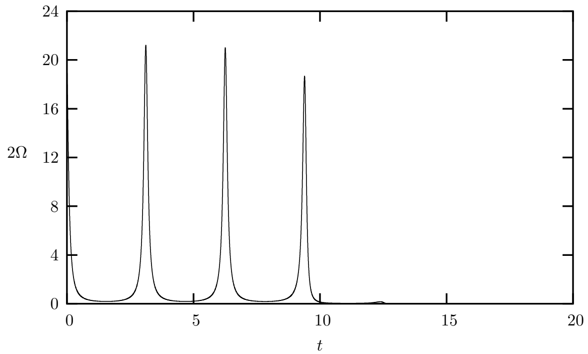
1) For $\rho > 0$ the vorticity $\nabla \wedge \mathcal{A}$ does not go to zero monotonically
(firstly conjectured by Guerra in 1992)
"gaussian solutions to the bidimensional harmonic oscillator"
(M. and Ugolini, AHP '94)



trajectory



energy vs. time

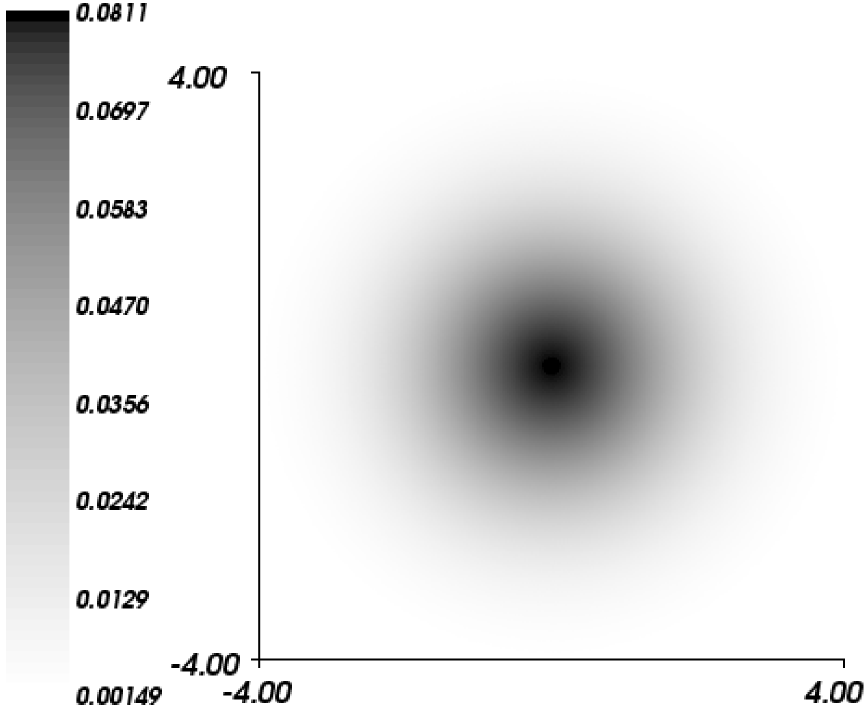


vorticity vs. time

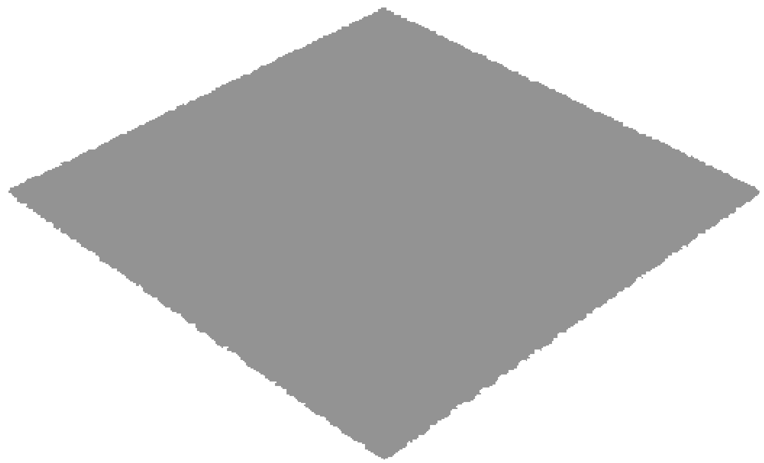
2) The vorticity can concentrate in the zeroes of the density

Non gaussian solutions to the bidimensional harmonic oscillator, numerical results:
[Caliari, Inverso and M. 2004, *New J. Phys.*, Vol 6, no. 69,
http://www.iop.org/EJ/journal/NJP]

Numerical experiment (t=0)

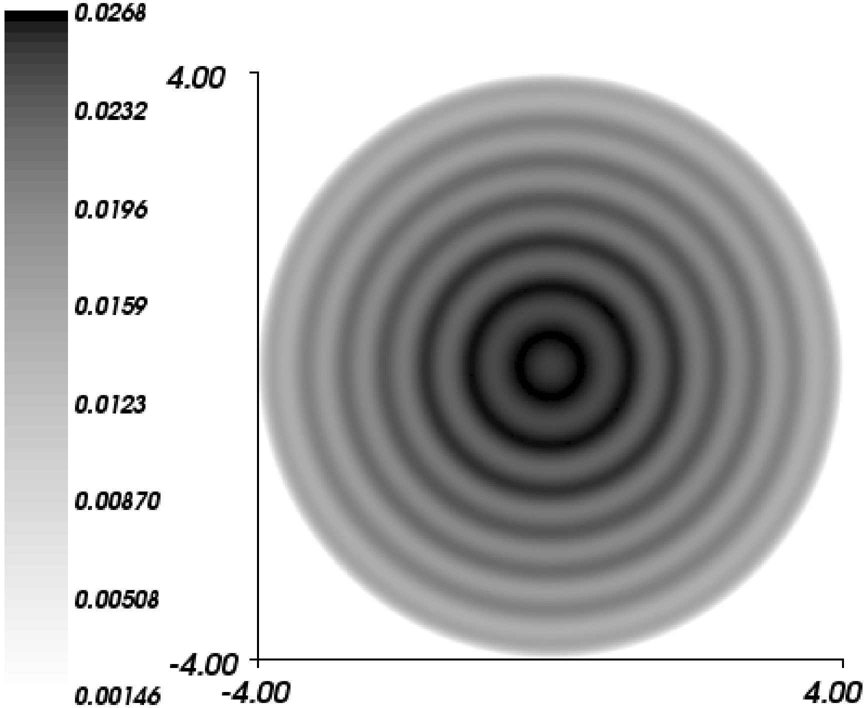


ρ at time $t = 0$, $E = 195$

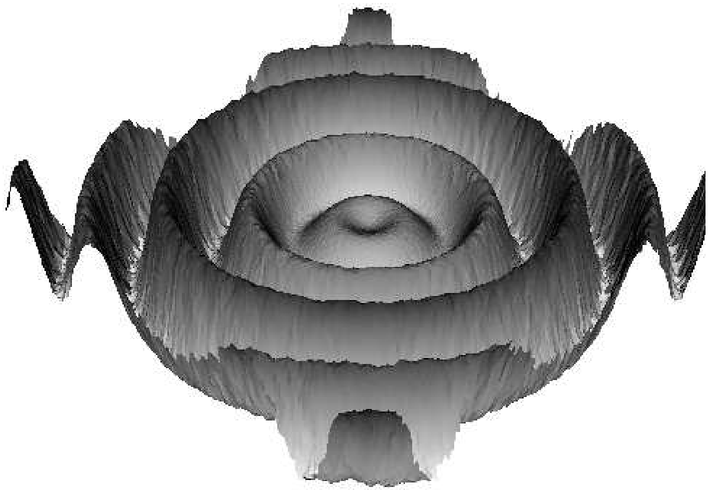


$-\nabla \wedge v = 2\Omega_o$

Numerical experiment (t=0.08)

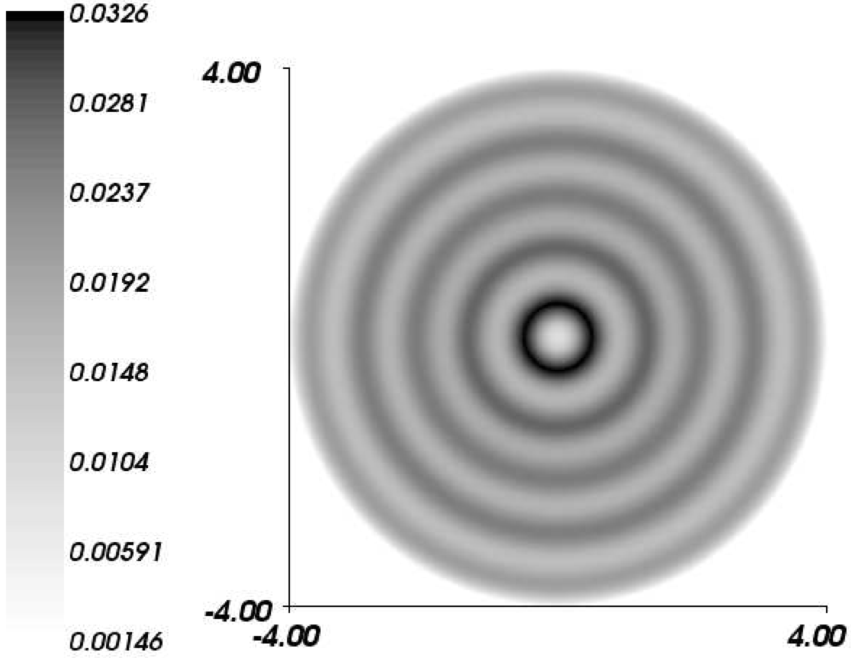


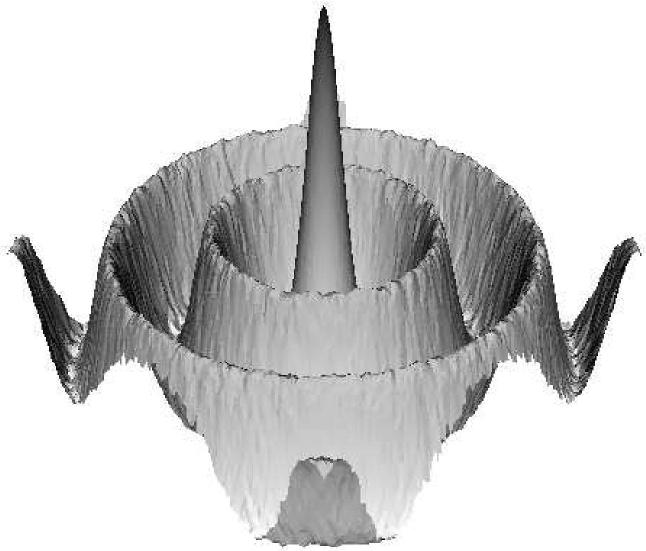
ρ at time $t = 0.08$, $E = 43$



$-\nabla \wedge v$

Numerical experiment (t=0.14)

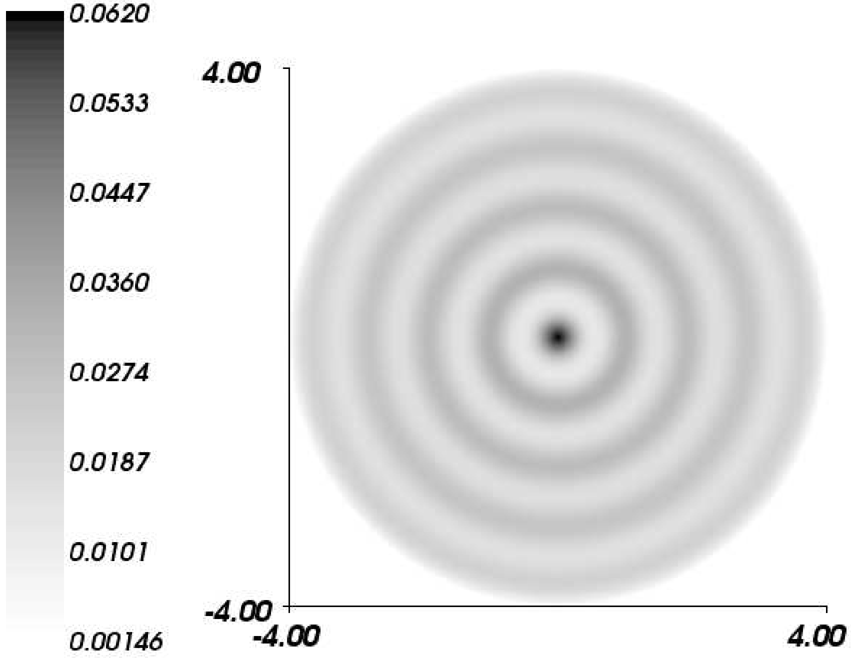




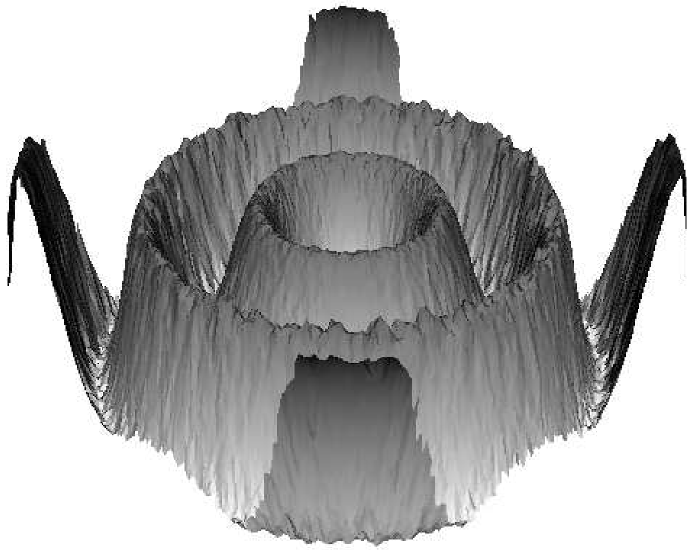
ρ at time $t = 0.14$, $E = 17$

$-\nabla \wedge v$

Numerical experiment (t=0.16)

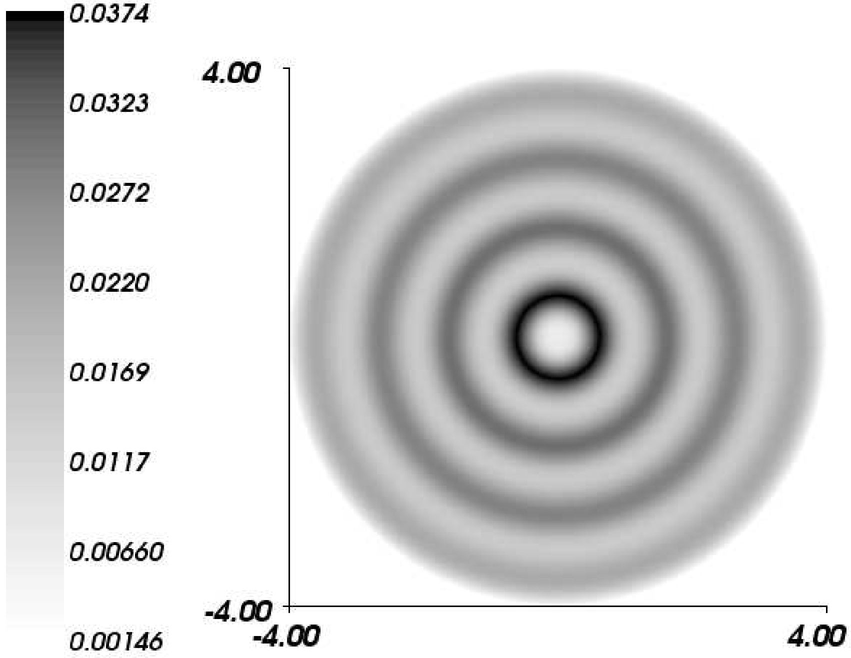


ρ at time $t = 0.16$, $E = 15$

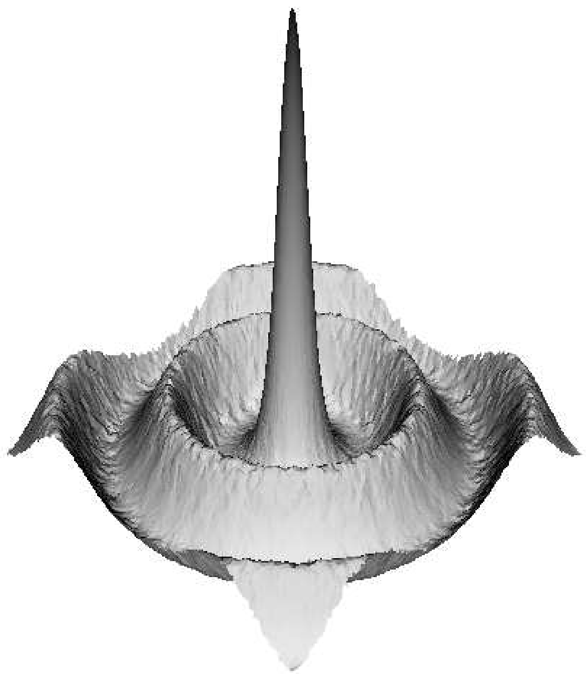


$-\nabla \wedge v$

Numerical experiment (t=0.19)

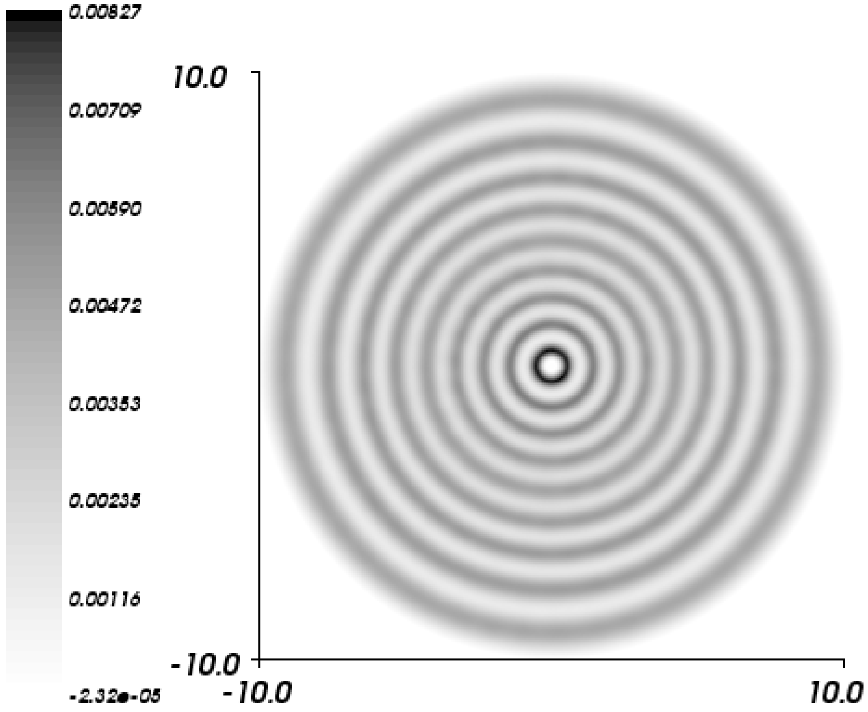


ρ at time $t = 0.19$, $E = 11$

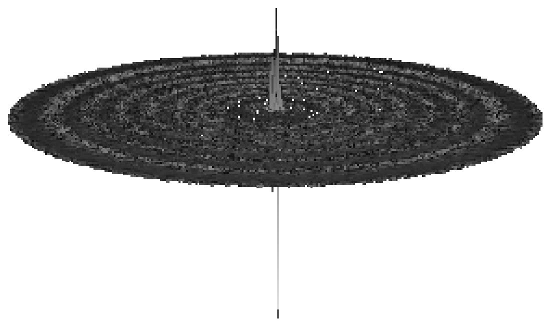


$-\nabla \wedge v$

Numerical experiment (t=0.23)



ρ at time $t = 0.23$, $E = 9$



$-\nabla \wedge v$

Rotational G.P. equation ?

Proposal (from first principles !!) : near dynamical equilibrium (see p. 10)

- $\bar{\Psi} := \bar{\rho}^{\,\frac{1}{2}} \mathrm{e}^{\frac{\imath}{\hbar} S}, \qquad \mathcal{A} := m\mathbf{v} - \nabla S$

$$\begin{cases} \imath\,\hbar\partial_t \bar{\Psi} = \frac{1}{2m}(\imath\nabla + \mathcal{A})^2 \bar{\Psi} + (K\alpha|\bar{\Psi}|^2 + \Phi)\bar{\Psi} \\ \partial_t \mathcal{A} = v_- \wedge (\nabla \wedge \mathcal{A}) - \frac{\hbar}{2m} \nabla \wedge (\nabla \wedge \mathcal{A}) \end{cases}$$

$$v_- := \frac{1}{m}[\nabla S - \mathcal{A} - \frac{\hbar}{2} \nabla \ln |\bar{\Psi}|^2]$$

NOTICE: DISSIPATION OUT OF DYNAMICAL EQUILIBRIUM !

(Loffredo and M., to appear)

Effort. . .

Numerical simulations of the “rotational G.P. equation”, with rotating asymmetric potential, by spectral methods (Caliari, Zuccher, . . .)

(In the literature huge amount of numerical simulations leading to formation of vortices, but with “rotating boundary conditions”. Stationary arrays need dissipative devices)

Conclusions

Stochastic Quantization of N identical interacting Bosons by Lagrangian Variational Principle

• Ancillary stochastic description : general one-particle Bose dynamics. Derivation of G.P. eq. from the N-body problem and new analysis of the G.P. model.

• Possible rotational dynamics with dissipation and concentration of vorticity in the zeroes of the density