Inhomogeneities and temperature effects in Bose-Einstein condensates

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New Challenges in Mathematical Modelling
and Numerical Simulation of Superfluids
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Bose-Einstein condensation

Dilute gaz of Bosons, cooled to temperature close to absolute zero
$\rightsquigarrow$ macroscopic part of atoms in lowest quantum state

Predictions : S.N. Bose, 1924 (photons), A. Einstein, 1925 (atoms)

First experiments : 1995 : Cornell, Wieman, ^{87}Rb ; Ketterle, ^{23}Na

Wave function :

$$\tilde{\psi}(t, x_1, \cdots, x_N) = \Pi_{j=1}^{N} \psi(t, x_j)$$

then if only two-body interactions and N large, ψ satisfies the Gross-Pitaevskii equation :

$$i\hbar\partial_t\psi(t,x) = -\frac{\hbar}{2m}\Delta\psi + V(x)\psi + \frac{4\pi\hbar^2 a}{m}|\psi|^2\psi$$

V : confining potential

Aim : take into account stochastic aspects (fluctuations) in the dynamics

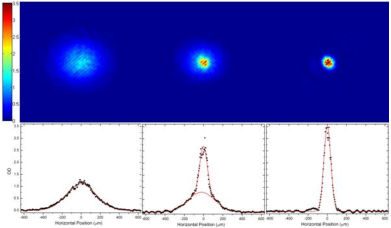


FIGURE: False-color plots of ^{87}Rb atoms undergoing Bose-Einstein condensation in a combined magnetic and optical potential. By Danny McCarron, Daniel Jenkin, Hung Wen Cho and Simon Cornish.

Mainly two sources of fluctuations in physics literature :

- Fluctuations of the laser parameters (optical confinement)
- Non zero temperature (e.g. Weiler et al. Nature, 2008)

Random variations of the confining potential

Random variations of the confining potential :

Gross-Pitaevskii with stochastic potential :

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(t,\mathbf{r})\psi + g|\psi|^2\psi$$

Abdullaev, Baizakov, Konotop, Nonlinearity and Disorder, 2001,
Garnier, Abdullaev, Baizakov, Phys. Rev. A, 2004

V : confining potential (laser) harmonic, with random fluctuations in time

$$V(t,\mathbf{r}) = \frac{m\omega_0}{2}|\mathbf{r}|^2(1+\xi(t))$$

with $\omega_0^2 = \alpha I/(2m\ell_0^2)$, depends on laser intensity I

$\xi(t)$: fluctuations of parameters

Assumptions : $\xi(t)$ is δ-correlated and with zero mean : $\langle\xi(t)\rangle = 0$, $\langle\xi(t)\xi(t')\rangle = \sigma_0^2\delta(t-t')$

Remark : The "white noise" assumption may be relaxed : $\xi(t)$ stationary, $\langle \xi(t)\xi(t') \rangle = c(t - t')$, with c sufficiently decaying ; Savard, O'Hara, Thomas, Phys. Rev. A, 1997

However, white noise is natural under some scaling.

Model studied in the attractive case ($g < 0$) by :

- Moments methods : (Abdullaev, Baizakov, Konotop, 2001) $\rightsquigarrow$ qualitative considerations about collapse
- "Variational" methods (Gaussian profile + asymptotic analysis) and simulations (Garnier, Abdullaev, Baizakov, 2004) $\rightsquigarrow$ density of collapse time τ and mean of τ as a function of the power P (or the number of atoms N)

Numerical simulations from Garnier et al. 2004 :

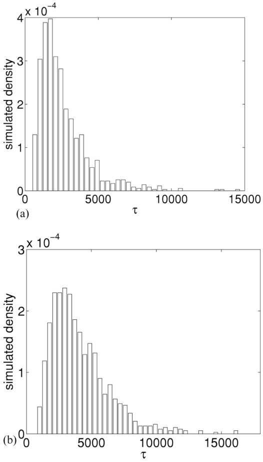


FIG. 3. Histograms of the collapse time obtained from series of 1000 simulations. (a) P=0.1; (b) P=0.05.

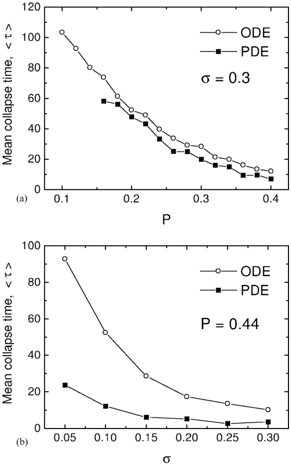


FIG. 7. Mean collapse time is calculated from stochastic PDE simulations (solid squares) and compared with the corresponding stochastic ODE simulations (open circles). Each mean is computed by averaging over a series of 100 simulations. (a) Mean collapse time as a function of P for a white noise strength σ=0.3. (b) Mean collapse time as a function of σ for a nonlinear parameter P =0.44 close to the critical value P_c=0.459.

Mathematical results :

AdB, R. Fukuizumi, Nonlinearity 2012

$$id\psi + \frac{1}{2}(\Delta\psi - V(x)\psi - 2g|\psi|^2\psi)dt = \frac{\sigma_0}{2}V(x)\psi \circ dW$$

Gauge transformation : $\psi(t,x) = e^{-i\frac{|x|^2}{2}(\sigma_0 W(t)+t)}u(t,x)$ leads to

$$i\partial_t u = -\frac{1}{2}(\nabla u - ix(\sigma_0 W(t) + t))^2 u + g|u|^2 u$$

Schrödinger equation with (random) magnetic field

- $d = 1$ and ψ_0 square integrable (in x) : existence of a unique adapted global square integrable solution ψ ; conservation of the number of atoms ; preservation of regularity.
- $\psi_0 \in \Sigma$, and $d = 2$ or 3 : existence of a stopping time T^* and of a unique adapted solution ψ a.s. in $C([0, T^*); \Sigma)$.

Global existence, or not :

Energy :

$$H(\psi) = \frac{1}{4}\int_{\mathbf{R}^d} (|\nabla\psi|^2 + V(x)|\psi|^2 + g|\psi|^4)dx$$

For the stochastic evolution : if $\tau < T^*$ a.s.

$$\begin{aligned} H(\psi(\tau)) &= H(\psi_0) + \sigma_0^2 \int_0^\tau \int_{\mathbf{R}^d} |x|^2 |\psi(x)|^2 dx dt \\ &\quad - \sigma_0 \mathrm{Im} \int_0^\tau \int_{\mathbf{R}^d} x \cdot \nabla\psi(x)\bar{\psi}(x) dx dW, \quad \text{a.s;} \end{aligned}$$

and

$$|x\psi(\tau)|_{L^2}^2 = |x\psi_0|_{L^2}^2 + \mathrm{Im} \int_0^\tau \int_{\mathbf{R}^d} x\bar{\psi} \cdot \nabla\psi dx dt,$$

- If $g > 0$, the solution is global i.e. $T^* = +\infty$, a.s.
- If $g < 0$, blow up occurs

Diffusion approximation :

Let $d = 1$ and $g \in \mathbf{R}$. Let $m(t)$ be e.g. stationary, ergodic, with some mixing conditions.

Then, for any $\varepsilon > 0$ and $\psi_0 \in L^2(\mathbf{R})$ there exists a unique global solution ϕ_ε, with continuous paths in $L^2(\mathbf{R})$, of

$$i\partial_t \phi = \frac{1}{2}(-\Delta\phi + V(x)\phi) + g|\phi|^2\phi + \frac{1}{2\varepsilon} m\Big(\frac{t}{\varepsilon^2}\Big) V(x)\phi,$$

with $\phi(0) = \psi_0$.

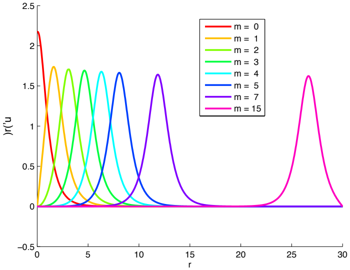
Moreover the process ϕ_ε converges in law in $C([0,T], L^2)$ as ε tends to zero, to the solution ψ of

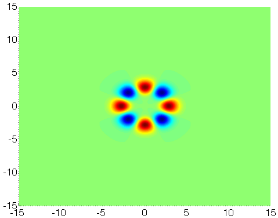
$$id\psi = \frac{1}{2}(-\Delta\psi + V(x)\psi)dt + g|\psi|^2\psi dt + \frac{\sigma_0}{2} V(x)\psi \circ dW,$$

with $\psi(0) = \psi_0$.

Vortices of the deterministic GP equation

Assume $g = 1$ (repulsive condensate), $V(x) = |x|^2$, $\sigma_0 = 0$, and $d = 2$





Centered ***m*-vortex :** $x = re^{i\theta} \in \mathbf{R}^2$, and $\mu > \lambda_m = 2m + 2$; then $\psi_{\mu,m}$ nonnegative solution of (GP) with

$$\psi_{\mu,m}(t, x) = e^{i\mu t} e^{im\theta} \varphi_{\mu,m}(r)$$

Dynamics of the stochastic equation

Consider the stochastic equation with small noise :

$$id\psi + \frac{1}{2}(\Delta\psi - |x|^2\psi)dt - |\psi|^2\psi dt = \frac{\varepsilon}{2}|x|^2\psi \circ dW$$

with $\psi(0,x) = \psi_{\mu,m}(x) = e^{im\theta}\varphi_{\mu,m}(r)$.

Question : how does the solution behaves asymptotically for small ε, and for t not "too large" ?

AdB, Fukuizumi, Poncet 2015

- The m-equivariance of the solution is preserved by the noise
- We may write the solution of the stochastic equation as

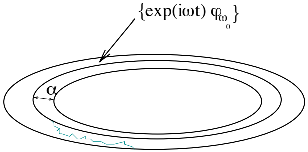
$$\psi^\varepsilon(t,x) = e^{i\xi^\varepsilon(t)}e^{im\theta}[\varphi_{\mu,m}(r) + v^\varepsilon(t,r)]$$

as long as $\|v^\varepsilon(t)\|_\Sigma \leq \alpha$, for some $\alpha > 0$, sufficiently small.

Estimate on the exit time

Question : Can we estimate the time τ_α^ε, with

$$\tau_\alpha^\varepsilon = \inf\{t > 0, \|v^\varepsilon\|_\Sigma \geq \alpha\}?$$



Result : there is a $C(\alpha, \mu) > 0$, such that for all $T > 0$, and all $\varepsilon \leq \varepsilon_0$,

$$\mathbf{P}(\tau_\alpha^\varepsilon \leq T) \leq e^{-C/\varepsilon^2 T}$$

Remark : if τ is the exit time of the solution, then $\mathbf{E}(\tau) < +\infty$.

Central limit Theorem

Let $v^\varepsilon(t,x) = \varepsilon\eta^\varepsilon(t,x)$. Then, for any $T > 0$, the process $(\eta^\varepsilon(t))_{t\in[0,T\wedge\tau_\alpha^\varepsilon]}$ converges in probability, as ε goes to zero, to a process η satisfying

$$d\eta = J\mathcal{L}_{\mu,m}\eta dt - (I - P_{\mu,m}) \begin{pmatrix} 0 \\ |x|^2\varphi_{\mu,m} \end{pmatrix} dW,$$

with $\eta(0) = 0$, where $P_{\mu,m}$ is the spectral projection onto the generalized null space of $J\mathcal{L}_{\mu,m}$. The convergence holds in $C([0,\tau_\alpha^\varepsilon \wedge T], L^2)$.

At first order in ε, the equations for the modulation parameter is given by

$$d\xi^\varepsilon(t) = \mu dt - \varepsilon \frac{(|x|^2\varphi_{\mu,m}, \partial_\mu\varphi_{\mu,m})}{(\varphi_{\mu,m}, \partial_\mu\varphi_{\mu,m})} dW + o(\varepsilon)$$

Numerical results

$$id\psi + (\Delta\psi - |x|^2\psi)dt = |\psi|^2\psi dt + \varepsilon|x|^2\psi \circ dW$$

Use equivariance symmetry : $\psi(t,x) = e^{-im\theta} r^m f(t,r)$

Numerical scheme :

- Crank-Nicolson (mid-point) for the linear terms (derived from Bao-Du, 2004)
- Relaxation for the nonlinear term (Besse, 1998) :

$$\frac{1}{2}(Q_j^{n+1/2} + Q_j^{n-1/2}) = |f_j^n|^{2\sigma}$$

- Mid-point discretization of the noise (Stratonovich) :

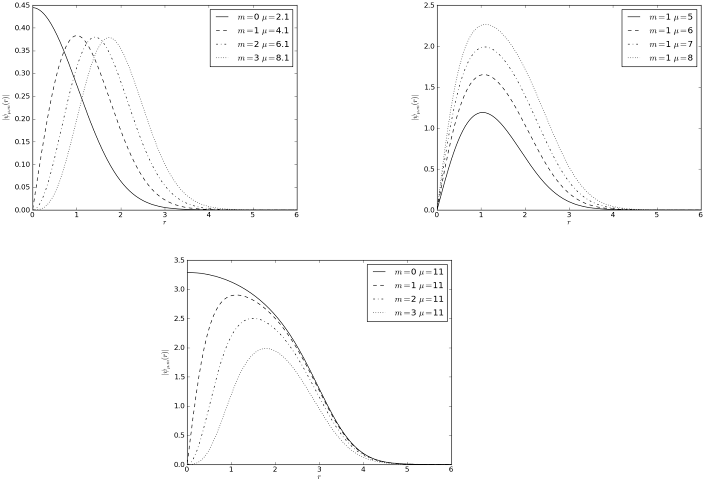
$$\varepsilon r_j^{m+2} f(r_j) \circ dW \sim \varepsilon r_j^{m+2} f_j^{n+1/2} \sqrt{\delta t}\chi_n$$

  where (χ_n) is a family of independent $\mathcal{N}(0,1)$
- Dirichlet boundary conditions

Initial data :

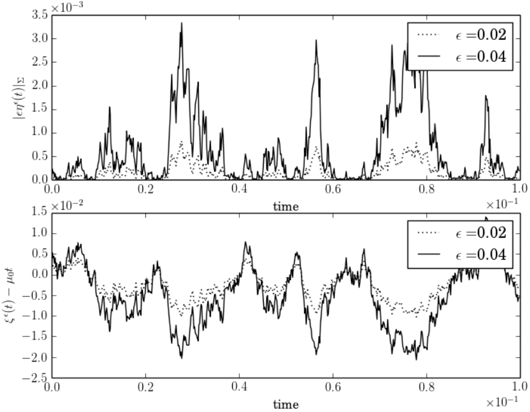
Profiles computed with shooting methods + 4^{th} order RK

$$\psi(0,x) = e^{-im\theta} r^m f_{\mu,m}(r)$$



Modulation parameter and remainder :

$$\xi^\varepsilon(t) = -\arg\left(\int_0^\infty \psi^\varepsilon(t)\phi_{\mu_0,m} r\,dr\right), \quad \varepsilon\eta^\varepsilon = \psi^\varepsilon e^{i\xi^\varepsilon(t)} - \phi_{\mu_0,m}$$



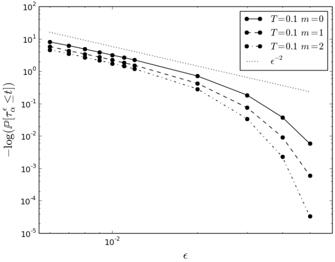
Evolution of $\xi^\varepsilon(t) - \mu_0 t$ and $|\varepsilon\xi^\varepsilon(t)|_\Sigma$ for two different values of ε for the same realization of the BM ($m = 2$, $\mu_0 = 2m + 3$)

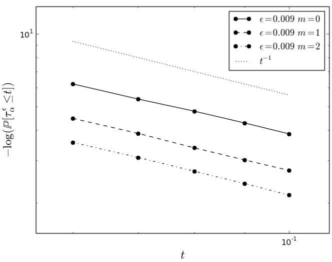
Estimate on the exit probabilities (Monte Carlo method) :

$$\mathbb{P}(\tau_\alpha^\varepsilon \leq t) \sim \widehat{Y}^{\alpha,\varepsilon}_{\Delta r,\Delta t,N} = \frac{1}{N}\sum_{k=1}^{N} Y^{\alpha,\varepsilon,(k)}_{\Delta r,\Delta t}$$

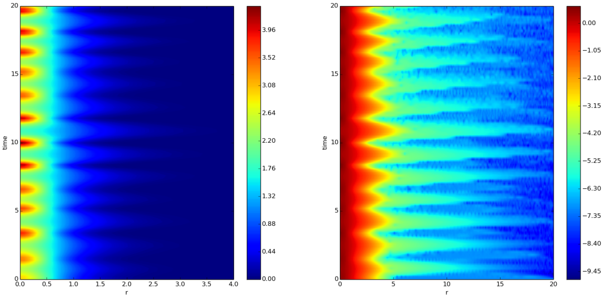
with

$$Y^{\alpha,\varepsilon,(k)}_{\Delta r,\Delta t} = \mathbf{1}_{\left\{|(\varepsilon\eta^\varepsilon_{\Delta r,\Delta t})^{(k)}|_{L^\infty((0,T);\Sigma)} > \alpha\right\}}$$



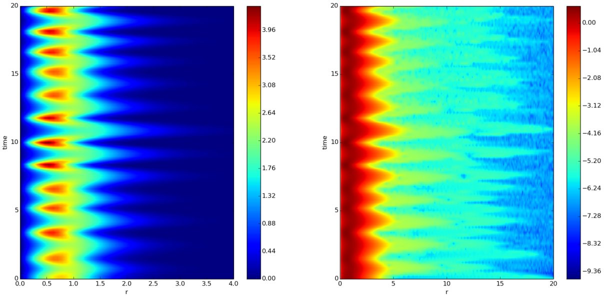


Trajectories of solutions : one realization of the noise



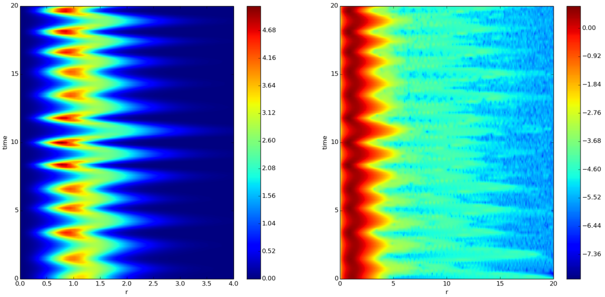
One realization of the solution for $\varepsilon = 0.1$, $m = 0$

Trajectories of solutions : one realization of the noise



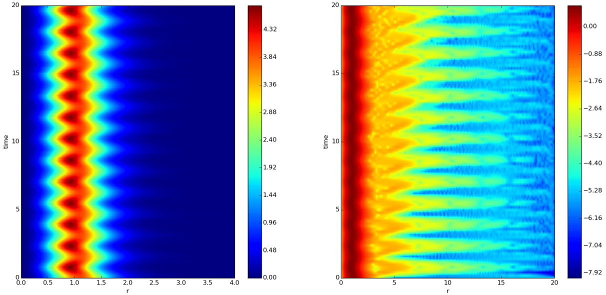
One realization of the solution for $\varepsilon = 0.1, m = 1$

Trajectories of solutions : one realization of the noise



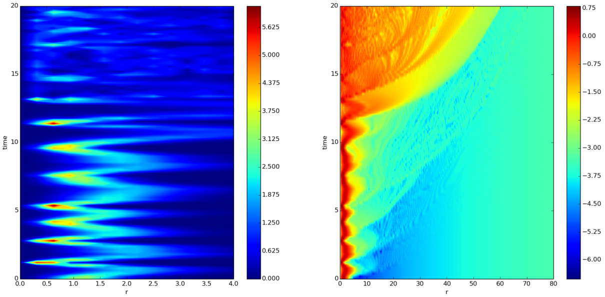
One realization of the solution for $\varepsilon = 0.1, m = 2$

Trajectories of solutions : deterministic solution with perturbed initial data



One realization of the solution for $\varepsilon = 0, m = 2$

Trajectories of solutions : one realization of the noise



One realization of the solution for $\varepsilon = 0.5, m = 2$

Finite temperature model : the projected stochastic GPE

Evaporative cooling

Weiler, Neely, Scherer, Bradley, Davis ; Nature, 2008

Experiment :

- ^{87}Rb atoms in magnetic trap
- evaporative cooling $\rightsquigarrow$ close to critical point
- relaxation of trap frequencies $\rightsquigarrow$ phase transition

Simulations :

- Use of stochastic projected GP equation
- Start with temperature $T_i = 45nK > T_c$, chemical potential μ_i $\rightsquigarrow$ reach equilibrium state
- Change temperature to $T_f = 34nK$, and larger μ_f $\rightsquigarrow$ spontaneous vortex formation

Stochastic projected GPE

ψ : wave function for the condensed atoms

$$L_{GP} = -\frac{\hbar^2}{2m}\Delta + V(x) + g|\psi(t,x)|^2$$

where m is the atomic mass, $g = \frac{4\pi\hbar^2 a}{m}$ and a the (positive) s-wave scattering length. Then

$$d\psi = \mathcal{P}_c\big[-\frac{i}{\hbar}L_{GP}\psi dt + \frac{\gamma}{k_B T}(\mu - L_{GP})\psi dt + dW_\gamma(t,x)\big]$$

where μ is the chemical potential, and $\mathcal{P}_c$ is a cut-off (low energy modes)

$$\langle dW_\gamma^*(t,x) dW_\gamma(t',x')\rangle = 2\gamma\delta(t-t')\delta(x-x')dt$$

Additional terms : interaction thermal cloud–condensate

Equilibrium state :

Energy : ψ_c projected wave function (d_c-dimensional)

$$H(\psi_c) = \frac{\hbar^2}{2m}|\nabla\psi_c|^2_{L^2} + |V(x)\psi_c|^2_{L^2} - \mu|\psi_c|^2_{L^2} + g|\psi_c|^4_{L^4}$$

with

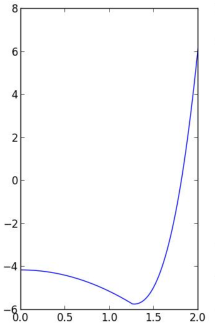
$$V(x) = \frac{m}{2}\omega^2 x^2.$$

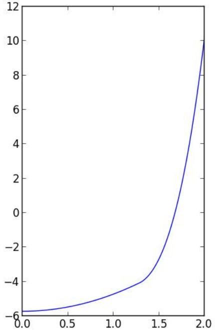
Ground state (T=0) : Symmetry breaking at $\mu = \hbar\omega$

Gibbs measure ($T > 0$) :

$$\pi_T(d\psi_c) = \alpha_c \exp\Big(-\frac{H(\psi_c)}{k_B T}\Big) d\psi_c$$

Convergence to equilibrium with geometric rate Roberts, Tweedie, 1996





Sections of coefficients of H

Numerical experiment

- Initial state distributed according to π_{T_i} with T_i above T_c and μ_i small ; then dynamical simulations with T_f below T_c and larger μ_f
- plot of isovalues of $|\psi_c(t,x)|^2$
- Euler + spectral + Hermite transform ; 35 to 40 modes

Infinite dimensional model

$$d\psi = (i+\gamma)\Big[\Delta\psi - x^2\psi + \mu\psi - |\psi|^2\psi\Big]dt + \sqrt{\gamma}dW$$

$\psi(t,x)$ is the wave function ; $\gamma > 0$; W is a cylindrical Wiener process : $(h_n)_{n\in\mathbf{N}}$ real valued c.o.s. of $L^2(\mathbf{R})$ s.t.

$$(-\Delta + x^2)h_n = \lambda_n^2 h_n, \quad \lambda_n^2 = 2n+1, \quad n \in \mathbf{N}$$

then W may be written as

$$W(t,x) = \sum_{k\in\mathbf{N}} \beta_k(t)h_k(x)$$

with $(\beta_k)_k$ sequence of independent complex valued BM

- $0 \le \mu < \lambda_1 = 1$ (take $\mu = 0$ for simplicity)
- Only dimension one in x is allowed

Invariant measure : Burq, Thomann, Tzvetkov, 2013

Let

$$\phi(x,\omega) = \sum_{n=0}^{+\infty} \frac{\sqrt{2}}{\lambda_n} g_n(\omega) h_n(x),$$

with $(g_n)_{n\in\mathbf{N}}$ independent $\mathbf{C}$-valued $\mathcal{N}(0,1) \rightsquigarrow$ law of ϕ is a Gaussian measure ρ with $\rho(A) = \mathbf{P}(\phi(\cdot,\omega) \in A)$. Then

$$\mathbf{P}(\phi \in L^p(\mathbf{R})) = \rho(L^p(\mathbf{R})) = \begin{cases} 0 \text{ if } p < 4 \\ 1 \text{ if } p \geq 4 \end{cases}$$

The Gibbs measure π is then defined on $L^4(\mathbf{R})$:

$$\pi(du) = \Gamma^{-1} \exp\Big(- \frac{1}{4} |u|_{L^4}^4 \Big) \rho(du)$$

and is abs. continuous with respect to ρ.

Note : Solutions are locally in time well defined in $L^4(\mathbf{R})$.

Global (a.s.) well posedness and convergence result :

dB, Debussche, Fukuizumi, 2016

- There exists a measurable set $\mathcal{O} \in L^4(\mathbf{R})$ s.t. $\pi(\mathcal{O}) = 1$, and for any $\psi_0 \in \mathcal{O}$, there is a unique solution ψ which is a.s. continuous with values in $L^4(\mathbf{R})$).
- For any F continuous and bounded in $L^4(\mathbf{R})$, define $U(t, \psi_0) = \mathbf{E}(F(\psi(t, \psi_0)))$ with ψ sol. of (CGL) with initial state ψ_0 ; then $U(t, \cdot)$ converges exponentially to

$$\bar{F} = \int_{L^4(\mathbf{R})} F(u)\pi(du)$$

in $L^2(L^4, d\pi)$ that is for some positive α,

$$\int_{L^4(\mathbf{R})} |U(t, u) - \bar{F}|^2 \pi(du) \leq Ce^{-\alpha t}$$

Conclusion and open problems

- Improve numerical methods for finite dimensional simulations (MC and statistics) ; in particular simulations of π, phase transition,...
- Finite dimensional dynamics : slow-fast dynamics ?
- Infinite dimensional dynamics : what about chemical potential μ larger than one ?
- More realistic space dimensions ($x \in \mathbf{R}^d$, $d = 2$ or 3) $\rightsquigarrow$ needs refined methods

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