Aspects of Open Quantum Systems and the Hartree Equation

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Physics, Analysis, Numerics

Time-*In*dependent Hartree Equation

1. One motivation from physics: Bose-Einstein condensation (BEC) in trapped gases
2. Symmetry breaking regime at finite coupling
3. Numerical approach to symmetry breaking

Time-Dependent Hartree Equation

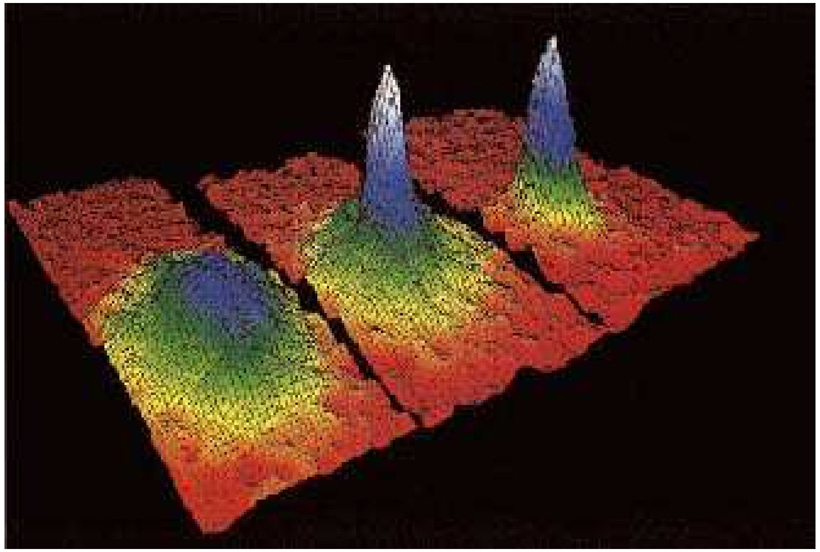
1. Weak coupling limit of bosonic system and Newtonian limit of Hartree equation
2. Analysis of numerical scheme
3. Numerical approach to long-time behavior

Time In-Dependent Hartree Equation

1. Motivation from physics: Bose-Einstein condensation (BEC) in trapped gases

• Series of seminal experiments 1995 on rubidium Rb_{87}, sodium Na_{23}, lithium Li_7: sharp peak in velocity distribution !
[Anderson et al. 95],[Davis et al. 95],[Bradley et al. 95]

• Rigorous description of BEC for very dilute gases based on analysis of weak coupling limit of large bosonic systems
[Hepp 74], [Lieb,Seiringer,Yngvason 99], [Fröhlich,Tsai,Yau 00]
$\Rightarrow$ Hartree theory !



Images of the velocity distribution by Anderson *et al.* (1995), taken by means of the expansion method. The left frame corresponds to a gas at a temperature just above condensation; the center frame, just after the appearance of the condensate; the right frame, after further evaporation leaves a sample of nearly pure condensate. The field of view is $200\mu m \times 270\mu m$, and corresponds to the distance the atoms have moved in about $1/20s$. The color corresponds to the number of atoms at each velocity, with red being the fewest and white being the most.

• Condensate wave function ψ is solution of Hartree eigenvalue problem

$$\begin{aligned} \left(-\frac{\hbar^2}{2m}\Delta + v + \gamma V * |\psi|^2\right)\psi &= \epsilon\psi \\ \|\psi\|_2^2 &= N \end{aligned}$$

m: mass of boson
v: external potential: the trap
γ: Hartree coupling
V: two-body potential of boson-boson interaction
N: number of bosons in the system

• BEC-scenario: mean interboson distance $d \gg$ range of V, V repulsive $\Rightarrow V = \delta$: [Gross-Pitaevskii] (GP)

• Regime of very dilute and cold gas:
[Low energy scattering theory]$\Rightarrow$ details of V irrelevant, boson-boson interaction characterized by scattering length a alone:

$$\gamma \propto a$$

• Rescaling to dimensionless variables:
energy unit: ground state energy $\hbar\omega_v$ of linear operator $-\frac{\hbar^2}{2m}\Delta + v$
length unit: $\Delta_v := (\frac{\hbar}{m\omega_v})^{1/2}$

$$\begin{aligned} \left(-\frac{1}{2}\Delta + v + g|\psi|^2\right)\psi &= E\psi \\ \|\psi\|_2^2 &= 1 \end{aligned}$$

with

$$g \propto N\frac{a}{\Delta_v}$$

• Mainly interested in attractive interatomic forces:
Li_7 has $a = -1.45 \cdot 10^{-9} m$!
[Abraham et al. 95]

• Bosons with *attractive* interactions may collapse into clusters of very high density:
Propose reintroduction of less coarse-grained resolution of boson-boson interaction:

$$\begin{aligned}\left(-\frac{1}{2}\Delta + v + gV * |\psi|^2\right)\psi &= E\psi \\ \|\psi\|_2^2 &= 1\end{aligned}$$

where V is of positive type and $g < 0$
(short range attractive)

- Experiment: Li_7-gas undergoes collective collapse, if $N > N_c$
- Minimizer Φ^{GP} of GP functional (p=3)

$$\mathcal{H}_g^{GP}[\bar{\psi}, \psi] := \frac{1}{2}\|\nabla\psi\|_2^2 + g\|\psi\|_{p+1}^{p+1}$$

For $g < 0$:

$$\mathcal{H}_g^{GP}[\bar{\psi}_\lambda, \psi_\lambda] = \lambda^2 \,\|\nabla\psi\|_2^2 + g\lambda^{d/2(p-1)}\,\|\psi\|_{p+1}^{p+1}$$

for $\psi_\lambda(x) := \lambda^{d/2}\psi(\lambda x)$, $x \in \mathbb{R}^d$, $\lambda \in \mathbb{R}^+$:

$$p < 1 + \frac{4}{d}$$

$\Rightarrow$ for $p = 3$, $d \geq 2$: bottom drops out !

$\Rightarrow$ GP theory breaks down at the collapse point of the condensate if $g < 0$!

• Unlike GP, minimizers Φ of Hartree functional

$$\mathcal{H}_g[\bar{\psi}, \psi] := \frac{1}{2}\|\nabla\psi\|_2^2 + (\psi, v\psi)_2 + \frac{1}{2}g(\psi, V * |\psi|^2\psi)_2$$

exist for $g < 0$ if $g_c < |g|$ for some *positive* g_c, even for $v = 0$!
Length scale Δ_H set by Hartree minimizer Φ in trap v of same order as Δ_v

$$\Delta_H \approx \Delta_v, \quad \text{for } |g| < g_c, \quad g < 0$$

whereas Φ still exists, and

$$\Delta_H \ll \Delta_v, \quad \text{for } g_c < |g|, \quad g < 0$$

and Δ_H *independent* of trap v.

• *neglect*:
- Inelastic collisions and recombination close to collapse, as well as interactions of electrons and nuclei with em field
- Short range *repulsive* interactions between bosons
$\Rightarrow$ two-body forces *purely attractive*
$\Rightarrow$ system *not* thermodynamically stable ($g < 0$ fixed, ground state energy scales like $-O(N^2)$ as $N \to \infty$)

• In *mean-field regime*, $N \to \infty$ and κN constant, a dilute gas of bosons well discribed by Hartree theory !
[Hepp 74],[Fröhlich,Tsai,Yau 00]

• Hartree theory meaningful at collpase point and *beyond*
$\Rightarrow$ serves to describe *qualitatively* features of system close to collapse!
None of these processes can be described by GP !

2. Symmetry breaking regime at finite coupling

• Symmetry properties minimizer Φ of Hartree functional for large negative coupling g,

$$\mathcal{H}_g[\bar{\psi}, \psi] = \frac{1}{2}\|\nabla \psi\|_2^2 + (\psi, v\psi)_2 + \frac{1}{2} g(\psi, V * |\psi|^2 \psi)_2$$

• Existence of g_c: variational methods

[Lieb 77]

• Size of g_c: [Birman-Schwinger]$\Rightarrow$ $g_c > 0$ for V short range, $d \geq 3$

E.g. [Cwikel-Lieb-Rozenblujm bound]
Let $d \geq 3$ and let $N(W)$ denote the number of bound states of $-\Delta + W$ on $L^2(\mathbb{R}^d)$. Then, there exists a constant $c_d \in \mathbb{R}^+$ such that

$$N(W) \leq c_d \int_{\mathbb{R}^d} d^d x \, |W_-(x)|^{d/2}.$$

$g_c = 0$ for V long range, $d \geq 3$, and for $d = 1, 2$!

• Non-uniqueness of Hartree minimizer Φ for sufficiently large coupling [Aschbacher,Fröhlich,Graf,Schnee,Troyer 00]

Theorem 1 (Symmetry breaking)
Let $V = |x|^{-1}$ in $\mathbb{R}^d$, $d \geq 2$, $v \in C_b(\mathbb{R}^d)$.
If, for some G in the group of Euclidian motions $E(d)$, any v-minimizing sequence $x_k \in \mathbb{R}^d$

$$\lim_{k\to\infty} v(x_k) = \inf_{x\in\mathbb{R}^d} v(x) \quad \text{fulfills} \quad \liminf_{k\to\infty} |Gx_k - x_k| > 0 \ (S),$$

then, for sufficiently large N, any minimizer Φ of the Hartree functional satisfies

$$|\Phi \circ G|^2 \neq |\Phi|^2.$$

In particular: If v has symmetry $G \in E(d)$
$\Rightarrow$*minimizer breaks symmetry of v for sufficiently large coupling* !

- Examples:

(1) Potential well at origin

(2) Potential well *not* at origin

(3) Mexican hat at origin

(4) Double well symmetric w.r.t origin

- Propose experiments for symmetry breaking with magnetic traps !

Remark

Theorem 1 also holds true for $V \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ is of *positive type*

- Sketch for Proof of Theorem 1

"Free" functional:

$$\mathcal{E}_g[\bar{\psi},\psi] := \frac{1}{2}\|\nabla\psi\|_2^2 + \frac{1}{2}g(\psi, V * |\psi|^2\psi)_2$$
$$E[N,g] := \inf\{\mathcal{E}_g[\bar{\psi},\psi] \,|\, \psi \in W^{1,2}(\mathbb{R}^d), \|\psi\|_2^2 = N\}$$

Step 1: Concentration

Given $\delta > 0$, there is $\eta > 0$ such that, for N large enough, any wave function ψ with $\|\psi\|_2^2 = N, \mathcal{E}_{-1}[\bar{\psi},\psi] \leq (1-\eta)E[N,-1]$ (η-approximate minimizer) fulfills, for some $y \in \mathbb{R}^d$,

$$\int_{B(y,\delta)} d^dx\, |\psi(x)|^2 \geq (1-\delta)\,N.$$

Step 2: Localization

Let $v \in C_b(\mathbb{R}^d)$ and $\epsilon, \delta > 0$ be fixed.
Then, for N large enough, any minimizer Φ of

$$\begin{aligned} \mathcal{H}_{-1}[\bar{\psi}, \psi] &= \mathcal{E}_{-1}[\bar{\psi}, \psi] + (\psi, v\psi)_2 \\ \|\psi\|_2^2 &= N \end{aligned}$$

satisfies

$$(i) \qquad \int_{B(y,\delta)} d^d x \, |\Phi(x)|^2 \geq (1-\delta) N$$

$$(ii) \qquad \inf_{x \in B(y,\delta)} v(x) \leq \inf_{x \in \mathbb{R}^d} v(x) + \epsilon$$

Step 3: Theorem 1

Reductio ad absurdum
$\square$

• Uniqueness of the Hartree minimizer Φ for sufficiently small coupling [Aschbacher,Fröhlich,Graf,Schnee,Troyer 00]

Theorem 2 (Positive critical coupling in $d \geq 1$)
Let $V \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ be real-valued, $v \in C_b(\mathbb{R}^d)$, $d \in \mathbb{N}$, such that

$$H_0 := -\frac{1}{2}\Delta + v$$

has an isolated ground state.
Then, for sufficiently small coupling $|g|$, there exists a unique nonlinear ground state ψ, $\|\psi\|_2 = 1$, of

$$H_g^{(\psi)} := H_0 + gV * |\psi|^2. \tag{1}$$

This implies that, in any dimension $d \geq 1$, symmetry breaking occurs above a strictly positive critical coupling g_* only, $|g| > g_*$.

• Sketch for Proof of Theorem 2

Step 1: Linear part and analytic perturbation theory

[Weyl]$\Rightarrow$ $\sigma_{ess}(H_0) = [0, \infty[$

By assumption: $E_0 := \inf \sigma\,(H_0) \in \sigma_p(H_0)$ isolated in $\sigma(H_0)$

$\Rightarrow$ $E_0 \in \sigma_d(H_0)$, i.e. $\dim \operatorname{Ran} P^{H_0}(E_0) < \infty$

e^{-tH_0} positivity improving for all $t > 0$

[Perron-Frobenius]$\Rightarrow$ E_0 is *nondegenerate* with strictly positive eigenfunction ψ_0

For $|g|$ sufficiently small: $H_g^{(\psi)}$ is *analytic family in the sense of Kato*

[Kato-Rellich]$\Rightarrow$ $\exists!$ isolated nondegenerate eigenvalue $E_g^{(\psi)}$ of $H_g^{(\psi)}$ near E_0 and $E_g^{(\psi)}$ is analytic in g

Step 2: Nonlinear part and contraction mapping principle

$$\begin{aligned} \mathcal{S} &:= \{\psi \in L^2(\mathbb{R}^d) \,|\, \|\psi\|_2 = 1\} \\ P_g : \mathcal{S} &\to \mathcal{S} \\ \psi &\mapsto P_g[\psi] := \frac{1}{c_g^{(\psi)}} \frac{1}{2\pi i} \oint_{\mathcal{C}_\varepsilon} dz \, [H_g^{(\psi)} - z]^{-1} \psi_0 \end{aligned}$$

with $\mathcal{C}_\varepsilon := \{z \in \mathbb{C} \,|\, |E_0 - z| = \varepsilon\}$ and normalization $c_g^{(\psi)}$

[Banach]$\Rightarrow$ *Fixed point* of P_g: unique nonlinear ground state !

$\square$

3. Numerical approach to symmetry breaking

HARTREE-package:

- Numerics: dyadic mesh, bilinear Finite Elements
- Implementation: BLITZ++

[Veldhuizen 98]

Hartree eigenvalue problem:

$$h^{(n)^{-2}} \left[\frac{1}{2} A^{(N)} + v^{(N)} + g\, W^{(N)}[\psi^{(N)}] \right] \psi^{(N)} = E^{(N)}\, \psi^{(N)}$$

- MFFT Mixed Radix Fast Fourier Transform

[Petersen 84]

Fast evaluation of Hartree energy:
O(N log(N)) (MFFT), O(N) (Multigrid) in nonconforming approximation:

$$\tilde{W}^{(N)}\left[\psi^{(N)}\right]_{(i,j),(k,l)} = \delta_{ik}\delta_{jl}\,{h^{(n)}}^4 \sum_{i',j'=0}^{n-1} \left|\psi^{(N)}_{i'j'}\right|^2 \frac{e^{-\alpha h^{(n)}\sqrt{(i-i')^2+(j-j')^2}}}{h^{(n)}\sqrt{(i-i')^2+(j-j')^2+\delta}}$$

- Interlocking iterative procedures:

$$\Psi^{(N),p,q} \overset{\text{PM}}{\underset{q\to\infty}{\longrightarrow}} \Psi^{(N),p} \overset{\text{PC}}{\underset{p\to\infty}{\longrightarrow}} \Psi^{(N)}$$

for $\Psi^{(N),p,q} := (E^{(N),p,q}, \Phi^{(N),p,q})$
[Picard] (PC)$\Rightarrow$ p: solutions of sequence of *linearized* problems

$${h^{(n)}}^{-2}\left[\frac{1}{2}A^{(N)} + v^{(N)} + g\,\tilde{W}^{(N)}[\Phi^{(N),p}]\right]\Phi^{(N),p+1} = E^{(N),p+1}\,\Phi^{(N),p+1}$$

[Power Method] (PM)$\Rightarrow$ Underlying linear problem
([Lanczos]: Krylov subspace method
[Lanczos 50],[Cullum,Willoughby 85])

PM: Linear real symmetric operator H on a complex finite N-dimensional Hilbert space $\mathcal{H}$, $\psi^0 = \sum_{k=0}^{N-1} c_k\phi_k$:

$$\psi^j := \frac{H^j\psi^0}{\|H^j\psi^0\|} = \sum_{k=0}^{N-1} \frac{c_k\left(\frac{E_k}{E_*}\right)^j}{\left(|c_*|^2 + \sum_{l=0,l\neq *}^{N-1} |c_l|^2 \left(\frac{E_l}{E_*}\right)^{2j}\right)^{1/2}} \phi_k \stackrel{j\to\infty}{\longrightarrow} \frac{c_*}{|c_*|}\phi_*$$

with

$$|E_*| = \max\left\{|E_k| \mid E_k \in \sigma\left(H|_{span\{\phi_k \,|\, c_k\neq 0\}}\right)\right\}$$

- Stopping criterion:

$$\left\| \frac{H_s \psi^j - \left(\psi^j, H_s \psi^j\right) \psi^j}{\left(\psi^j, (H_s - s\mathbb{I}) \psi^j\right)} \right\| \leq \epsilon_{rel}$$

s: energy shift

- Convergence speed:

$$q_{\tilde{k}}(s) := \left(\frac{E_{\tilde{k}} + s}{E_* + s} \right)^j$$

$\tilde{k} \in \{0, ..., N-1\}$: quotient closest to 1
Level spacing:

$$\Delta E = O(g^2)$$

$\Rightarrow$ Estimate on j !

- Simulation 1 Double well potential

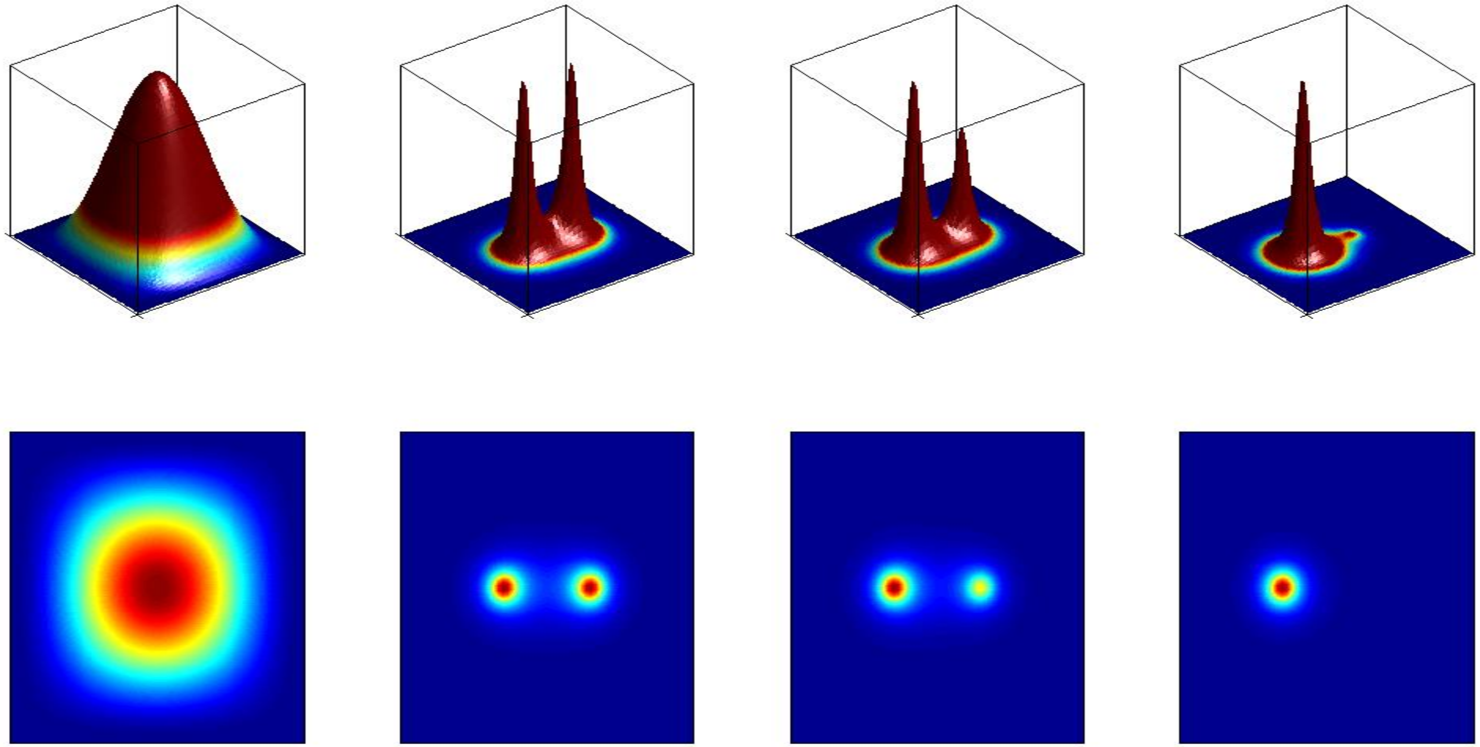
- Parameters (for the figure):

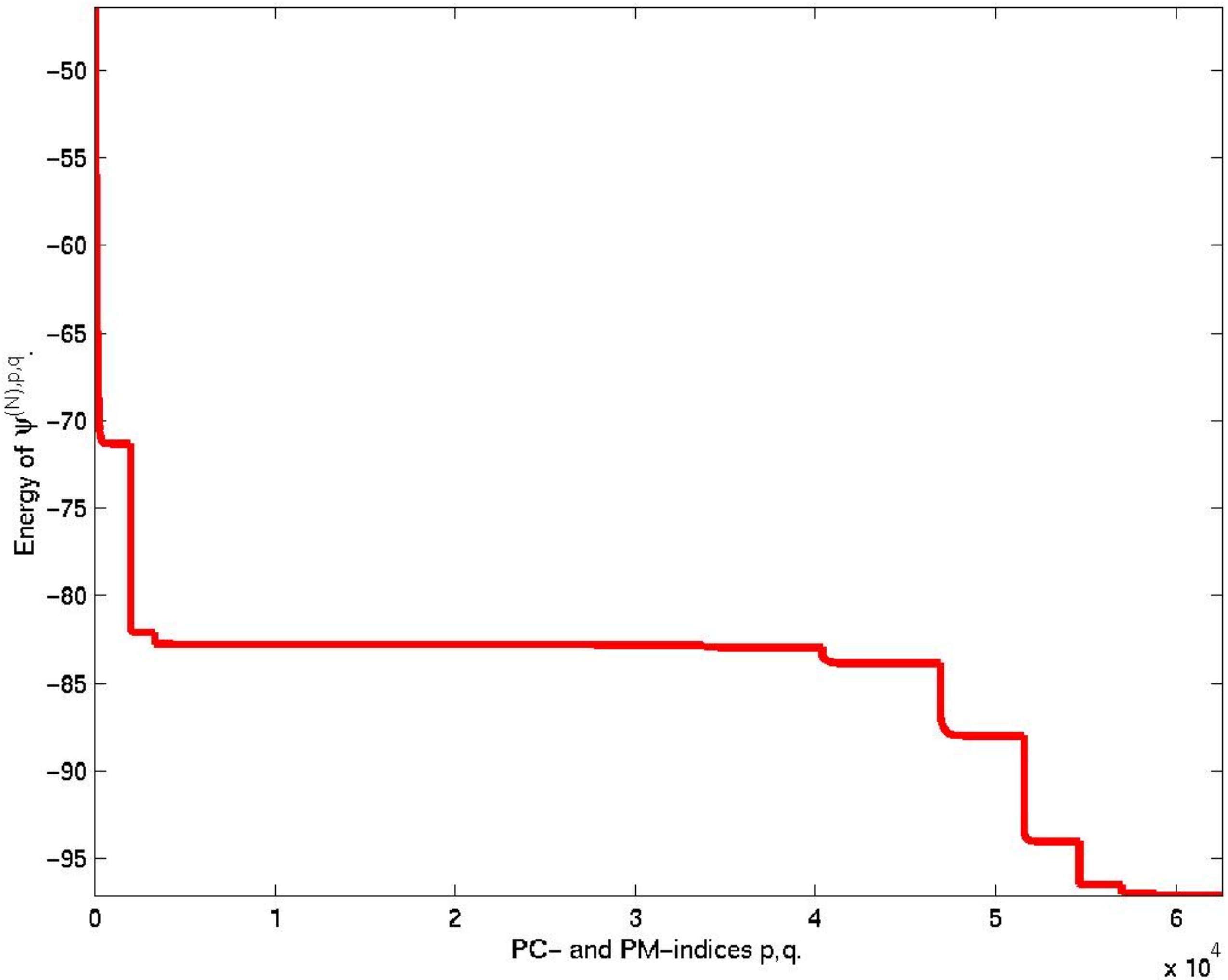
Number of grid points: $n = 2^m$ (here: m=6; confirmed for higher m)
External potential: $v(x, y) = V_0/\cosh((x - x_0)^2/a^2 + (y - y_0)^2/b^2)$
$((x_1)_0, (y_1)_0) = (0.35, 0.5)$, $((x_2)_0, (y_2)_0) = (0.65, 0.5)$
$(a_1, b_1) = (a_2, b_2) = (0.03, 0.03)$, $(V_1)_0 = (V_2)_0 = -0.1$
Two-body potential: $\alpha = 0$ and $\delta = 0.1$
Coupling constant: $g = -16$
Tolerance: $\epsilon_{rel} = 0.000001$

- Iteration: $q = \infty$: $q = O(10) - O(10^2)$, $p = \infty$: $p = O(10)$

- Starting guesses:

$$\Phi^{(N),p+1,0} := \Phi^{(N),p,\infty}$$





Energy of $\psi^{(N),p,q}$.
−50
−55
−60
−65
−70
−75
−80
−85
−90
−95
0
1
2
3
4
5
6
PC- and PM-indices p,q.
x 10^4

Time Dependent Hartree Equation

1. Weak coupling limit of bosonic system and Newtonian limit of Hartree equation

• Large system of weakly interacting nonrelativistic bosons
[Hepp 74], [Ginibre,Velo 79,80]

State space: $\mathcal{H}^{(N)} := \frac{1}{N!}\sum_{\pi\in\sigma(N)} U_\pi\, L^2(\mathbb{R}^{3N})$ (Pauli principle)
Hamiltonian:

$$H^{(N)} := \sum_{j=1}^{N}\left[-\frac{1}{2}\Delta_j + v(x_j)\right] - \kappa \sum_{1\le i<j\le N} V(x_i - x_j)$$

with $\kappa > 0$.
Example: $V(x) \simeq |x|^{-6} + \alpha|x|^{-1}$, $\alpha \ll 1$, $|x| \gg$ diameter of atom

Second quantization formalism:

Fock space over state space: $\mathcal{F}_b := \bigoplus_{N=0}^{\infty} \mathcal{H}^{(N)}$, $\mathcal{H}^{(0)} := \mathbb{C}$

Annihilatiors: $(a(f)\Psi)^{(N)}(x_1, ..., x_N) \propto \int dx\, \bar{f}(x)\, \Psi^{(N+1)}(x, x_1, ..., x_N)$

CCR: $[a(f), a(g)] = [a^\dagger(f), a^\dagger(g)] = 0$, $[a(f), a^\dagger(g)] = (f, g)$

Theorem

$$\lim_{\kappa \to 0} \langle \theta_\kappa, \prod_{j=1}^{m} A_\kappa^*(f_j, t_j) A_\kappa(g_j, s_j) \theta_\kappa \rangle = \prod_{j=1}^{m} \bar{\psi}(f_j, t_j) \psi(g_j, s_j)$$

with $\theta_\kappa := c_\kappa\, (a^\dagger(\psi_0))^{[\kappa^{-1}]} \phi$, $\psi(f, t) := \int dx\, \bar{f}(x)\, \psi(x, t)$, and $\psi(x, t)$ is solution of

$$i\partial_t \psi = \left[-\frac{1}{2}\Delta + v - V * |\psi|^2 \right] \psi$$

with $\psi(x, 0) = \psi_0$!

• Newtonian Limit

[Fröhlich,Tsai,Yau 00]

Hamiltonian nature of Hartree equation: phase space $W^{1,2}(\mathbb{R}^3)$, symplectic 2-form $\omega = \frac{i}{2} d\psi \wedge d\bar{\psi}$

Gauge invariance and Galilei symmetries !

Hartree equation as Hamilton's equation of motion from Hartree functional or Euler-Lagrange equation from action

$$\mathcal{S}[\bar{\psi}, \psi] = \int_{t_1}^{t_2} dt \left[\frac{i}{2} \int_{\mathbb{R}^d} d^d x \; \bar{\psi}_t \dot{\psi}_t - \mathcal{H}[\bar{\psi}_t, \psi_t] \right]$$

Action on perturbed superposition of minimizers Φ_{N_j}

$$\psi_t(x) = \sum_{j=1}^{k} \Phi_{N_j(t)}(x - r_j(t)) e^{i\theta_j(x,t)} + h_t^\varepsilon(x)$$

$\Rightarrow$ On time scale $O(\varepsilon^{-1})$:

$$\mathcal{S}[\bar\psi, \psi] \;=\; \frac{1}{2}\mathcal{S}_{Nwt} + \frac{1}{2}\int_{t_1}^{t_2} dt \sum_{j=1}^{k} \left[\frac{i}{2}\dot N_j - N_j \dot\vartheta_j - 2\mathcal{H}[\Phi_{N_j(t)}, \Phi_{N_j(t)}] + R^\varepsilon\right]$$

$$\mathcal{S}_{Nwt} \;=\; \int_{t_1}^{t_2} dt \sum_{j=1}^{k} \left[\frac{N_j}{2}\dot r_j^2 - N_j w^\varepsilon(r_j) + \frac{1}{2}\sum_{i=1, i\neq j}^{k} N_i N_j V^{long}(\varepsilon(r_i - r_j))\right]$$

S_{Nwt}: k point particles, masses $N_1, ..., N_k$, external potential $v = w^\varepsilon$, two-body interaction $N_i N_j V^{long}(\varepsilon(r_i - r_j))$
$R^\varepsilon = o(\varepsilon)$: remainder

Variations w.r.t. r_j
$\Rightarrow$ Newton's equation of motion !

$$\ddot{r}_j = -\varepsilon \nabla w(\varepsilon r_j) + \varepsilon \frac{1}{2} \sum_{i=1, i \neq j}^{k} N_i \nabla V^{long}(\varepsilon(r_i - r_j)) + a_j$$

$|a_j(t)| = o(\varepsilon)$: from R^ε

Variations w.r.t. ϑ_j
$\Rightarrow$ Approximate conservation N_j: $\dot{N}_j = o(\varepsilon)$

$\Rightarrow$ Point particle limit for $\varepsilon \downarrow 0$!

I.e.:
Motion of extended particle in shallow external potential interacting weakly with dispersive medium, exchanging mass and energy !

• Applications in physics:

Dynamics of BEC

Structure formation in universe from cold dark matter dynamics

Measurement process in quantum mechanics

2. Analysis of numerical scheme

Hartree initial-boundary value problem:

$$\begin{aligned} i\partial_t \psi_t &= \left(-\frac{1}{2}\Delta + v + g\, V *_{\Omega_c} |\psi_t|^2\right)\psi_t,\ \ t > 0 \\ \psi_t|_{\partial\Omega_c} &= 0,\ \ t \geq 0, \\ \psi_0 &= \psi_{in} \end{aligned}$$

- Space (FE) and time discretization [IFD]:

$$\begin{aligned} i\frac{1}{t^{(s)}}\left(\phi^{(N)}, \psi^{(N)}_{k+1} - \psi^{(N)}_{k}\right)_2 &= \frac{1}{2}\left(\nabla\phi^{(N)}, \nabla\psi^{(N)}_{\tilde{k}}\right)_2 + \left(\phi^{(N)}, v\psi^{(N)}_{\tilde{k}}\right)_2 \\ &\quad + g\left(\phi^{(N)}, F_{ic,\psi^{(N)}_k}\left[\psi^{(N)}_{\tilde{k}}\right]\right)_2 \\ \psi^{(N)}_0 &= \psi^{(N)}_{in} \end{aligned}$$

where $F_{ic,\phi}[\psi] := \frac{1}{2}(W[2\,\psi - \phi] + W[\phi])\psi,\ W[\varphi] := V * |\varphi|^2$

• Theorems Existence, uniqueness, and accuracy

Theorem 4 (Accuracy)
Let $V \in W^{2,1}(\mathbb{R}^2)$, $v \in W^{2,2}(\Omega_s)$, and

$$\left\|\psi_{in} - \psi_{in}^{(N)}\right\|_2 \leq c_{in}\, {h^{(n)}}^2$$

for some $c_{in} \in \mathbb{R}^+$.
Then, the L^2-error of the discretization is controlled by

$$\max_{k \in \{0,\ldots,s-1\}} \left\|\psi_k - \psi_k^{(N)}\right\|_2 \leq c_{ic} \left({t^{(s)}}^2 + {h^{(n)}}^2\right)$$

for some $c_{ic} = c_{ic}(\|\psi\|_{m,2})$, $m = 0, 1, 2, 4, 6$.

• Sketch for Proof of Theorem 4

Step 1: Replacement

Locally Lipschitz problem $\mapsto$ globally Lipschitz problem:

$$\begin{aligned}
\tilde{F}_{ic}[\psi_1, \psi_2] &:= \frac{1}{2}(W[\psi_1] + W[\psi_2])\frac{1}{2}(\psi_1 + \psi_2) \\
T^{\delta}_{ic} &:= \left\{\varphi \in L^2(\Omega) \,|\, \exists t \in \bar{\tau} : \|\psi_t - \varphi\|_2 \leq \delta\right\}^{\times 2} \\
\tilde{F}^{\delta}_i|_{T^{\delta}_i} &:= \tilde{F}_i|_{T^{\delta}_i} \\
\|\tilde{F}^{\delta}_{ic}[\psi_1, \phi_1] - \tilde{F}^{\delta}_{ic}[\psi_2, \phi_2]\|_2 &\leq L_{ic}(\|\psi_1 - \psi_2\|_2 + \|\phi_1 - \phi_2\|_2)
\end{aligned}$$

Step 2: Accuracy for globally Lipschitz problem

Step 3: Approximation

Globally Lipschitz solution within world tube for *sufficiently small* $t^{(s)}, h^{(n)}$

$\square$

- a priori estimate on $c_{ic} = c_{ic}(\|\psi\|_{m,2})$, $m = 0, 1, 2, 4, 6$?

Theorem (Regularity of Global Solution):
$\psi \in C([0, \infty[, W^{2,2}(\Omega)) \cap C^1([0, \infty[, L^2(\Omega))$, $\Omega \subset \mathbb{R}^2$
But: polynomial decay in time of higher Sobolev norms
[Bourgain 95], [Staffilani 97]

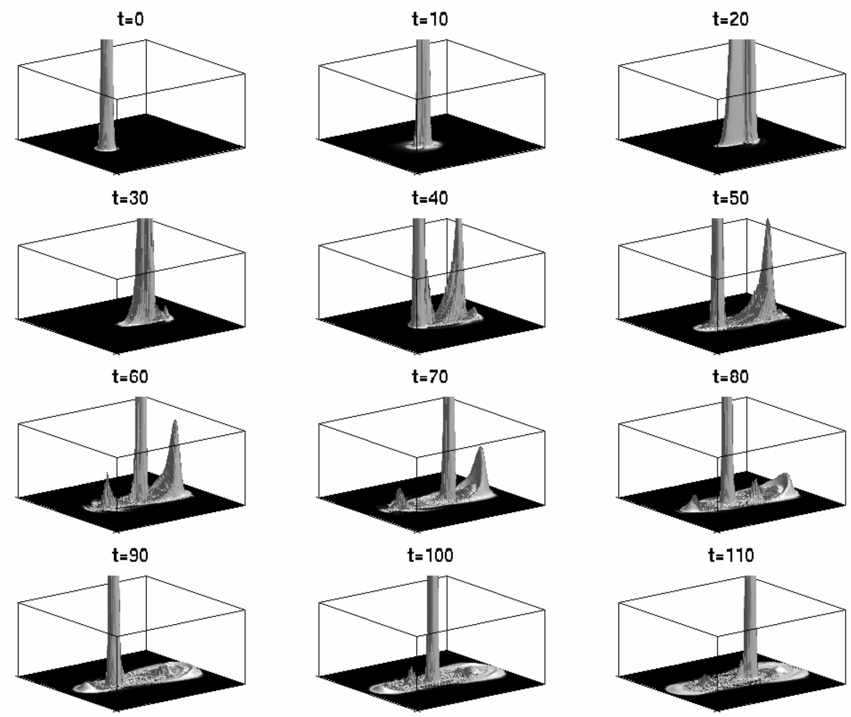
3. Numerical approach to long-time behavior

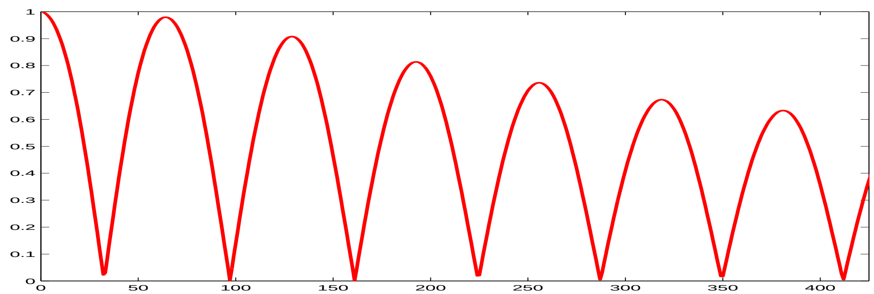
[Aschbacher,Fröhlich,Interlandi,Troyer 01]

• Simulation 2 Damped oscillation into potentials minimum

Loss of mass and energy from particle into dispersive waves: dissipation through radiation

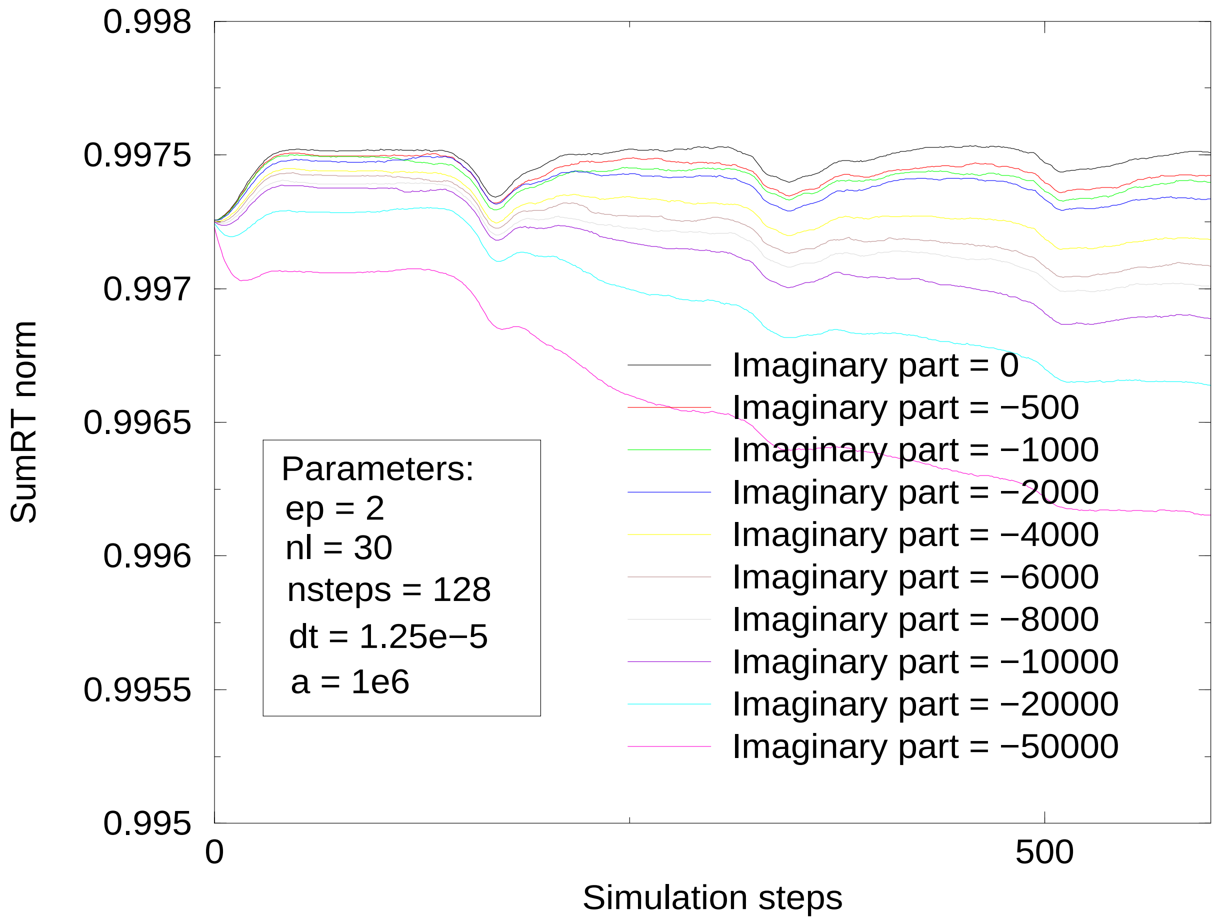
$\Rightarrow t \to \infty$: trajectory expected to approach minimum of external potential !

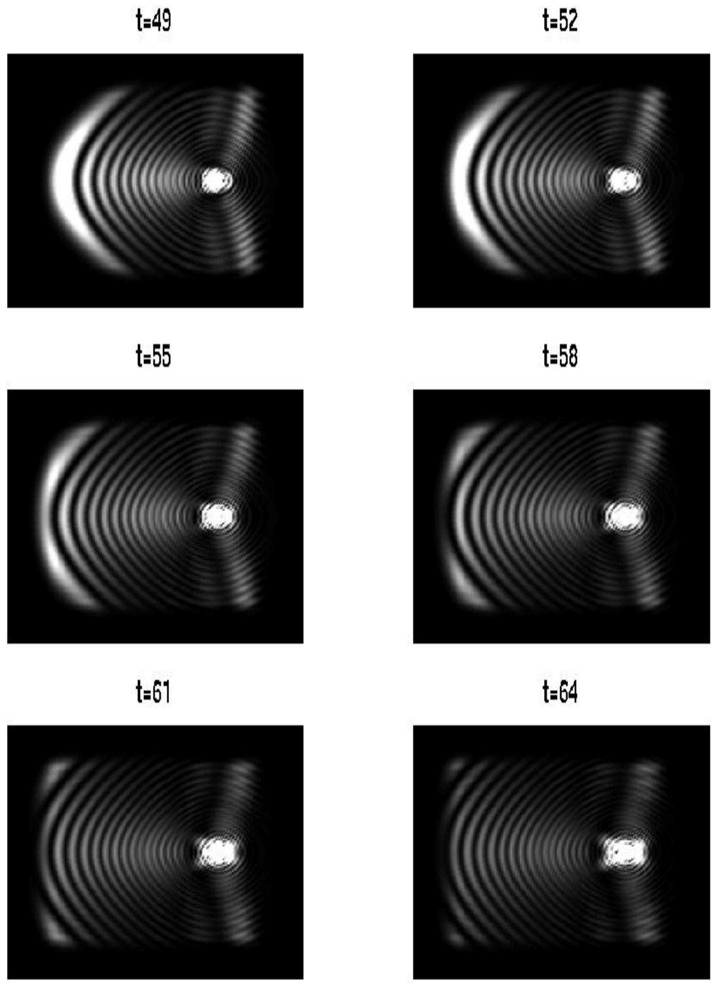




Return to equilibrium

SumRT norm for different imaginary parts





Absorbing boundaries

Outlook

• Coherent picture of measurement process
Ingredients: proof relaxation to ground state, scattering theory,...

• Simulations: Mirror charge model, Young double slit,...

• Higher regularity of global solutions in more general cases
$\Rightarrow$ *a priori* estimates on accuracy

Summary

Physics: Interpretations
(BEC, bosonic CDM, measurement process,...)

Analysis: Results on continuous and discretized Hartree equation
(Uniqueness and non-uniqueness of Hartree minimizers, accuracy of approximation schemes, regularity of global solutions, ...)

Numerics: High performance *implementation* of Hartree eigenvalue problem and Hartree dynamics in external potentials
(Soliton dissipation through emission of radiation, binary collapse, measurement process,...).