The Boson system: An introduction. II.

Dionisios Margetis

Department of Mathematics, & IPST, & CSCAMM

Applied PDE & Particle Systems RITs
22 September 2014

Why is BEC in atomic gases is interesting?

High-dimensional PDE !
Impractical for predictions

$$\hat{H}_N \Psi_N(t,\vec{x}) = i\partial_t \Psi_N(t,\vec{x}), \quad \vec{x} = (x_1, \dots, x_N)$$

$$\hat{H}_N = \sum_{j=1}^{N} [-\Delta_j + V_e(x_j)] + \sum_{j<l} \mathcal{V}(x_j, x_l) \qquad (\hbar = 2m = 1)$$

Usually short-ranged, repulsive, symmetric, $\mathcal{V} = V(|x_j - x_l|)$

- What macroscopic description, **mean field limit**, emerges, and in what sense, in **3 dimensions** as $N \to \infty$?

- What corrections exist beyond this limit for large but finite N, in a controllable ``PDE sense''?

Digression: Second quantization: Bosonic Fock space $\mathbb{F}$

- Elements of $\mathbb{F}$ (space with indefinite number of Bosons):

$Z = \{Z^{(n)}\}_{n\geq 0}$ where $Z^{(0)}$: complex number, $Z^{(n)} \in L^2_s(\mathbb{R}^{3n})$. Inner product: $\langle Z, \Psi\rangle_{\mathbb{F}} = \sum_{n\geq 0}\int_{\mathbb{R}^{3n}} Z^{(n)}(x)\Psi^{(n)*}(x)\mathrm{d}x$.

adjoint

- Annihilation & creation operators for 1-part. state Φ are $a_\Phi, a^*_\Phi : \mathbb{F} \to \mathbb{F}$.

$$(a^*_\Phi Z)^{(n)}(\vec{x}_n) = n^{-1/2}\sum_{j=1}^{n}\Phi(x_j)Z^{(n-1)}(x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_n)\ ,$$

$$(a_\Phi Z)^{(n)}(\vec{x}_n) = \sqrt{n+1}\int_{\mathbb{R}^3}\mathrm{d}x_0\,\Phi^*(x_0)Z^{(n+1)}(x_0,\vec{x}_n)\ ,\ \vec{x}_n := (x_1,\ldots,x_n)$$

Commutation relation: $[a_\Phi, a^*_\Phi] = a_\Phi a^*_\Phi - a^*_\Phi a_\Phi = \|\Phi\|^2_{L^2}$.

- Periodic bc's: Momentum creation and annihilation operators:

a^*_k and a_k, for $\Phi(x) = (1/\sqrt{|\text{-}\;|})e^{ik\cdot x}$.

$$[a_k, a^*_{k'}] = \delta_{k,k'}$$

- Vacuum (no particles): $|\mathrm{vac}\rangle = \{1,0,0,\ldots\}$. $\quad a_\Phi|\mathrm{vac}\rangle = 0,\ a^*_\Phi|\mathrm{vac}\rangle = |\Phi\rangle$

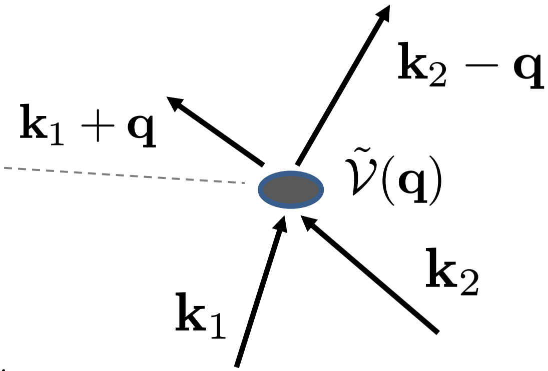
Weakly interacting Bosons in a periodic box Ω, T=0: Statics

[Bogoliubov, 1947; Lee, Huang, Yang, 1957]

PDE Hamiltonian:

$$\hat{H}_N = \sum_{j=1}^{N}(-\Delta_j) + \frac{1}{2}\sum_{\substack{j,l=1\\ j\neq l}}^{N} \underbrace{\mathcal{V}(x_j - x_l)} \qquad (\hbar = 2m = 1)$$

Compactly supported, smooth



This is replaced by Hamiltonian in Fock space:

$$\mathcal{H} = \sum_k k^2\, \underbrace{a_k^* a_k} + \frac{1}{2\underbrace{|\text{-}|}} \sum_{k_1,k_2,q} a^*_{k_1+q} a^*_{k_2-q}\, \tilde{\mathcal{V}}(q)\, a_{k_1} a_{k_2}$$

Operator for number of Bosons at mom. k; volume

$$\tilde{\mathcal{V}}(q) = \int \mathcal{V}(x)\, e^{-iq\cdot x}\, dx$$

In a dilute gas, the actual form of $\mathcal{V}$ *is not important. What matters is an effective potential that reproduces the correct low-energy behavior in the far field.*

Low-energy scattering length

Lee, Huang, and Yang set: $\mathcal{V}(x_i - x_j) \to \mathcal{V}' = 8\pi a \delta(x_i - x_j)\frac{\partial}{\partial r_{ij}} r_{ij}, \quad r_{ij} = |x_i - x_j|$

Fermi pseudopotential

Length a comes from solving: $-\Delta w + (1/2)\mathcal{V}(x) w = 0, \qquad \lim_{|x|\to\infty} w = 1$

In particular, $w(x) \sim 1 - \frac{a}{|x|} \quad \text{as } |x| \to \infty$

Definition of a

[Blatt, Weiskopf, 1952]

Weakly interacting Bosons in a periodic box Ω, T=0 (cont.)

$\mathcal{V}'$ is replaced by $8\pi a \delta(x_i - x_j)$

$$\mathcal{H}' = \sum_k k^2 a_k^* a_k + |\text{-}\ |^{-1} 4\pi a \sum_{k_1, k_2, q} a_{k_1+q}^* a_{k_2-q}^* a_{k_1} a_{k_2}$$

$$\sim a_0^* a_0^* a_0 a_0 + \sum_{k \neq 0} (4 a_0^* a_k^* a_0 a_k + a_k^* a_{-k}^* a_0 a_0 + a_0^* a_0^* a_k a_{-k})$$

pair excitation

$$k_1 = 0, k_2 = k, q = 0$$
$$k_1 = k, k_2 = 0, q = 0$$
$$k_1 = 0, k_2 = k, q = k$$
$$k_1 = k, k_2 = 0, q = -k$$

$$\sim (a_0^* a_0)^2 = \left(N - \sum_{k \neq 0} a_k^* a_k\right)^2 \sim N^2 - 2N \sum_{k \neq 0} a_k^* a_k$$

Many-body state vec.
In Fock space

$$N = \underbrace{\langle \Psi, (a_0^* a_0) \Psi \rangle}_{\mathcal{O}(N)} + \underbrace{\langle \Psi, \left(\sum_{k \neq 0} a_k^* a_k \right) \Psi \rangle}_{o(N)}, \quad \text{or} \quad N = a_0^* a_0 + \sum_{k \neq 0} a_k^* a_k$$

$$\Rightarrow \mathcal{H}' \sim \underbrace{4\pi a \rho_0 N}_{\mathcal{O}(N)} + \underbrace{\sum_{k \neq 0} (k^2 + 8\pi a \rho_0) a_k^* a_k + 4\pi a \rho_0 \sum_{k \neq 0} (a_k a_{-k} + a_k^* a_{-k}^*)}_{\mathcal{O}(N\sqrt{\rho_0 a^3})} + o(N\sqrt{\rho_0 a^3}); \quad \rho_0 = N / |\text{-}\ |$$

Weakly interacting Bosons in a periodic box Ω, T=0 (cont.)

$$\mathcal{H}_{app} = 4\pi a\rho_0 N + 2\sum{}'(k^2+8\pi a\rho_0)[\tfrac{1}{2}(a_k^* a_k + a_{-k}^* a_{-k}) + \zeta_k(a_k a_{-k} + a_k^* a_{-k}^*)]$$

$\sum{}'$: $\{all\ k \neq 0 :\ k_z > 0\}$

$\zeta_k = 4\pi a\rho_0 (k^2 + 8\pi a\rho_0)^{-1}$

Quadratic in a_{-k} , a_k

How can one diagonalize it?

Digression: Toy Hamiltonian:

$$\mathcal{H}_{toy} = \tfrac{1}{2}(\mathcal{A}^*\mathcal{A}+\mathcal{B}^*\mathcal{B})+\zeta(\mathcal{A}\mathcal{B}+\mathcal{A}^*\mathcal{B}^*); \quad [\mathcal{A},\mathcal{A}^*]=1=[\mathcal{B},\mathcal{B}^*],\ [\mathcal{A},\mathcal{B}]=0=[\mathcal{A}^*,\mathcal{B}]$$

Define:

$$\breve{\mathcal{H}}_{toy} \equiv e^{\beta\mathcal{A}\mathcal{B}}\mathcal{H}_{toy}e^{-\beta\mathcal{A}^*\mathcal{B}^*} = (\tfrac{1}{2}-\beta\zeta)(\mathcal{A}^*\mathcal{A}+\mathcal{B}^*\mathcal{B})+\zeta\mathcal{A}\mathcal{B}-\beta\zeta+(\zeta-\beta+\beta^2\zeta)\mathcal{A}^*\mathcal{B}^*$$

Harmonic-oscillator-type: $(\mathcal{A}^*\mathcal{A}+\mathcal{B}^*\mathcal{B})$; eliminate: $(\zeta-\beta+\beta^2\zeta)\mathcal{A}^*\mathcal{B}^*$ (struck through)

Same eigenvalues as $\mathcal{H}_{toy}$; eigenstates $e^{\beta\mathcal{A}^*\mathcal{B}^*}\Psi_{toy}$

Determine β so that : $\zeta-\beta+\beta^2\zeta=0$

→ Spectrum of $\mathcal{H}_{toy}$: $\lambda_{n_1,n_2} = -\tfrac{1}{2}+\tfrac{1}{2}(1-4\zeta^2)^{1/2}(1+n_1+n_2), \qquad n_{1,2}=0,\,1,\,\ldots$

Back to $\mathcal{H}_{app}$: To obtain ground state energy :

Set $\mathcal{A}=a_k,\quad \mathcal{B}=a_{-k},\ n_1=n_2=n=0.$ Take $\sum{}'$

Weakly interacting Bosons in a periodic box Ω, T=0 (cont.)

$$\mathcal{H}_{app} = 4\pi a\rho_0 N + 2\sum_{\substack{k\neq 0\\ k_z>0}} (k^2 + 8\pi a\rho_0)[\tfrac{1}{2}(a_k^* a_k + a_{-k}^* a_{-k}) + \zeta_k(a_k a_{-k} + a_k^* a_{-k}^*)]$$

$\zeta_k = 4\pi a\rho_0(k^2 + 8\pi a\rho_0)^{-1}$

Quadratic in a_k , a_{-k}

- Ground state energy :

$$E_{N,0} = 4\pi a\rho_0 N\left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho_0 a^3}\right]; \qquad \rho_0 a^3 \ll 1 \text{ (dilute gas)}$$

- Ground state vector:

$$\Psi_{app} \approx \mathfrak{N}\exp\left[-\frac{1}{2N}\sum_{k\neq 0}\beta_k a_k^* a_{-k}^* a_0^2\right]\Psi_0^0$$

Annihilates 2 particles from 0 momentum state; and creates 2 particles at momenta *k*, *-k*

Mean field

$$\Psi_0^0 = (N!)^{-1/2} {a_0^*}^N |\text{vac}\rangle$$

All particles at 0 momentum

Rigorously via variational approach in Fock sp. by Yau, Yin (2009).

How can this approach be extended to non-periodic, time-dependent settings ?

Lack of translation invariance:

- The macroscopic 1-particle quantum state (condensate) is not known a priori; it must be determined.
- There is no sense of opposite momenta in scattering of particles from condensate to other states.

BEC in non-periodic setting: Mean field limit

[Gross, 1961; Pitaevskii, 1961; Wu, 1961, 1998]

$$H_N = \sum_{j=1}^{N} [-\Delta_j + V_e(x_j)] + 4\pi a \sum_{i \neq j} \delta(x_i - x_j) \qquad (\hbar = 2m = 1)$$

Many-body wave function ≈ Tensor product of 1-particle states ?

Condensate wave function

If $\Psi_N(0, \vec{x}_N) = \prod_{j=1}^{N} \Phi_0(x_j)$ (at t=0), is it possible that $\Psi_N(t, \vec{x}_N) \approx \prod_{j=1}^{N} \Phi(t, x_j)$,

for some appropriate $\Phi(t,x_j)$, for $t > 0$? $\quad (N!)^{-1/2} {a_\Phi^*}^N |\text{vac}\rangle$

Answer: Yes.

Heuristically: Gross [1961], Pitaevskii [1961], Wu [1961]

Mean field PDE for **Φ** is **nonlinear Schroedinger-type in 3D.**

BEC in non-periodic setting: Beyond MF: **Pair excitation**

[Wu, 1961, 1998]

$$\Psi_N^0[\Phi](t,\vec{x}_N) \equiv \prod_{j=1}^{N} \Phi(t,x_j); \qquad \vec{x}_N = (x_1, x_2, \ldots, x_N)$$

Pair Excitation **Ansatz** (beyond mean field limit):

$$\Psi_N(t,\vec{x}_N) \approx \mathfrak{N}(t)\, e^{\mathcal{B}[K]} \Psi_N^0[\Phi](t,\vec{x}_N)$$

unknown ($\mathcal{B}[K]$)   unknown (Φ)

- $\mathcal{B}$[K] : Operator that describes scattering of particles from Φ to other states *in pairs*. K=$K(t,x,y)$: ***pair excitation kernel***
- Ψ_N looks roughly as $\Phi(t,x_1)\Phi(t,x_2)\cdots\Phi(t,x_N)\prod_{i,j} f(t,x_i,x_j)$
- Φ satisfies a nonlinear Schroedinger-type PDE; K satisfies nonlocal PDE

Mean field limit

3D

Effective mean field potential

$$i\partial_t \Phi(t,x) = [-\Delta + 8\pi a|\Phi|^2 + V_e(x) - 4\pi a\zeta(t)]\Phi(t,x)$$

``Gross-Pitaevskii (GP) eq.''

$$\zeta(t) = N^{-1}\int_{\mathbb{R}^3} |\Phi(t,x)|^4\,dx; \qquad N^{-1}\int |\Phi(t,x)|^2\,dx = 1$$

Digression: Second quantization: Boson field operators

Operator-valued distributions, $\psi^*(x)$ and $\psi(x)$ in Fock space:

$$a_\Phi^*(t) = N^{-1/2} \int dx\, \Phi(t,x)\, \psi^*(x)\ , \qquad a_\Phi(t) = N^{-1/2} \int dx\, \Phi^*(t,x)\, \psi(x)$$

Canonical commutation relations:

$$[\psi(x), \psi^*(y)] = \delta(x-y)\ ,\ [\psi^*(x), \psi^*(y)] = [\psi(x), \psi(y)] = 0$$

Hamiltonian in Fock space:

$$\mathcal{H} = \int dx\, \psi^*(x)[-\Delta_x + V_e(x)]\psi(x) + \frac{1}{2}\int dx\, dy\ \psi^*(x)\psi^*(y)\mathcal{V}(x,y)\psi(y)\psi(x)$$

- Field operator splitting:

$$\psi(x) = \underbrace{\psi_0(t,x)}_{N^{-1/2} a_\Phi(t)\ \Phi(t,x)} + \overbrace{\psi_1(t,x)}^{N^{-1/2}\sum_{j=1}^{\infty} a_{\varphi_j}(t)\ \varphi_j;\quad \varphi_j \perp \Phi}$$

Pair excitation operator [Wu, 1961]:

$$\mathcal{B}[K] = (2N)^{-1} \int dx\, dy\, \underbrace{\psi_1^*(t,x)\psi_1^*(t,y)}_{\text{Creates 2 particles at states } \perp \Phi}\, K(t,x,y)\, \underbrace{a_\Phi^2}_{\text{Annihilates 2 particles from } \Phi}$$

Difficulty for rigorous treatment:

This operator does not have any ``nice" properties; errors estimates become too hard.

BEC in non-periodic setting: Pair excitation

[Wu, 1961, 1998]

Pair Excitation Ansatz:

$$\Psi_N(t,\vec{x}_N) \approx \mathfrak{N}(t)\, e^{\mathcal{B}[K]}\, \Psi_N^0[\Phi](t,\vec{x}_N)$$

$$[i\partial_t - E(t)]K(t,x,y)$$
$$= \{\mathfrak{L}[\Phi](t,x) + \mathcal{L}[\Phi](t,y) + 8\pi a[|\Phi(t,x)|^2 + |\Phi(t,y)|^2]\}K(t,x,y)$$
$$+8\pi a\Phi(t,x)^2\delta(x-y) + 8\pi a \int_{\mathbb{R}^3} dz\, \Phi^*(t,z)^2\, K(t,x,z)\, K(t,y,z)$$

$$\mathfrak{L}[\Phi](t,x) = -\Delta_x + V_e(x) + 8\pi a|\Phi(t,x)|^2 - \bar{\zeta}(t) - 8\pi a\zeta(t) - \zeta_e(t)$$

$$E(t) = iN^{-1}\int \{\partial_t \Phi(t,x)\}\, \Phi^*(t,x)\, dx$$

$$\zeta(t) = N^{-1}\int |\Phi(t,x)|^4\, dx, \quad \bar{\zeta}(t) = N^{-1}\int |\nabla\Phi|^2\, dx, \quad \zeta_e(t) = N^{-1}\int V_e(x)\, |\Phi(t,x)|^2\, dx$$

Some recent rigorous results:

The time evolution problem

Mean Field: Mathematical theme

$$\hat{H}_N \Psi_N(t, \vec{x}) = i\partial_t \Psi_N(t, \vec{x})$$

$$\hat{H}_N = \sum_{j=1}^{N} [-\Delta_j] + (2N)^{-1} \sum_{\substack{j,l=1 \\ j \neq l}}^{N} N^{3\alpha} v(N^\alpha(x_j - x_l))$$

PDE Hamiltonian

$$0 \cdot \ \alpha \cdot \ 1, \quad v > 0$$

If $\Psi_N(0, \vec{x}_N) = \prod_{j=1}^{N} \Phi_0(x_j)$ (at t=0), is it possible that $\Psi_N(t, \vec{x}_N) \approx \prod_{j=1}^{N} \Phi(t, x_j)$,

for some appropriate $\Phi(t,x_j)$, for t >0, large N ?

$$(N!)^{-1/2} {a_\Phi^*}^N |\text{vac}\rangle$$

Mean field PDE

$$i\partial_t \Phi(t,x) = -\Delta\Phi + q_\alpha(|\Phi|^2)\Phi; \quad \Phi(0,x) = \Phi_0(x)$$

$$q_0 = \underbrace{\upsilon \star |\Phi|^2}_{Hartree\ evol.}\ ; \quad q_\alpha = \underbrace{(\int \upsilon)|\Phi|^2}_{NLS\,evol.},\ 0 < \alpha < 1; \quad q_1 = \underbrace{8\pi a|\Phi|^2}_{\substack{\textbf{Gross-Pitaevskii}\ evol; \\ a:\ \textbf{sc. length}}}.$$

- ESY [06-07]: For $0 < \alpha \cdot\ \ 1$, PDE is justified in the sense that

$$\|\gamma_N^{(1)} - \Phi\quad\Phi^*\|_{HS}^2 = \iint dxdx'\ |\gamma_N^{(1)}(t,x,x') - \Phi(t,x)\Phi^*(t,x')|^2 \to 0 \text{ as } N \to \infty$$

via **coupled PDEs** (“BBGKY hierarchies”) for marginal densities $\gamma_N^{(k)}$ $(k \geq 1)$;
$\gamma_N^{(k)}(t,\vec{x}_k,\vec{x}'_k) = \int d\vec{y}_{N-k}\ \Psi_N^*(t,\vec{x}_k,\vec{y}_{N-k})\Psi_N(t,\vec{x}'_k,\vec{y}_{N-k})$ [**k-part. marg. dens.**]

- Rodnianski, Schlein [2009]: Rate of convergence for $\alpha = 0$ via **Fock space**:

$$\|\gamma_N^{(1)} - \Phi\quad\Phi^*\|_{HS} \cdot\ \ e^{ct}/N \quad \text{for large } N$$

Note: On the hierarchy approach by Yau et al

What is a good norm for *N*-particle product quantum state?

L^2-norm is preserved by the N-body Hamlt. flow. BUT it is too strong.

Example 1 [Yau] Let $\|f\|_{L^2(\mathbb{R}^3)} = \|\tilde{f}\|_{L^2(\mathbb{R}^3)} = 1$, with

$$\Psi_N := f(x_1)\cdots f(x_N), \quad \tilde{\Psi}_N := \tilde{f}(x_1)\cdots\tilde{f}(x_N); \quad \|\Psi_N\|_{L^2(\mathbb{R}^{3N})} = \|\tilde{\Psi}_N\|_{L^2} = 1.$$

$$\Rightarrow \|\Psi_N - \tilde{\Psi}_N\|^2_{L^2(\mathbb{R}^{3N})} = 2 - \left(\langle f, \tilde{f}\rangle\right)^N \to 2 \quad \text{as } N \to \infty$$

Other norms seem ``hopeless'' $\langle f, \tilde{f}\rangle = 0$

Example 2 [Yau] Let $\Psi_N = \mathrm{Symm}[f \quad \bigotimes_{j=2}^N g]$ and $\tilde{\Psi}_N = \mathrm{Symm}[\tilde{f} \quad \bigotimes_{j=2}^N g]$

$$\Rightarrow \|\Psi_N - \tilde{\Psi}_N\|^2_{L^2(\mathbb{R}^{3N})} = \|f - \tilde{f}\|^2_{L^2(\mathbb{R}^3)} = 2$$

BUT:

$$\gamma_N^{(1)}(x,y) = N^{-1}[f(x)f^*(y) + (N-1)g(x)g^*(y)] \Rightarrow \mathrm{Tr}\left[\gamma_N^{(1)} - \tilde{\gamma}_N^{(1)}\right] = \mathcal{O}(N^{-1})$$

Can one rigorously study effects beyond MF? Issues…

- M. G. Grillakis, M. Machedon, DM (2010), *Second-order corrections to mean field evolution of weakly interacting Bosons. I*, Comm. Math. Phys. **294**, pp. 273-301.

- M. G. Grillakis, M. Machedon, DM (2011), *Second-order corrections to mean field evolution of weakly interacting Bosons. II*, Advances Math. **228**, pp. 1788-1815.

- DM (2013), *Bose-Einstein condensation beyond mean field: Many-body bound state of periodic microstructure*, (SIAM) Multisc. Modeling Simul. **10**, pp. 383-417.

Case α=0 (Hartree dynamics) [Grillakis, Machedon, DM, 2011, 12]

- **Coherent state in Fock space:** Define operators $\mathcal{A}(\Phi)$, $\mathcal{W}(\Phi)$:

$$\mathcal{W}(\Phi) = e^{-\sqrt{N}\mathcal{A}(\Phi)}, \quad \mathcal{A}(\Phi) = a_\Phi - a^*_\Phi .$$

Coherent state at $t = 0$: $\Psi_{coh} = \mathcal{W}(\Phi_0)\,|\text{vac}\rangle = \overbrace{(\ldots, c_n \prod_{j=1}^{n} \Phi_0(x_j), \ldots)}^{\text{State in Fock space}}$

Mean field corresponds to $\Psi_{MF}(t) = \mathcal{W}(\Phi(t))|\text{vac}\rangle$

- **"Pair excitation":** Define $\Psi_{app}(t) = \overbrace{e^{-\mathcal{B}(K)}}^{\textbf{unitary}} \overbrace{\mathcal{W}(\Phi(t))|\text{vac}\rangle}^{\text{coherent at } t>0}$ where

$$\mathcal{B}(K) = \int dxdy \left\{K^*(t,x,y)\psi(x)\psi(y) - K(t,x,y)\psi^*(x)\psi^*(y)\right\}; \; K|_{t=0} = 0.$$

Task: Start with Ψ_{coh} at $t = 0$. We want to **compare** exact dynamics $\Psi_{ex}(t) = e^{-it\mathcal{H}}\Psi_{coh}$ to approximate dynamics $\Psi_{app}(t)$.

Goal: We will show that $\overbrace{\|\Psi_{ex}(t) - \Psi_{app}(t)\|_{\mathbb{F}}}^{\text{Abs. error}} \cdot \; C\sqrt{1+t}/\sqrt{N}$ for large N.

Strategy:

- Notice that $\|\Psi_{ex}(t) - \Psi_{app}(t)\|_{\mathbb{F}} = \|\overbrace{\Psi_{red}(t) - |\text{vac}\rangle}^{\Psi_{err}}\|_{\mathbb{F}}$ where

$$\Psi_{red}(t) = \mathcal{W}^*(\Phi(t))e^{\mathcal{B}(K(t))}e^{-it\mathcal{H}_N}\mathcal{W}(\Phi_0)|\text{vac}\rangle \; ; \; \Psi_{red}(0) = |\text{vac}\rangle$$

- Compute "reduced Hamiltonian" $\mathcal{H}_{red}$ such that

$$\left(i\frac{\partial}{\partial t} - \mathcal{H}_{red}\right)\Psi_{red} = 0 \iff \left(i\frac{\partial}{\partial t} - \mathcal{H}_{red}\right)\Psi_{err} = \mathcal{H}_{red}|\text{vac}\rangle$$

$$(\Psi_{err}(0) = 0)$$

- Find PDEs for Φ, K such that $\|\mathcal{H}_{red}|\text{vac}\rangle\|_{\mathbb{F}}$ be small.

Elements of proof

- (Polynomial-type) Structure of ``reduced Hamiltonian'':

Elimination of $\psi^* \psi^*$ leads to integro-PDE for K

Tempted to Neglect

Absorbed in phase fac.

Quadratic

$$\mathcal{H}_{\rm red} = N\, e_0 + \sqrt{N}\mathfrak{H}_1 + N^0\ \mathfrak{H}_2 + N^{-1/2}\ \mathfrak{H}_3 + N^{-1}\ \mathfrak{H}_4$$

Linear in ψ and ψ^*

$()\psi^*\psi^*$
$+()\psi^*\psi$
$+()\psi\psi$

Cubic

Quartic

Elimination leads to mean field Φ

- Show that PDE for K has global in time solution in appropriate space.
- Estimate error for Ψ from last two terms, $\mathfrak{P}_3$ and $\mathfrak{P}_4$.

In particular: Stationary mean field dynamics:

$$\mathfrak{H}_1 = \int_{\mathbb{R}^3} dx \, \{h(x)\psi^*(x) + h^*(x)\psi(x)\}$$

$$h(x) = -\Delta_x \Phi + (\upsilon \star |\Phi|^2)\Phi - \lambda\Phi$$

Elimination of $\mathfrak{H}_1$ by $h(x) = 0$:

$\Rightarrow$ Mean field Hartree dynamics as approximation for $N \gg 1$

Note: operator algebra for $\mathcal{H}_{red}$

This involves computing

$$\frac{\partial}{\partial t}\left(e^{\sqrt{N}\mathcal{A}(t)}e^{\mathcal{B}(t)}e^{-it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(0)}|\mathrm{vac}\rangle\right)$$

Note that

$$\left(\frac{\partial}{\partial t}e^{\mathcal{B}(t)}\right)e^{-\mathcal{B}(t)} = \dot{\mathcal{B}} + \frac{1}{2!}[\dot{\mathcal{B}},\mathcal{B}] + \dots$$

Observation: This computation can be facilitated by using a nice one-to-one mapping from algebra of 2x2 matrices to that of Boson operators in Fock space

$$M \mapsto \mathcal{I}(M) \in \mathbb{F}$$

2x2 matrix

``Lie algebra isomorphism''

In particular,

Easy to compute

$$\mathcal{B} = \mathcal{I}(\mathfrak{K}), \quad \mathfrak{K} = \begin{pmatrix} 0 & K^* \\ K & 0 \end{pmatrix}: \quad \left(\frac{\partial}{\partial t}e^{\mathcal{B}(t)}\right)e^{-\mathcal{B}(t)} = \mathcal{I}\left(\left(\frac{\partial}{\partial t}e^{\mathfrak{K}(t)}\right)e^{-\mathfrak{K}(t)}\right)$$

Open questions

- Error estimate for Gross-Pitaevskii dynamics (α=1)?

Partial results by Grillakis, Machedon (2014) for 0<α<1/3.

- Rigorous derivation with a trapping potential?

$$\textbf{Conjecture}: \quad \|\Psi_{N,ex}(t) - \Psi_{N,app}(t)\|_{\mathbb{F}} < \frac{C(t)}{\sqrt{N}}, \quad N \gg 1$$

- How can one go beyond the pair excitation ansatz?

Issues of timescale.

- What is the corresponding pair-excitation formalism for finite temperatures below the phase transition?

Emergence of quantum fluids: Navier-Stokes-type PDEs do not hold.