Uniform in N estimates for a Bosonic system of Hartree-Fock-Bogoliubov type

Joint work with **M. Grillakis**

Overview of the problem:

Approximate symmetric solutions to the many-body problem

$$\frac{1}{i}\frac{\partial}{\partial t}\psi_N(t, x_1, \cdots x_N) = H_N \psi_N(t, x_1, \cdots x_N)$$
$$\psi_N(0, x_1, \cdots x_N) = (\text{or} \sim)\phi_0(x_1)\phi_0(x_2)\cdots\psi_0(x_N)$$

where

$$H_N = \sum_{j=1}^{N} \Delta_{x_j} - \frac{1}{N}\sum_{i<j} v_N(x_i - x_j)$$

N is large but fixed, $x_k \in \mathbb{R}^3$, $v \in \mathcal{S}$, and $0 < \beta \leq 1$ and $v_N(x) = N^{3\beta} v(N^\beta x)$. Approximate ψ_N with combinations of solutions to a non-linear PDE in much fewer variables

One answer: NLS and Gross-Pitaevskii equations

$$\psi_N(t, x_1, \cdots x_N) \sim \phi(t, x_1)\phi(t, x_2)\cdots\phi(t, N)$$

where ϕ satisfies

$$\frac{1}{i}\frac{\partial}{\partial t}\phi - \Delta\phi + c|\phi|^2\phi = 0$$

The coupling constant changes from
$\beta < 1$ ($c = \int v$)
to $\beta = 1$ ($c =$ scattering length of v).

Rigorous work by Erdös, Schlein and Yau.

A proposed more detailed answer than NLS: "Hartree-Fock-Bogoliubov equations".

The approximation involves not only a $\phi(t,x)$ but also a function $k(t,x,y)$.

Something like this is well-known. Usually, ϕ is taken to be a solution to NLS, while k is determined by an elliptic equation involving ϕ.

TDHFB equations for Bosons also address this, and are not well-known. They are a coupled system of Schrödinger type equations in $3+1$ variables and $6+1$ variables.

The equations were derived by M. Grillakis and me (2013) and are closely related to those derived independently by **Bach, Breteaux, T. Chen, Fröhlich and Sigal** .

They are similar in spirit to the Hartree-Fock-Bogoliubov equations used in the Physics literature for Fermions.

Our work is based on earlier work with D. Margetis.

HFB equations share common features with BBGKY.

Background: BBGKY and the work of Erdös, Schlein and Yau.

For ψ satisfying

$$\frac{1}{i}\frac{\partial}{\partial t}\psi_N(t, x_1, \cdots x_N) = H_N \psi_N(t, x_1, \cdots x_N)$$

Consider $\bar{\psi}_N(t, \mathbf{x})\psi_N(t, \mathbf{y})$, average out most variables, and look at the marginal density "matrices"

$$\gamma_N^{(k)}(t, \mathbf{x_k}, \mathbf{y_k})$$
$$= \int \bar{\psi}_N(t, \mathbf{x_k}, \mathbf{x_{N-k}})\psi_N(t, \mathbf{y_k}, \mathbf{x_{N-k}})\mathbf{dx_{N-k}}$$

These satisfy a hierarchy of equations, for all N $\gamma_N^{(k)}$ "matrices":

$$\left(\frac{1}{i}\frac{\partial}{\partial t}+\Delta_{x_1}-\Delta_{y_1}\right)\bar{\gamma}_N^{(1)}(t,x_1;y_1)$$
$$=\frac{N-1}{N}\int v_N(x_1-x_2)\bar{\gamma}_N^{(2)}(t,x_1,x_2;y_1,x_2)dx_2$$
$$-\frac{N-1}{N}\int v_N(y_1-y_2)\bar{\gamma}_N^{(2)}(t,x_1,y_2;y_1,y_2)dy_2$$

$$\left(\frac{1}{i}\frac{\partial}{\partial t}+\left(\Delta_{x_1,x_2}-\frac{1}{N}v_N(x_1-x_2)\right)\right.$$
$$\left.-\left(\Delta_{y_1,y_2}-\frac{1}{N}v_N(y_1-y_2)\right)\right)\bar{\gamma}_N^{(2)}(t,x_1,x_2;y_1,y_2)$$
$$=\frac{N-2}{N}\int v_N(x_1-x_3)\bar{\gamma}_N^{(3)}(t,x_1,x_2,x_3;y_1,y_2,x_3)dx_3$$
$$+\frac{N-2}{N}\int v_N(x_2-x_3)\bar{\gamma}_N^{(3)}(t,x_1,x_2,x_3;y_1,y_2,x_3)dx_3$$
$$-\frac{N-2}{N}\int v_N(y_1-y_3)\bar{\gamma}_N^{(3)}(t,x_1,x_2y_3;y_1,y_2,y_3)dy_3$$
$$-\frac{N-2}{N}\int v_N(y_2-y_3)\bar{\gamma}_N^{(3)}(t,x_1,x_2y_3;y_1,y_2,y_3)dy_3$$
$$\ldots$$

Formally, as $N \to \infty$,

$$\gamma_N^{(k)} \to \gamma^{(k)}$$

satisfies Gross-Pitaevskii hierarchy

$$\left(\frac{1}{i}\frac{\partial}{\partial t} + \Delta_{x_1} - \Delta_{y_1}\right)\bar{\gamma}^{(1)}(t, x_1; y_1)$$
$$= c\bar{\gamma}^{(2)}(t, x_1, x_1; y_1, x_1)$$
$$- c\bar{\gamma}_N^{(2)}(t, x_1, y_1; y_1, y_1)$$
$$\cdots$$

which admits solutions

$$\bar{\gamma}^{(1)} = \phi(t, x_1)\bar{\phi}(t, y_1)$$
$$\bar{\gamma}^{(2)} = \phi(t, x_1)\phi(t, x_2)\bar{\phi}(t, y_1)\bar{\phi}(t, y_2)$$

where

$$\left(\frac{1}{i}\frac{\partial}{\partial t} + \Delta\right)\phi - c|\phi|^2\phi = 0$$

The well-known work of Elgart, Erdos, Schlein and Yau: this is true for $\beta < 1$ with $c = \int v$, and c scattering length of v for $\beta = 1$.

Heuristically, the change of coupling constant when $\beta = 1$ comes from the fact that the true form of $\gamma_N^{(2)}$ is closer to

$$
\begin{aligned}
&\bar{\gamma}_N^{(2)} \\
=&\phi(t, x_1)\phi(t, x_2) f_N(x_1, x_2) \\
&\bar{\phi}(t, y_1)\bar{\phi}(t, y_2) f_N(y_1, y_2)
\end{aligned}
$$

and f_N accounts for correlations.

In previous work, f_N (related to our k) is determined by an elliptic equation

$$\left(-\Delta + \frac{1}{2N} v_N(x)\right) f_N(x) = 0$$
$$\lim_{x \to \infty} f_N(x) = 1$$

(Green will always refer to objects determined by this type of elliptic equation, while blue will be reserved to objects determined through HFB.)

The HFB equations are a coupled system of Schrödinger-type PDEs for for ϕ_N (denoted ϕ, representing "the condensate"), $\Gamma_N = \Gamma$ (a Fock space $\gamma_N^{(1)}$ matrix)
and $\Lambda_N(t, x_1, x_2) = \Lambda(t, x_1, x_2)$ which plays the role of $\phi_N(t, x_1)\phi_N(t, x_2) f_N(x_1, x_2)$,
but also allows the correlations to form dynamically in time.

The HFB equations are derived in Fock space, which has been used in order to get estimates for the rate of convergence of the approximation to the exact solution.

First one for marginal densities $\gamma_N^{(k)}$: Rodnianski and Schlein (2009).

First one for $L^2(\mathbb{R}^N)$ through Fock space: Grillakis, M, Margetis (2010).

Efficient direct estimates in $L^2(\mathbb{R}^N)$ (using Fock space type estimates) Lewin, Nam and Schlein (2015).

Inspired by older work of Hepp (1974), Ginibre and Velo (1979).

One model (analysts' Fock space), which suggests useful analogies:

$$
\begin{aligned}
&\mathcal{F} = L^2(\mathbb{R}^n) \\
&\Omega = e^{-\frac{|x|^2}{2}} \\
&a_i^* = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial x_i} + x_i\right) \\
&a_i = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x_i} + x_i\right) \\
&[a_i, a_j^*] = \delta_{ij}
\end{aligned}
$$

Exponentials of skew-Hermitian linear and quadratic expressions in creation and annihilation operators are well-known to analysts. (I learned them from Folland's book "Harmonic analysis in phase space").

Switch to physicists' symmetric Fock space (different space, same algebra)

$\mathcal{F} = \{(\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \psi_3(x_1, x_2, x_3), \cdots)\}$

with $l^2(L^2)$ inner product and norm. For $f \in L^2(\mathbb{R}^3)$ the (unbounded, closed, densely defined) creation operator $a^*(f) : \mathcal{F} \to \mathcal{F}$ and annihilation $a(\bar{f}) : \mathcal{F} \to \mathcal{F}$ are defined by

$$\left(a^*(f)\psi_{n-1}\right)(x_1, x_2, \cdots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\psi_{n-1}(x_1, \cdots, x_{j-1}, x_{j+1}, \cdots x_n)$$

and

$$\left(a(\overline{f})\psi_{n+1}\right)(x_1, x_2, \cdots, x_n) = \sqrt{n+1} \int \psi_{(n+1)}(x, x_1, \cdots, x_n)\overline{f}(x)dx$$

Also, define the operator valued distributions a_x^* and a_x defined by

$$a^*(f) = \int f(x) a_x^* dx$$
$$a(\overline{f}) = \int \overline{f}(x) a_x dx$$

These satisfy the canonical relations

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

$H_N : \mathcal{F} \to \mathcal{F}$ defined by

$$H_N = \int a_x^* \Delta a_x dx - \frac{1}{2N} \int v(x - y) a_x^* a_y^* a_x a_y dx dy$$

H_N is a diagonal operator on $\mathcal{F}$ which acts on each component ψ_n as a PDE Hamiltonian

$$H_{N,n} = \sum_{j=1}^{n} \Delta_{x_j} - \frac{1}{N} \sum_{i<j} v(x_i - x_j)$$

Let $\phi \in L^2(\mathbb{R}^3)$ Define

$$A(\phi) = a(\overline{\phi}) - a^*(\phi)$$
$$e^{-\sqrt{N}A(\phi)} \text{ (= Weyl operator)}$$

(Stone-von Neumann representation of the "Heisenberg group" $= L^2(\mathbb{R}^n, \mathbb{C}) \times \mathbb{R}$ with symplectic inner product $\Im \int f\bar{g}$)
Let $\Omega = (1, 0, 0, \cdots) \in \mathcal{F}$ and

$$e^{-\sqrt{N}A(\phi)}\Omega$$
$$= e^{-N/2}\left(1, \cdots, \left(\frac{N^n}{n!}\right)^{1/2} \phi(x_1)\cdots\phi(x_n), \cdots\right)$$

is a coherent state, similar to a wave packet in classical PDEs/analysis.

Introduce the pair excitation function $k(t,x,y)$ via

$$\mathcal{B} = \frac{1}{2}\int \left(\overline{k}(t,x,y)a_x a_y - k(t,x,y)a_x^* a_y^*\right) dxdy$$

$$e^{\mathcal{B}} = \text{ metaplectic representation}$$

of the "real" symplectic matrix,

$$\exp\begin{pmatrix} 0 & \overline{k} \\ k & 0 \end{pmatrix} = \begin{pmatrix} \text{ch}(k) & \overline{\text{sh}(k)} \\ \text{sh}(k) & \overline{\text{ch}(k)} \end{pmatrix}$$

called Bogoliubov transformations by mathematical physicists. Here

$$\text{ch}(k)(t,x,y) = \delta(x-y) + \frac{1}{2}\overline{k} \circ k + \cdots$$

In the analysts' Fock space, this is related to $e^{it\,(\Delta+|x|^2)}$, and the lens transform.

Interesting to note that the theory of Bogoliubov transformations or metaplectic representation evolved independently in Physics and Math.

Shale's 1962 paper "Linear symmetries of free Boson fields" makes no reference to Bogoliubov.

Bogoliubov's 1947 paper makes no reference to the Stone and Von Neumann theorem from 1931. This states that any two unitary irreducible representations of the (finite dimensional) Heisenberg group (with an additional assumption) are conjugated by (the implementation/representation of a) Bogoliubov transformation.

Formal derivation of HFB equations

Start with initial conditions which are pure tensor products

$$e^{-\sqrt{N}A(\phi_0)}\Omega$$
$$= e^{-N/2}\left(1, \cdots, \left(\frac{N^n}{n!}\right)^{1/2} \phi_0(x_1)\cdots\phi_0(x_n), \cdots\right)$$

or more general initial conditions which include correlations

$$e^{-\sqrt{N}A(\phi_0)}e^{B(k_0)}\Omega = (?, ??, \cdots)$$

(similar to the above, but also include th$(k)(x_i, x_k)$). Evolve these under the exact Hamiltonian

$$\Psi_{exact} = e^{itH_N}e^{-\sqrt{N}A(\phi_0)}e^{B(k_0)}\Omega$$

and impose two PDEs for ϕ and k so Ψ_{exact} is approximated, in Fock space, by

$$\Psi_{approx} = e^{-\sqrt{N}A(\phi(t))}e^{-B(k(t))}\Omega$$

Early papers: Hartree equation for ϕ plus an equation for k with coefficients depending on ϕ. Provide a Fock space approximation for $\beta < 1/3$ (Grillakis, M) and $\beta < 1/2$ (**Kuz**). Extended/adapted by **Nam and Napiorkowski** for Hartree states (fixed N).

Hartree states approach: **Lewin, Nam and Schlein**.

Alternative approach: **Benedikter, de Oliveira and Schlein (2015)**, as well as **Bocatto, Cenatiempo and Schlein (2017)**, : Impose the expected GP equation for ϕ and define k by an explicit formula.

For $\beta = 1$, the formula is in the spirit of

$$k(t, x, y) = -N\phi(t, x)\phi(t, y)w(N(x - y)$$

where

$$\left(-\Delta + \frac{1}{2}v\right)(1 - w) = 0$$

while for $\beta < 1$ this has to be modified but is similar in spirit.
Then $\Psi_{approx} = e^{-\sqrt{N}A(\phi(t))}e^{-B(k(t))}\Omega$ provides an approximation for Ψ_{exact} in the sense of marginal densities if $\beta = 1$. Also Ψ_{approx} modified by an additional unitary transformation provides a Fock space norm approximation if $\beta < 1$.

k accounts for correlations, and these have to be present in the initial conditions.

Our approach: the Hartree-Fock-Bogoliubov PDEs:

$$\|e^{it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(\phi_0)}e^{-\mathcal{B}(k(0))}\Omega - e^{-\sqrt{N}\mathcal{A}(\phi(t))}e^{-\mathcal{B}(k(t))}\Omega\|$$
$$= \|e^{\mathcal{B}(k(t))}e^{\sqrt{N}\mathcal{A}(\phi(t))}e^{it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(\phi_0)}e^{-\mathcal{B}(k(0))}\Omega - \Omega\|$$

This leads to
$U(t) = e^{\mathcal{B}(k(t))}e^{\sqrt{N}\mathcal{A}(\phi(t))}e^{it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(\phi_0)}e^{-\mathcal{B}(k(0))}$
which satisfies an evolution equation in Fock space:

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \mathcal{H}_{\text{red}}\right)U(t)\Omega = 0$$
$$U_{\text{red}}(0)\Omega = \Omega$$

($\mathcal{H}_{\text{red}} =$ " reduced Hamiltonian", can be computed explicitly.)

$U(t)\Omega = \Omega$ would correspond to an exact solution, which would follow if Ω satisfied the same equation as $U_{\text{red}}(t)\Omega$, namely

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \mathcal{H}_{\text{red}}\right)\Omega = 0$$

This, of course, is not possible

In reality, Ω satisfies

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \mathcal{H}_{\text{red}}\right)\Omega = -\mathcal{H}_{\text{red}}\Omega$$
$$= (X_0, X_1, X_2, X_3, X_4, 0, \cdots)$$

($X_i = X_i(\phi, k)$, can be computed explicitly). Impose two equations in two unknowns (ϕ and k).

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \mathcal{H}_{\text{red}}\right)\Omega = -\mathcal{H}_{\text{red}}\Omega$$
$$= (X_0, 0, 0, X_3, X_4, 0, \cdots)$$

$$X_1 = 0 \text{ and } X_2 = 0.$$

are the time-dependent Hartree-Fock-Bogoliubov equations in abstract form.

Based on just this one can see that the expected number of particles

$$\left\langle e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))}\Omega, \mathcal{N} e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))}\Omega \right\rangle$$

(where $\mathcal{N} = \int a_x^* a_x dx$ is the number operator), as well as the energy

$$\left\langle e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))}\Omega, \mathcal{H} e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))}\Omega \right\rangle$$

and energy are preserved by the approximate evolution. (Explicit formulas are also available). Also, the equations are E.L. equations for $\int X_0$.

Similar results were obtained by Bach, Breteaux, Chen, Fröhlich and Sigal.

In their most concrete elegant form , the HFB equations are expressed in terms of the "generalized marginal density matrices" (fix some of the variables, average in the rest)

$$\mathcal{L}_{m,n}(t, x_1, \ldots, x_m; y_1, \ldots, y_n) := \frac{1}{N^{\frac{n+m}{2}}} \left\langle a_{x_1}, \cdot, a_{x_m} e^{-\sqrt{N}\mathcal{A}} e^{-\mathcal{B}} \Omega,\ a_{y_1}, \cdot, a_{y_n} e^{-\sqrt{N}\mathcal{A}} e^{-\mathcal{B}} \Omega \right\rangle$$

Also, it turns out that

$$\mathcal{L}_{0,1}(t, x) = \phi(t, x)$$

$$\mathcal{L}_{1,1}(t, x, y) = \overline{\phi}(t, x)\phi(t, y) + \frac{1}{N}(\overline{\mathrm{sh}(k)} \circ \mathrm{sh}(k))(t, x, y)$$

$$:= \Gamma(t, x, y)$$

$$\mathcal{L}_{0,2}(t, x, y) = \phi(t, x)\phi(t, y) + \frac{1}{2N}\mathrm{sh}(2k)(t, x, y)$$

$$:= \Lambda(t, x, y)$$

and all the higher $\mathcal{L}$ matrices can be expressed in terms of these.

Explicitly, the three Hartree-Fock-Bogoliubov equations are:

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \Delta_{x_1}\right)\mathcal{L}_{0,1}(t,x_1)$$
$$= -\int v_N(x_1-x_2)\mathcal{L}_{1,2}(t,x_2;x_1,x_2)dx_2$$

$$\left(\frac{1}{i}\frac{\partial}{\partial t} + \Delta_{x_1} - \Delta_{y_1}\right)\mathcal{L}_{1,1}(t,x_1;y_1)$$
$$= \int v_N(x_1-x_2)\mathcal{L}_{2,2}(t,x_1,x_2;y_1,x_2)dx_2$$
$$- \int v_N(y_1-y_2)\mathcal{L}_{2,2}(t,x_1,y_2;y_1,y_2)dy_2$$

(BBGKY, with $\mathcal{L}_{i,i} = \gamma_N^{(i)}$!)

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \Delta_{x_1} - \Delta_{x_2} + \frac{1}{N}v_N(x_1-x_2)\right)\mathcal{L}_{0,2}(t,x_1,x_2)$$
$$= -\int v_N(x_1-y)\mathcal{L}_{1,3}(t,y;x_1,x_2,y)dy$$
$$- \int v_N(x_2-y)\mathcal{L}_{1,3}(t,y;x_1,x_2,y)dy$$

The similarity with BBGKY has been exploited by **Jacky Chong** in his thesis. Following work by **T. Chen, Pavlovic and Tzirakis** on the G-P hierarchy, he obtained Morawetz and interaction Morawetz type estimates for solutions to HFB.

More explicit form of HFB: First equation

$$
\begin{aligned}
&\left(\frac{1}{i}\partial_t - \Delta_{x_1}\right)\phi(x_1)\\
&= -\left(\int \left(v_N(x_1-y)\Gamma(y,y)\right)dy\right)\phi(x_1)\\
&- \int v_N(x_1-y)\Gamma(y,x_1)\phi(y)dy\\
&+ \int v_N(x_1-y)\Lambda(x_1,y)\overline{\phi}(y)dy
\end{aligned}
$$

In the pure tensor product case ($k = 0$), if one forgets the coupling and sets

$$\Gamma(t, x, y) = \overline{\phi}(t, x)\phi(t, y)$$
$$\Lambda(t, x, y) = \phi(t, x)\phi(t, y)$$

the RHS of the previous equation is just $-\left(v_N * |\phi|^2\right)\phi$, and the equation would just be Hartree:
$\left(\frac{1}{i}\partial_t - \Delta\right)\phi + \left(v_N * |\phi|^2\right)\phi = 0$

Second equation, which rules out $k = 0$:

$$\left(\frac{1}{i}\partial_t - \Delta_{x_1} - \Delta_{x_2} + \frac{1}{N}v_N(x_1 - x_2)\right)\Lambda(x_1, x_2)$$
$$= -\left(\int v_N(x_1 - y)_{sym}\Gamma(y, y)dy\right)\Lambda(x_1, x_2)$$
$$-\int \Big(v_N(x_1 - y)\Big)_{sym}\Big(\Lambda(x_1, y)\Gamma(y, x_2)\Big)_{sym}dy$$
$$+ 2\int dy\left\{\Big(v_N(x_1 - y)\Big)_{sym}|\phi(y)|^2\phi(x_1)\phi(x_2)\right\}$$

$$\Big(f(x_1, x_2)_{sym} = f(x_1, x_2) + f(x_2, x_1)\Big).$$

In a hypothetical tensor product case,

$$\Gamma(t,x,y) = \overline{\phi}(t,x)\phi(t,y)$$
$$\Lambda(t,x,y) = \phi(t,x)\phi(t,y)$$

the RHS would be $-(v_N{*}|\phi|^2)(x_1)\phi(x_1)\phi(x_2) - (v_N{*}|\phi|^2)(x_2)\phi(x_2)\phi(x_1)$, but the potential forces correlations to form and rules out tensor product solutions.

The expectation is that Λ, for $t > 0$, should behave like

$$\Lambda(t,x,y) \sim \phi(t,x)\phi(t,y)(1 - N^{1-\beta}\omega(N^{\beta}(x-y)$$

even if $\Lambda(0,x,y) = \phi_0(x)\phi_0(y)$.

$$
\begin{aligned}
&\Big(\frac{1}{i}\partial_t - \Delta_{x_1} + \Delta_{x_2}\Big)\overline{\Gamma}(x_1, x_2)\\
&= -\int dy\left\{v_N(x_1-y)_{a-sym}\Lambda(x_1,y)\overline{\Lambda}(y,x_2)\right\} +\\
&- \int dy\Big\{v_N(x_1-y)_{a-s}\Big(\overline{\Gamma}(x_1,y)\overline{\Gamma}(y,x_2)\\
&+ \overline{\Gamma}(y,y)\overline{\Gamma}(x_1,x_2)\Big)\Big\}\\
&+ 2\int dy\left\{v_N(x_1-y)_{a-sym}|\phi(y)|^2\phi(x_1)\overline{\phi}(x_2)\right\}
\end{aligned}
$$

Again, if $k = 0$, this is just the Hartree equation.

HFB are a generalization of the Hartree equation which includes the mechanism for correlation formation. They do not have C^∞ solutions (uniformly in N). This is a natural "existence with low regularity" problem. The window between the minimum regularity needed ($H^{\frac{1}{2}}$ for ϕ, $H^{\frac{1}{2},\frac{1}{2}}$ for Λ and Γ and the maximum regularity allowed seems to be very small.

If $\phi = \Lambda = 0$ and some of the signs (and scaling) are changed, this is HFB for Fermions.

Conserved quantities: Conservation of the number of particles and energy

The total number of particles (divided by N) is

$$\int \Gamma(t,x,x)dx = \|\phi(t)\|^2_{L^2(dx)} + \frac{1}{N}\|\mathrm{sh}(k)(t)\|^2_{L^2(dxdy)}$$

This allows, in principle, for $\|\mathrm{sh}(k)(t)\|^2_{L^2(dxdy)}$ to become as large as N in finite time, which seems wrong, if one believes

$$\begin{aligned} k(t,x,y) =&\sim N\phi(t,x)\phi(t,y)w(N(x-y) \\ &\sim \frac{\phi(t,x)\phi(t,y)}{|x-y|} \end{aligned}$$

where ϕ satisfies NLS with $H^{\frac{1}{2}}$ data, and w is bounded and $w(Nx) \sim \frac{1}{N|x|}$ if $N|x|$ is large.

The estimates that follow will show that in fact,

$\|\mathrm{sh}(k)(t)\|_{L^\infty([0,T])L^2(dxdy)} \leq C(T)$ (indep of N)

The energy is

$$\int \nabla_x \cdot \nabla_y \Gamma(t,x,y)\Big|_{x=y} dx + (positive)$$
$$= \|\nabla \phi(t)\|^2_{L^2(dx)} + \frac{1}{2N}\|\nabla_x \mathrm{sh}(k)\|^2_{L^2(dxdy)}$$
$$+ \frac{1}{2N}\|\nabla_y \mathrm{sh}(k)\|^2_{L^2(dxdy)} + (positive)$$

In particular,

$$\|\phi(t)\|_{L^2(dx)} + \|\nabla\phi(t)\|_{L^2(dx)} \le C$$
$$\|\Gamma(t)\|_{L^2(dxdy)} + \|\nabla_x\nabla_y\Gamma(t)\|_{L^2(dxdy)} \le C$$
$$\|\Lambda(t)\|_{L^2(dxdy)} + \||\nabla_x|^{\frac{1}{2}}|\nabla_y|^{\frac{1}{2}}\Lambda(t)\|_{L^2(dxdy)} \le C$$

uniformly in time and N, and in fact

$$\||\nabla_x|^{\frac{1}{2}+\epsilon}|\nabla_y|^{\frac{1}{2}+\epsilon}\Lambda(t)\|_{L^2(dxdy)} \le C(1+t)^\delta$$

This is significant because NLS is locally well-posed locally in time in $H^{\frac{1}{2}}$ (but not below) in 3+1 dimensions.

Therefore, well-posedness for HFB requires at least $\nabla_x^{1/2}\phi_0$
and $\nabla_x^{1/2}\nabla_y^{1/2}\Lambda_0 \in L^2$
and $\nabla_x^{1/2}\nabla_y^{1/2}\Gamma_0 \in L^2$.

The theorem to be stated in the next few slides (for $\beta < 1$) requires initial conditions of regularity within epsilon of these conserved quantities. The conserved energy for Γ scales like H^2, while the conserved energy for Λ scales like H^1. The low regularity of Λ comes from k

$$\Lambda(t,x,y) = \phi(t,x)\phi(t,y) + \frac{1}{2N}\mathrm{sh}(2k)(t,x,y)$$

and

$$\frac{1}{\sqrt{N}} \| |\nabla_x|^{\frac{1}{2}} |\nabla_y|^{\frac{1}{2}} \mathrm{sh}(2k) \|_{L^2(dxdy)} \leq C$$

uniformly in time. But there is "extra regularity" in N.

One can also show, if the initial conditions are sufficiently smooth,

$$\|\|\nabla_x \nabla_y \mathsf{sh}(2k)\|_{L^2(dxdy)} \lesssim (1+t)N^{power}$$

This was done by Jacky Chong for $\beta < 2/3$, but the argument also works for $\beta < 1$. An interpolation argument shows

$$\|\,|\nabla_x|^{\frac{1}{2}+\epsilon}|\nabla_y|^{\frac{1}{2}+\epsilon}\Lambda\|_{L^2(dxdy)} \leq C(1+t)^{\delta}$$

The main result.

The norms

Fix $\alpha > \frac{1}{2}$, so that $2\alpha\beta < 1$. $0 < T < 1$ and $c(t)$ = characteristic function of $[0, T]$.

$$
\begin{aligned}
& N_T(\Lambda) \\
=& \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} c(t)\Lambda \|_{L^2(dt)L^6(dx)L^2(dy)} \\
& + \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} c(t)\Lambda \|_{L^\infty(dt)L^2(dx)L^2(dy)} \\
& + \text{same norm with } x \text{ and } y \text{ reversed} \\
& + \sup_w \| < \nabla >^{\alpha} c(t)\Lambda(t, x, x+w) \|_{L^2(dtdx)} \\
& + \sup_w \| \left|\partial_t\right|^{\frac{1}{4}} c(t)\Lambda(t, x, x+w) \|_{L^2(dtdx)}
\end{aligned}
$$

$$
\begin{aligned}
& \dot{N}_T(\Gamma) \\
=& \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} c(t)\Gamma \|_{L^2(dt)L^6(dx)L^2(dy)} \\
& + \text{same norms with } x \text{ and } y \text{ reversed} \\
& \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} c(t)\Gamma \|_{L^\infty(dt)L^2(dx)L^2(dy)} \\
& + \sup_w \| < \nabla >^{\alpha - \frac{1}{2}} |\nabla|^{\frac{1}{2}} c(t)\Gamma(t, x, x+w) \|_{L^2(dtdx)}
\end{aligned}
$$

$$
\begin{aligned}
& N_T(\phi) \\
=& \| < \nabla_x >^\alpha c(t)\phi \|_{L^2(dt)L^6(dx)} \\
& + \| < \nabla_x >^\alpha c(t)\phi \|_{L^\infty(dt)L^2(dx)}
\end{aligned}
$$

The non-linear theorem:

Assume v is a Schwartz function with $\widehat{v}$ supported in the unit ball, such that $|\widehat{v}| \leq \widehat{w}$ with w a Schwartz function. Then there exists, $N_0 \in \mathbb{N}$ and T_0 such that, if $0 < T < T_0$ and $N \geq N_0$,

$$
\begin{aligned}
&N_T\,(\Lambda) + \dot{N}_T\,(\Gamma) + N_T\,(\phi) \\
&\lesssim \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} \Lambda(0,\cdot) \|_{L^2} + \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} \Gamma \\
&+ \| < \nabla_x >^{\alpha} \phi(0,\cdot) \|_{L^2}
\end{aligned}
$$

Similar estimates hold for differences, and derivatives which commute with the potential.

It is not clear if something like this holds for $\beta = 1$.

The RHS evaluated at T (rather than 0) grows sub-linearly in time, so this provides global estimates.

To prove this, $X^{s,b}$ spaces are needed.

Denote

$$\mathbf{S} = \frac{1}{i}\partial_t - \Delta_x - \Delta_y$$

so that he symbol of $\mathbf{S}$ is $\tau + |\xi|^2 + |\eta|^2$ Recall

$\|\Lambda\|_{X^\delta} = \| < \tau + |\xi|^2 + |\eta|^2 >^\delta \widehat{\Lambda}(\tau, \xi, \eta)\|_{L^2(d\tau d\xi d\eta)}$

The theorem follows from linear estimate:

Let

$$\mathbf{S}\Lambda = \frac{1}{N} v_N(x-y)\Lambda + F$$
$$\Lambda(0) = \Lambda_0$$

Then for all $\delta > 0$ sufficiently small, the following holds, uniformly in N.

$$N_T(\Lambda) \lesssim_\delta \| < \nabla_x >^\alpha < \nabla_y >^\alpha \Lambda_0 \|$$
$$+ \| < \nabla_x >^\alpha < \nabla_y >^\alpha c(t) F \|_{X^{-\frac{1}{2}+\delta}}$$
$$+ \max\{ \| < \nabla_x >^\alpha < \nabla_y >^{\alpha - \frac{1}{2}} c(t) F \|_{X^{-\frac{1}{4}-\delta}},$$
$$\| < \nabla_x >^{\alpha - \frac{1}{2}} < \nabla_y >^\alpha c(t) F \|_{X^{-\frac{1}{4}-\delta}} \}$$

The presence of $X^{-\frac{1}{4}}$ on the RHS, and $|\partial_t|^{\frac{1}{4}}$ on the LHS, is unusual. They are related.

Ingredients in the proof:
Let $\left(\frac{1}{i}\partial_t - \Delta_{x_1} + \Delta_{x_2}\right)\Gamma = 0$.
Estimating $\|\Gamma(t,x,x)\|_{L^2(dtdx)}$ using space-time Fourier transform: going back to estimates for the wave equation from the early 90s **Klainerman-M, Beals-Bezard**. More recently **T. Chen-Pavlovic, X. Chen -Holmer** . Another approach for

$$\|\Gamma(t,x,x)\|_{L^{p/2}(dt)L^{q/2}(dx)} \lesssim \|\Gamma_0\|_{Schatten\ norm}$$

due to **Frank and Sabin**.

The two methods give different types of results (except in 1+1 dimensions, where they almost agree).

If $\left(\frac{1}{i}\partial_t - \Delta_{x_1} - \Delta_{x_2}\right)\Lambda = 0$, estimates for $\|\Lambda(t,x,x)\|_{L^2(dtdx)}$ can also be obtained using the space-time Fourier transform using "old" techniques. Explicitly, If $\mathbf{S}\Lambda = 0$ then

$$\sup_z \||\nabla|_x^{1/2}\Lambda(t,x,x+z)\|_{L^2(dtdx)}$$
$$\lesssim \||\nabla|_x^{1/2}|\nabla|_y^{1/2}\Lambda_0(x,y)\|_{L^2(dxdy)}$$

Also, if $\alpha > \frac{1}{2}$, $\delta > 0$ then

$$\sup_z \| < \nabla_x >^{\alpha} \Lambda(t,x,x+z)\|_{L^2(dtdx)}$$
$$\lesssim \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} \Lambda\|_{X^{1/2+\delta}}$$

Estimates for

$$\sup_w \| \left|\partial_t\right|^{\frac{1}{4}} c(t)\Lambda(t,x,x+w)\|_{L^2(dtdx)}$$

are new:

Let $c = \chi_{[0,1]}$, $\alpha > \frac{1}{2}$, and let $\Lambda(t,x,y)$, $F(t,x,y)$ such that

$$\Lambda = e^{it\Delta}\Lambda_0 + \int_{-\infty}^{\infty} c(t-s)e^{i(t-s)\Delta}F(s,\cdot)ds$$

(this agrees with Duhamel for $t \in [0,1]$). Then there exists $\epsilon > 0$ such that

$$\begin{aligned} &\sup_w \| \left|\partial_t\right|^{\frac{1}{4}} \left(\Lambda(t,x,x+w)\right) \|_{L^2} \\ &\lesssim \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} \Lambda_0\|_{L^2} \\ &+ \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha} F\|_{X^{-\frac{1+\epsilon}{2}}} \\ &+ \| < \nabla_x >^{\alpha} < \nabla_y >^{\alpha-\frac{1}{2}} F\|_{X^{-\frac{1+2\epsilon}{4}}} \end{aligned}$$

Notice there are no time derivatives on the RHS or the data.

Imposing estimates (say L^2) of time derivatives of the data is restrictive:

If

$$\left(\frac{1}{i}\partial_t - \Delta_x - \Delta_y + \frac{1}{N}v_N(x-y)\right)\Lambda(t,x,y) = 0$$
$$\Lambda(0) = \Lambda_0$$

then

$$\frac{1}{i}\partial_t \Lambda\Big|_{t=0} = \left(\Delta_x + \Delta_y - \frac{1}{N}v_N(x-y)\right)\Lambda_0 \in L^2$$

Λ_0 smooth does not satisfy this (uniformly in N). Correlation must be present in the initial conditions, such as

$$\Lambda_0(x,y) = \phi_0(x)\phi_0(y)(1 - N^{\beta-1}w(N^\beta(x-y))$$

where

$$\left(-\Delta + \frac{1}{2}v\right)(1-w) = 0$$

The main difficulties in proving the linear theorem come from
$\frac{1}{N}v_N(x-y) = N^{3\beta-1}v(N^\beta(x-y))$.

Recall

$$\mathbf{S}\Lambda = \frac{1}{N}v_N(x-y)\Lambda + F$$

Strichartz estimates (say $L^2(dt)L^6(d(x-y))L^2(d(x+y))$ would be easy, but if we differentiate,

$$\begin{aligned}
&\mathbf{S} < \nabla_x >^\alpha < \nabla_y >^\alpha \Lambda \\
&= \frac{1}{N}(< \nabla_x >^\alpha < \nabla_y >^\alpha v_N(x-y))\Lambda + \cdots \\
&\sim \delta(x-y)f(t,x+y) + \cdots
\end{aligned}$$

$(f(t,x+y) = \Lambda(t,\frac{x+y}{2},\frac{x+y}{2}))$. Away from the paraboloid, the space-time Fourier transform of $< \nabla_x >^\alpha < \nabla_y >^\alpha \Lambda$ includes the term

$$\frac{\tilde{f}(\tau,\xi+\eta)}{\tau+|\xi|^2+|\eta|^2}$$

No matter how nice $\tilde{f}$ is,

$$< \tau + |\xi|^2 + |\eta|^2 >^\delta \frac{\tilde{f}(\tau, \xi + \eta)}{\tau + |\xi|^2 + |\eta|^2}$$

will not be in L^2 is $\delta \geq \frac{1}{4}$, so the contribution from this term is only in $X^{\frac{1}{4}-\epsilon}$ in the region where $\xi - \eta$ is big.

The PDE cannot be treated the usual way, estimating the solution in an $X^{1/2}$ type space, and the RHS in an $X^{-1/2}$.

This theorem is proved by using more sophisticated norms which also take frequency localization into account (so that derivatives can hit the high frequency terms):

$$\mathcal{N}(\Lambda) = \| < \nabla_x >^\alpha < \nabla_y >^\alpha P_{|\xi-\eta| \gtrsim N^{\beta'}} c(t)\Lambda\|_{X^{\frac{1}{2}-}}$$
$$+ \| < \nabla_x >^\alpha < \nabla_y >^\alpha P_{|\xi+\eta| \gtrsim N^{\beta'}} c(t)\Lambda\|_{X^{\frac{1}{2}-}}$$
$$+ \| < \nabla_x >^\alpha < \nabla_y >^\alpha P_{|\xi\pm\eta| \lesssim N^{\beta'}} c(t)\Lambda\|_{L^2(dt)L^6(dx)L^2(dy)}$$
$$+ \| < \nabla_x >^\alpha < \nabla_y >^\alpha P_{|\xi\pm\eta| \lesssim N^{\beta'}} c(t)\Lambda\|_{L^\infty(dt)L^2(dx)L^2(dy}$$
$$+ \text{same norm with } x \text{ and } y \text{ reversed}$$
$$+ \sup_w \| < \nabla >^\alpha c(t)\Lambda(t, x+w, x-w)\|_{L^2(dtdx)}$$
$$+ \sup_w \| \left|\partial_t\right|^{1/4} c(t)\Lambda(t, x+w, x-w)\|_{L^2(dtdx)}$$
$$+ \|c(t)\Lambda\|_{X^{\frac{1}{2}-}} + N^{-1}\| < \nabla_x >^\alpha < \nabla_y >^\alpha P_{|\xi-\eta| \lesssim N^{\beta'}, |\xi+\eta}$$

$(\beta < \beta' < 1)$

In other words, the high ($> N^{\beta'}$) frequency part of Λ can be estimated in $X^{\frac{1}{2}-}$, and this implies both the Strichartz and collapsing estimates.

In the low frequency part ($|\xi - \eta| \lesssim N^{\beta}$), the Strichartz estimates are obtained through $X^{\frac{1}{4}}$ + Sobolev techniques, while the collapsing estimates can be seen directly in Fourier space. In the model case, if

$$\mathbf{S}\Lambda = \frac{1}{N}\delta(x-y)f(t,x+y)$$

$\Big($where $f(t,x+y) = \Lambda(t, \frac{x+y}{2}, \frac{x+y}{2})\Big)$ is solved in $[0,1]$ by

$$u = \int_{-\infty}^{\infty} e^{i(t-s)(\Delta_x+\Delta_y)}\delta(x-y)c(s)f(s,x+y)dy$$

then

$$\left|P_{|\xi-\eta|\lesssim N^{\beta}}c(t)\widetilde{\Lambda(t,x,x)}\right| \lesssim \left|\tilde{c f}(\tau,\xi)\right|$$

Future work:

Using work of **Jacky Chong** in the case $\beta < 2/3$ globally in time, it is very likely that one can show, for $\beta < 1$,

$$\|e^{it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(\phi_0)}e^{-\mathcal{B}(k(0))}\Omega - e^{-\sqrt{N}\mathcal{A}(\phi(t))}e^{-\mathcal{B}(k(t))}\Omega\|$$

$$\leq C\frac{e^{t^{power}}}{N^{\frac{1-\beta}{2}}}$$

As stated above, the Fock space errors are of the same nature as those of **Bocatto, Cenatiempo and Schlein**, as well as **very recent L^2 estimates** of **Brennecke, Nam, Napiorkowski, and Schlein**. The main difference is that the proof is based on estimates to a PDE, and there is more freedom in the choice of initial conditions.

Also, $e^{t^{power}}$ may not be optimal. The issue is to get large time estimates for the solutions to HFB. The problem is completely open.

A hard question: what are the large time decay properties ϕ from HFB (uniformly in N)?

The problem involves both difficulties for NLS (Lin and Strauss, greatly simplified by new techniques) and Schrödinger with a potential. In the critical case $\beta = 1$, the potential $N^{3\beta-1}v(N^{\beta}(x-y)) \in L^{\frac{3}{2}}$ uniformly in N. This is more singular than the case considered by Journé, Soffer and Sogge.