Estimates for a system of Hartree-Fock-Bogoliubov type

Joint work with **Jacky Chong , Xin Dong, Manoussos Grillakis and Zehua Zhao, with generalizations by Xiaoqi Huang.**
Based on earlier work with **Dio Margetis**.

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, $x_k \in \mathbb{R}^3$, $v \in \mathcal{S}$, $v \geq 0$ (with additional assumptions) 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, i.e. NLS with a different coupling constant.

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

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 Elgart, 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 $k(t, x, y)$.

A function like k (but not the Schrödinger-like PDE I will talk about) is standard. Usually, ϕ is taken to be a solution to NLS, while k is determined by an elliptic equation involving ϕ.

The HFB equations are a coupled system of Schrödinger type equations in $3 + 1$ variables and $6 + 1$ variables.

The equations were derived in a paper by M. Grillakis and me (2013) and are closely related to those derived independently by **Bach, Breteaux, T. Chen, Fröhlich and Sigal** , and also **Benedikter, Sok, and Solovej** (2018).

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

HFB equations share common features with BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon), used by Elgart, 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":

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

$$\Big(\frac{1}{i}\frac{\partial}{\partial t} + \Big(\Delta_{x_1,x_2} - \frac{1}{N} v_N(x_1 - x_2)\Big)$$

$$- \Big(\Delta_{y_1,y_2} - \frac{1}{N} v_N(y_1 - y_2)\Big)\Big)\bar{\gamma}_N^{(2)}(t, x_1, x_2; y_1, y_2)$$

$$= \frac{N-2}{N}\int v_N(x_1 - x_3)\bar{\gamma}_N^{(3)}(t, x_1, x_2, x_3; y_1, y_2, x_3)dx_3$$

$$+ \frac{N-2}{N}\int v_N(x_2 - x_3)\bar{\gamma}_N^{(3)}(t, x_1, x_2, x_3; y_1, y_2, x_3)dx_3$$

$$- \frac{N-2}{N}\int v_N(y_1 - y_3)\bar{\gamma}_N^{(3)}(t, x_1, x_2 y_3; y_1, y_2, y_3)dy_3$$

$$- \frac{N-2}{N}\int v_N(y_2 - y_3)\bar{\gamma}_N^{(3)}(t, x_1, x_2 y_3; y_1, y_2, y_3)dy_3$$

$\ldots$

Formally, as $N \to \infty$, $v_N \to \delta$ and

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

satisfies the Gross-Pitaevskii hierarchy

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

which admits solutions

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

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.

Fock space 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:

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

Exponentials of skew-Hermitian linear in creation and annihilation (or position and momentum) used for "coherent states".

Exponentials of skew-Hermitian quadratic expressions in creation and annihilation operators: the metaplectic representation. (I learned these 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 by

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

These satisfy the canonical relations

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

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

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

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

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

of the "real" symplectic matrix,

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

($k \in L^2(dxdy)$) called Bogoliubov transformations by mathematical physicists. The conjugation

$e^{\mathcal{B}}\mathcal{A}(\phi)e^{-\mathcal{B}} = \mathcal{A}(symplectic\ transformation)(\phi, \bar{\phi})$

so this is a kind of Egorov theorem.

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

In the analysts' Fock space, $e^{\mathcal{B}}$ 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 a unitary "Bogoliubov transformation".

Formal derivation of HFB equations (Grillakis-M version).

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$(k)(x_i, x_k)$), coming from the "LDU" decomposition of e^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

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

(The linear PDE in N variables is approximated by PDEs in 3 and 6 variavles)

The approach of **Benedikter, de Oliveira and Schlein (2015)**, **Bocatto, Cenatiempo and Schlein (2017)**, and **Caraci, Oldenburg and Schlein (2024)** : Impose the expected NLS 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 $1 - w$, called f earlier,

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

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 $\beta < 1$. This seemed best possible. Very recently (2024), Caraci, Oldenburg and Schlein made a version of this approach give Fock space estimates in the case $\beta = 1$. There is a story here!

k accounts for correlations, and these have to be present in the initial conditions (pure tensor products won't work).

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

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

which satisfies an evolution equation in Fock space:

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

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

$U_{red}(t)\Omega = \Omega$ 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,

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

($X_i = X_i(\phi, k)$, can be computed explicitly). Impose 2 equations in 2 unknowns (ϕ and k).

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

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

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

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

are preserved by the approximate evolution.

Also, the equations are E.L. equations for $\int X_0$.

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

In their concrete 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 HFB 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 equation for Λ, which rules out $k = 0$:

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

$\left(f(x_1, x_2)_{sym} = f(x_1, x_2) + f(x_2, x_1)\right)$,
$v_N(x) = N^{3\beta}v(N^\beta x)$

In simplified form, as $N \to \infty$, and $v_N \to \delta$ on RHS,

$$\left(\frac{1}{i}\partial_t - \Delta_{x_1} - \Delta_{x_2} + \frac{1}{N}v_N(x_1 - x_2)\right)\Lambda(x_1, x_2)$$
$$= -\Gamma(t, x_1, x_1)\Lambda(x_1, x_2) + \cdots$$

with

$$\Gamma(t, x_1, x_2)$$
$$= \overline{\phi}(t, x_1)\phi(t, x_2) + \frac{1}{N}(\overline{\mathrm{sh}(k)} \circ \mathrm{sh}(k))(t, x_1, x_2)$$
$$\Lambda(t, x_1, x_2)$$
$$= \phi(t, x_1)\phi(t, x_2) + \frac{1}{2N}\mathrm{sh}(2k)(t, x_1, x_2)$$

If we neglect v and k, and ϕ satisfied NLS, then Λ and Γ satisfy the above equation. The nonlinearity requires $|\nabla_{x_1}|^{\frac{1}{2}}|\nabla_{x_2}|^{\frac{1}{2}}$ derivatives for well-posedness, and the natural coordinates for the nonlinearity are x_1 and x_2.

For the linear part, if v is "nice" and/or small and $\beta = 1$,
$\frac{1}{N} v_N(x-y) = N^2 v(N(x-y))$ is in the critical space $L^{\frac{3}{2}}(\mathbb{R}^3)$ uniformly in N and decay and Strichartz estimate are available (going back to Journe, Soffer and Sogge, and later Yajima, and more recent results, including those for v in the Kato class.)

But taking $|\nabla_x|^{\frac{1}{2}} |\nabla_y|^{\frac{1}{2}}$ changes the potential in the equation for Λ to (essentially)
$N^3 v(N(x-y))$ for which Strichartz type estimates do not apply - but have a special form, as pointed out by **Daniel Tataru**.

Also, the natural coordinates for the linear part are $x_1 - x_2$ and $x_1 + x_2$.

Part of the proof is going back and forth between x_1, x_2 coordinates and $x_1 - x_2$ and $x_1 + x_2$.

Another part is getting estimates with a RHS in $L^1(d(x-y))L^2(dt\, d(x+y))$ (with additional smoothness in time and $x+y$).

Conserved quantities: Conservation of the number of particles and energy, and an interaction Morawetz estimate

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

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

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 **main theorem** shows that in fact, for $\frac{2}{p}+\frac{3}{q}=\frac{3}{2}$, $2 \le p \le \infty$,

$\|\mathrm{sh}(k)(t)\|_{L^p(dt)L^q(dx)L^2(dy)} \leq C \log N$ (C indep of N) with corresponding estimates for $|\nabla_{x+y}|\mathrm{sh}(k)$ and $\partial_t \mathrm{sh}(k)$. ($\beta < 1$: **Chong, Dong, Grillakis, M. and Zhao**).

And, if $\beta = 1$ (the critical case)

$$\|\mathrm{sh}(k)(t)\|_{L^p(dt)L^q(dx)L^2(dy)} \leq C$$

(but no time derivatives yet). Due to **Xiaoqi Huang.**

Ingredients in the proof

(Elementary) Sobolev, Bernstein, square function estimates in rotated coordinates.

The argument is based on the following lemma:

Let

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -I & I \end{pmatrix}$$

so that $\|f \circ R\|_{L^p(dx)L^q(dy)} = \|f\|_{L^p(d(x-y))L^q(d(x+y))}$. Let $K = K(x)$ and denote $K\delta = K(x)\delta(y)$ (tensor product).

If

$$\|(K\delta) * f\|_{L^{p_1}(dx)L^q(dy)} \lesssim \|f\|_{L^{p_2}(dx)L^q(dy)}$$

Then

$$\|(K\delta) * f\|_{L^{p_1}(d(x-y))L^q(d(x+y))} \lesssim \|f\|_{L^{p_2}(d(x-y))L^q(d(x+y))}$$

Consequence: "Sobolev at an angle" estimate

Let $\alpha > 0$, $1 \leq p, q, \leq \infty$ and assume the Sobolev estimate $\|u\|_{L^p(dx)} \lesssim \|\left\langle \nabla_x \right\rangle^\alpha\|_{L^q(dx)}$ holds. Then

$$\|\Lambda\|_{L^p(d(x-y))L^2(d(x+y))}$$
$$\lesssim \min\{\|\left\langle \nabla_x \right\rangle^\alpha \Lambda\|_{L^q(d(x-y))L^2(d(x+y))},$$
$$\|\left\langle \nabla_y \right\rangle^\alpha \Lambda\|_{L^q(d(x-y))L^2(d(x+y))}\}$$

There are similar Bernstein estimates "at an angle". Also, estimates for a "double square function" in rotated coordinates:

Let $1 < p < \infty$. Then

$$\| \left(\sum_{k',k''} |P_{|\xi|\sim 2^k,\, |\eta|\sim 2^{k'}} f|^2 \right)^{\frac{1}{2}} \|_{L^p(d(x-y))L^2(d(x+y))}$$
$$\sim \|f\|_{L^p(d(x-y))L^2(d(x+y))}.$$

Another ingredient: Collapsing estimates, mix-and-match inhomogeneous Strichartz estimates, and "new" estimate:

Let $\left(\frac{1}{i}\partial_t - \Delta_{x_1} + \Delta_{x_2}\right)\Gamma = 0$.
(or $\frac{1}{i}\partial_t\Gamma - [\Delta, \Gamma] = 0$)

Collapsing estimates, using space-time Fourier transform: going back to estimates for the wave equation from the early 90s **Klainerman-M, Beals-Bezard** -around the same time as Chris made the local smoothing conjecture for the wave equation.

Collapsing estimate:

$$\||\nabla_x|^\alpha \Gamma(t,x,x)\|_{L^2(dtdx)} \le C\|\big\langle\nabla_x\big\rangle^\alpha\big\langle\nabla_y\big\rangle^\alpha\Gamma_0\|_{L^2(dxdy)}$$

True for $\alpha > \frac{1}{2}$, likely not true for $\alpha = \frac{1}{2}$. More generally,

$$\begin{aligned}&\||\nabla_{x+y}|^\alpha \Gamma\|_{L^\infty(d(x-y))L^2(dtd(x+y))}\\ &\le C\|\big\langle\nabla_x\big\rangle^\alpha\big\langle\nabla_y\big\rangle^\alpha\Gamma_0\|_{L^2(dxdy)}\end{aligned}$$

The method was further developed by **Thomas Chen, Younghun Hong and Natasa Pavlovic**, and several other authors.

A side remark: One cannot lower the $L^p(dt\,dx)$ norm on the LHS (**Xiumin Du, M.**)

If

$$\| |\nabla|_x^{\alpha} \Gamma(t,x,x) \|_{L^p(dt)L^q(dx)} \lesssim \| \Gamma_0(x,y) \|_{H^s(dxdy)}$$

for some $\alpha \geq 0, s \geq 0$. Then $p \geq 2$ and $q \geq 2$.

The proof uses estimates for sums of wave packet solutions.

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**. (p, q Strichartz exponents).

(Restriction theorems for orthonormal functions, strichartz estimates and uniform Sobolev estimates)

If $\Gamma(t,x,y) = \bar{\phi}(t,x)\phi(t,x)$ with ϕ satisfying a linear Schrödinger equation, the LHS can be estimates by Strichartz.

If the compact self-adjoint operator Γ has a diagonalization $\Gamma(t,x,y) = \sum_{i=1}^{\infty} \lambda_i \bar{\phi}(t,x)\phi(t,x)$ with ϕ_i orthonormal, the estimate

$$\|\Gamma(t,x,x)\|_{L^{p/2}(dt)L^{q/2}(dx)} \lesssim \sum |\lambda_i| = \|\Gamma_0\|_{Schatten(1)}$$

follows trivially. Such an estimate is not true (without extra derivatives on the LHS and RHS) with the RHS in $L^2 = H - S = Schatten(2)$.

Frank and Sabin found the optimal range of p, q and the optimal Schatten space. Their proof is based on Stein interpolation proof of the restriction theorem. Their method gives different types of results from the K-M method(except in $1+1$ dimensions, where they almost agree).

Their paper also extends uniform Sobolev estimates of Kenig, Ruiz, and Sogge in Schatten spaces.

The corresponding sharp collapsing estimate for the ++ Schrödinger equation holds (with the same type of proof):

If $\left(\frac{1}{i}\partial_t - \Delta_{x_1} - \Delta_{x_2}\right)\Lambda = 0$,

$$\| |\nabla|_{x+y}^{1/2} \Lambda \|_{L^\infty d((x-y)) L^2(dtd(x+y))} \lesssim \| |\nabla|_x^{1/2} |\nabla|_y^{1/2} \Lambda_0(x,y) \|_{L^2(dxdy)}$$

Another ingredient: Generalized Strichartz estimates.

If

$$\left(\frac{1}{i}\partial_t - \Delta_x\right) u = 0$$

$(x \in \mathbb{R}^3)$, $2 \leq p \leq \infty$ and

$$\frac{2}{p} + \frac{3}{q} = \frac{3}{2}$$

then

$$\|u\|_{L^p(dt)L^q(dx)} \leq C\|u_0\|_{L^2}$$

It is straightforward to generalize this to $u(t, x, y)$ satisfying

$$\left(\frac{1}{i}\partial_t - \Delta_x - \Delta_y\right) u = 0$$

then

$$\|u\|_{L^p(dt)L^q(dx)L^2(dy)} \leq C\|u_0\|_{L^2}$$

Such spaces were used by Xuwen Chen and Justin Holmer in the context of BBGKY.

In the proof of the main theorem, one needs "mix-and-match" inhomogeneous estimates: Let

$$\left(\frac{1}{i}\partial_t - \Delta_x - \Delta_y\right) u = f$$

(with initial conditions 0). Then

$$\max\Big\{\|u\|_{L^2(dt)L^6(dx)L^2(dy)}, \|u\|_{L^2(dt)L^6(dy)L^2(dx)},$$
$$\|u\|_{L^2(dt)L^6(d(x-y))L^2(d(x+y))}\Big\}$$
$$\lesssim \min\Big\{\|f\|_{L^2(dt)L^{\frac{6}{5}}(dx)L^2(dy)}, \|f\|_{L^2(dt)L^{\frac{6}{5}}(dy)L^2(dx)},$$
$$\|f\|_{L^2(dt)L^{\frac{6}{5}}(d(x-y))L^2(d(x+y))}\Big\}$$

All quantities on the LHS can be estimated easily for the homogeneous equation, and the non-endpoint inhomogeneous estimate follows by Christ-Kiselev.

Some of the double end-point results follow the Keel-Tao strategy, based on

$$\|u(t)\|_{L^\infty(dx)L^2(dy)} \lesssim \frac{1}{t^{3/2}}\|u(0)\|_{L^1(d(x-y))L^2(d(x+y)}$$

But the dispersive estimate does not hold when flipping x and y - yet Strichartz still works. The proof of this last case has not appeared in print yet.

Regarding

$$\|u(t)\|_{L^\infty(dx)L^2(dy)} \lesssim \frac{1}{t^{3/2}}\|u(0)\|_{L^1(d(x-y))L^2(d(x+y))}$$

after some reductions, this follows from, for any u_k,

$$\sup_{v_k \text{ orthonormal}} \left\| \sum \left(e^{it\Delta} u_k\right) e^{it\Delta} v_k \right\|_{L^2(\mathbb{R}^3)}$$
$$\lesssim \frac{1}{t^{3/2}} \left\| \left(\sum |u_k|^2\right)^{\frac{1}{2}} \right\|_{L^1(\mathbb{R}^3)}.$$

For any $A \in \mathcal{S}(\mathbb{R}^3)$, let $e^{-it\Delta}A(x)e^{it\Delta} = A(x + 2tD)$ where $D = p = \frac{1}{i}\frac{\partial}{\partial x}$, computed by Weyl quantization to have the kernel

$$K_t(x, y) = \frac{1}{(4\pi t)^3}\widehat{A}\left(\frac{-x + y}{2t}\right) e^{-i\frac{|x|^2}{4t}} e^{i\frac{|y|^2}{4t}}$$
$$= B_{t,x}(y) e^{-i\frac{|x|^2}{4t}} e^{i\frac{|y|^2}{4t}}$$

Notice

$$\|B_{t,x}\|_{L^2(dy)} = \frac{c}{t^{\frac{3}{2}}}\|A\|_{L^2}.$$

If $\|A\|_{L^2} = 1$, compute, by duality,

$$
\begin{aligned}
&= \int \sum \overline{e^{it\Delta} u_k}(x) A(x) e^{it\Delta} v_k(x) dx \\
&= \sum < e^{it\Delta} u_k, A e^{it\Delta} v_k > = \sum < u_k, e^{-it\Delta} A e^{it\Delta} v_k > \\
&= \sum < u_k, A(x + 2tD) v_k > \\
&= \sum \int \overline{e^{i\frac{|x|^2}{4t}} u_k(x)} B_{t,x}(y) e^{i\frac{|y|^2}{4t}} v_k(y) dx\, dy
\end{aligned}
$$

from which the estimate follows after additional standard reductions.

As an application of this type of mix-and-match end-point Strichartz estimates, if N_0 is fixed, v is small, one can show that solutions to

$$\left(\frac{1}{i}\partial_t - \sum_{i=1}^{N_0} \Delta_{x_i} + \sum_{i,j=1}^{N_0} N^2 v(N(x_i - x_j)\right) u = 0$$

satisfy

$$\|u\|_{L^p(dt)L^q(dx_1)L^2(dx_2\cdots dx_n)} \lesssim \|u(0)\|_{L^2}$$

(uniformly in N)

The original result of this type is due to **Younghun Hong** (2017), using X and Y spaces.

Our method also gives Strichartz estimates for the inhomogeneous equation.

"New" estimates, going beyond Strichartz Let

$$\left(\frac{1}{i}\partial_t - \Delta_x - \Delta_y\right) u = f$$

where f stands for $N^3 v(N(x-y)\Lambda(t,x,y)$. Then

$$\|u\|_{L^2(dt)L^6(dx)L^2(dy)}$$
$$\lesssim \||\partial_t|^{\frac{1}{4}} f\|_{L^1(d(x-y))L^2(dt)\,d(x+y))}$$
$$+ \||\nabla|^{\frac{1}{2}}_{x+y} f\|_{L^1(d(x-y))L^2(dt\,d(x+y)))}$$

Dyadic version, and non-shart global version : Chong, Dong, Grillakis, M., Zhao.

Strategy: divide by the symbol away from the characteristic set, in the spirit of $X^{s,b}$ spaces, and use Strichartz estimates when $\tau >> |\xi|^2 + |\eta|^2$

Sharp version, using clever additional dyadic decompositions: Xiaoqi Huang.

Linear estimate (Xiaoqi's sharp version) Let

$$\frac{1}{i}\left(\frac{\partial}{\partial t} - \Delta_x - \Delta_y + N^2 v(N(x-y))\right)\Lambda(t,x,y)$$
$$= G$$

($\widehat{v}$ compactly supported, small). Then

$$\|\left\langle \nabla_x \right\rangle^{\frac{1}{2}} \left\langle \nabla_y \right\rangle^{\frac{1}{2}} \Lambda\|_{L^p(dt)L^q(dx)L^2(dy)}$$
$$+ \|\left\langle \nabla_{x+y} \right\rangle^{\frac{1}{2}} \Lambda_{|\xi|,|\eta| \lesssim N}\|_{L^\infty(d(x-y))L^2(d(x+y)dt)}$$
$$+ \|\left|\partial_t\right|^{\frac{1}{4}} \Lambda_{|\xi|,|\eta| \lesssim N}\|_{L^\infty(d(x-y))L^2(d(x+y)dt)}$$
$$\lesssim \|G\|_{non-end-point\ dual\ Strichartz}$$
$$+ \|\left\langle \nabla_x \right\rangle^{\frac{1}{2}} \left\langle \nabla_y \right\rangle^{\frac{1}{2}} \Lambda_0\|_{L^2}$$

As things stand, the (UMD-affiliate) answer to the original approximation problem is: let $0 < \epsilon < \frac{1-\beta}{2}$. Then for all N sufficiently large,

$$\sup_{t\in[0,T]} \|\psi_{\text{exact}}(t) - e^{i\int_0^t X_0(s)ds}\psi_{\text{appr}}(t)\|_{Fock}$$
$$\lesssim_\epsilon N^{-\epsilon} + N^{-1}(1+T)^{\frac{1}{2}} \ .$$

In view of the results of Caraci, Oldenburg and Schlein, the truth (for $1 < \beta \leq 1$) is probably something like

$$\sup_{t\in[0,T]} \|\psi_{\text{exact}}(t) - e^{i\int_0^t X_0(s)ds}\psi_{\text{appr}}(t)\|_{Fock}$$
$$\lesssim C(t)N^{-\frac{1}{4}}$$

assuming $\frac{\partial}{\partial t}\left\langle\nabla_x\right\rangle^{\frac{1}{2}}\left\langle\nabla_y\right\rangle^{\frac{1}{2}}\Lambda_0 \in L^2$ or, equivalently, $\left(-\Delta_x-\Delta_y+N^2v(N(x-y))\right)\left\langle\nabla_x\right\rangle^{\frac{1}{2}}\left\langle\nabla_y\right\rangle^{\frac{1}{2}}\Lambda_0 \in L^2$ uniformly in N,
which imposes non-trivial but natural restrictions on the initial conditions.

This is work in progress!