On the pair excitation function.

Joint work with M. Grillakis
based on our 2013 and 2016 papers
"Beyond mean field: On the role of pair excitations in the evolution of condensates", Journal of fixed point theory and applications (2013), (The Yvonne Choquet-Bruhat Festschrift)
and
"Pair excitations and the mean field approximation of interacting Bosons, II"

which, in turn, are based earlier papers D. Margetis (2010, 2011)

The Hamiltonian

The mean field Hamiltonian is

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

N is large, but fixed.

The potential $v \geq 0$, $v \in C_0^\infty$, and $0 < \beta \leq 1$.

$$v_N = N^{3\beta} v(N^\beta x) \to (\int v)\delta(x)$$

In the presence of a trap the ground state of H_N looks like

$$\Psi_N(x_1, x_2, \cdots, x_N) \sim \phi_0(x_1)\phi_0(x_2)\phi_0(x_N)$$
$$+ \text{ very important corrections}$$

Rigorous results: Lieb, Seiringer:

$$\gamma_1^N(x, x') \to \phi_0(x)\overline{\phi_0}(x')$$

in trace norm, where

$$\gamma_1^N(x, x') = \int \Psi_N(x, x_2, \cdots, x_N)\overline{\Psi_N}(x', x_2, \cdots, x_N) dx_2 \cdots dx_N$$

Here $\|\phi_0\|_{L^2} = 1$ and ϕ_0 minimizes the Gross-Pitaevskii functional.

$$\int_{\mathbb{R}^3} |\nabla\phi|^2 + v_{externa}(x)|\phi|^2 + 4\pi a|\phi|^4$$

a= scattering length of v.

Incidentally,
$\gamma_2^N(x_1, x_2, x_1', x_2') \to$
$\phi_0(x_1)\phi_0(x_2)\overline{\phi_0(x_1')\phi_0(x_2')}$ in trace norm is automatic, but most likely not in higher Sobolev norms, so what about proving

$$\frac{\gamma_2^N(x_1, x_2, x_1', x_2')}{(1 - w(N(x_1 - x_2)))\overline{(1 - w)}}$$
$$\to$$
$$\phi_0(x_1)\phi_0(x_2)\overline{\phi_0(x_1')\phi_0(x_2')}$$

in a higher Sobolev norm? The term $w(N(x_1 - x_2)$ expected to come form the pair excitation function, and

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

The trap is removed and the evolution is observed.

$$\psi_N(t,\cdot) = e^{itH_N}\psi_N(0,\cdot)$$

where $\psi_N(0,\cdot)$ is "close" to the ground state in the presence of a trap. Crudely,

$$\psi_N(0,x_1,\cdots,x_N) \sim \phi_0(x_1)\phi_0(x_2)\cdots\phi_0(x_N)$$

goal

$$\psi_N(t,x_1,\cdots,x_N) \sim e^{iN\chi(t)}\phi(t,x_1)\phi(t,x_2)\cdots\phi(t,x_N)$$

(or a finer refinement) where

$$i\partial_t\phi + \Delta\phi - c\phi|\phi|^2 = 0$$

$c = 8\pi a$, $a =$ the scattering length of v if $\beta = 1$ (ϕ satisfies the Gross-Pitevskii equation),
$c = \int v$ if $0 < \beta < 1$ (NLS)
The meaning of $\sim$ is to be made precise.

This is a "classical PDE" problem, the number of particles stays fixed. For technical reasons we move over in Fock space where all possible numbers of particles are considered at the same time, and only at the end look at just the Nth component. The algebra is much easier in Fock space.

Alternative approach of Lewin, Nam and Schlein (2015), as well as Nam and Napiorkowski (2016) which address fluctuations around a Hartree state (pure tensor product).

The current version of our work is also related to a recent preprint of Bach, Breteaux, T. Chen, Fröhlich and Sigal (more about this later).

Fock space is a Hilbert space with a creation and annihilation operator satisfying the canonical commutation relations. There are several models of (Bosonic) Fock space

$L^2(\mathbb{R}^n)$ with $a_i = \frac{\frac{\partial}{\partial x_i}+x_i}{\sqrt{2}}$, $a_i^* = -\frac{\frac{\partial}{\partial x_i}+x_i}{\sqrt{2}}$, or

holomorphic functions on $\mathbb{C}^n$ with a weight with $a_i = \frac{\partial}{\partial z_i}$, $a_i^* = z_i$, etc.

There are strong analogies between these Fock spaces over a finite dimensional vector space and the physicists' Fock space over $L^2(\mathbb{R}^3)$.

Background on Physicists' Fock space

Symmetric Fock space $\mathcal{F}$ over $L^2(\mathbb{R}^3)$: The elements of $\mathcal{F}$ are vectors of the form

$$\boldsymbol{\psi} = (\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \cdots)$$

where $\psi_0 \in \mathbb{C}$ and $\psi_n \in L^2_s$ are symmetric in $x_1, \cdots, x_n$. The Hilbert space structure of $\mathcal{F}$ is given by $(\boldsymbol{\phi}, \boldsymbol{\psi}) = \sum_n \int \overline{\phi_n} \psi_n dx$.

We only care about the Nth component, but the algebra is much simpler if we carry all components. Extracting information about the relevant component may or may not be easy.

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

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

as well as 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

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

Fix N, define the Fock space Hamiltonian $H : \mathcal{F} \to \mathcal{F}$ 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

$$H_{N,n} = \sum_{j=1}^{n} \Delta_{x_j} - \frac{1}{2N} \sum_{1 \le i \ne j \le n} v(x_i - x_j)$$

Most interesting component: $n = N$.

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

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

$$[A(\phi), A(\psi)] = 2\Im \int \phi\overline{\psi}$$

(Stone-von Neumann representation of the "Heisenberg group" $= L^2(\mathbb{R}^n) \times \mathbb{R}$)
Let $\Omega = (1, 0, 0, \cdots) \in \mathcal{F}$ and

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

is a coherent state.

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

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

$e^B =$ Segal-Shale-Weil or metaplectic representation of the symplectic matrix,

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

called Bogoliubov transformations by physicists.

It satisfies

$$e^B(a(f) + a^*(g))e^{-B}$$
$$= \begin{pmatrix} f & g \end{pmatrix} \begin{pmatrix} \mathrm{ch}(k) & \overline{\mathrm{sh}(k)} \\ \mathrm{sh}(k) & \overline{\mathrm{ch}(k)} \end{pmatrix} \begin{pmatrix} a_x \\ a_x^* \end{pmatrix}$$

Bogoliubov used the RHS of this equation in his celebrated 1947 Physics paper. Stone and Von Neumann thm from the early 1930s.

Notice B is skew-Hermitian and e^B is unitary.
Our project, started in 2010 with Margetis:
Impose PDEs for ϕ and k so

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

is approximatex, in Fock space, by

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

The expectation is that, in the presence of a trap and suitable k_N, ϕ_N,

$$\|\Psi_{ground\ state} - e^{-\sqrt{N}A(\phi_N)}e^{-B(k_N)}\Omega\|_{\mathcal{F}} \to 0$$

as $N \to \infty$. This may be true for $\beta < 1$, not true for $\beta = 1$. I don't know of any such rigorous results. A different, non-unitary e^B (using only creation operators) used by Lee, Huang and Yang in physics (1959), and then, rigorously, by Erdös, Schlein and Yau (2009), and also Yau and Yin, to find an upper bound for ground state energy of H in a box, along the lines of results predicted by Lee, Huang and Yang.

The history of the construction

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

(as far as I know it). Compare

$$\Psi_{exact} = e^{it\mathcal{H}}e^{-\sqrt{N}A(\phi_0)}\Omega$$

with

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

via the fluctuations dynamics unitary operator

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

introduced by Hepp (1974), used by Ginibre and Velo (1979), then, 20 years later, by Rodnianski and Schlein (2009) to prove rigorously the rate of convergence of gamma matrices for Coulomb interactions.

Remarked recently by Ben Arous, Kirkpatrick and Schlein, (2013) that, under suitable assumption, $U_N(t)$ has a limit which can be written, abstractly, as a Bogoliubov transformation.

A different, non-unitary e^B used by Wu (1961), Margetis, together with a (different) equation for k to study the evolution problem.

Back to this particular e^B and approximation

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

If ϕ satisfies the Hartree equation and sh$(2k)$, ch$(2k)$ satisfy a coupled system of linear equations, then this construction provides a Fock space approximation for $\beta < 1/3$ (GM 2013) and for $\beta < 1/2$ (Elif Kuz, 2015). This is very likely as high as one can go with the linear equations. Very similar linear equations used by Nam and Napiorkowski adapting Fock space techniques to the classical PDE problem ($\beta < 1/2$) in 2016.

The construction (but not the PDE) has been used very successfully by Benedikter, de Oliveira, Schlein (2015) for the rate of convergence of gamma matrices for $\beta = 1$ and Boccato, Cenatiempo, and Schlein (2016) for Fock space estimates for $\beta < 1$. Their approximation

$$e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))} U_{2,N}(t)\Omega$$

where $k(t) = k(t, x, y)$ is explicit (and related but different from our $k(t)$) and $U_{2,N}(t)$ is an evolution in Fock space with a quadratic generator.

The current state of the project: approximate

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

This leads to

$U_{\text{red}\,2}(t) = e^{\mathcal{B}(k(t))}e^{\sqrt{N}\mathcal{A}(\phi(t))}e^{it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(\phi_0)}e^{-\mathcal{B}(k(0))}$

and a "doubly reduced Hamiltonian" $\mathcal{H}_{\text{red}\,2}$ such that

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \mathcal{H}_{\text{red}\,2}\right) U_{\text{red}\,2}(t)\Omega = 0$$
$$U_{\text{red}\,2}(0)\Omega = \Omega$$

Ideally, $U_{\text{red}\,2}(t)\Omega$ should be close to Ω, and Ω satisfies

$$\left(\frac{1}{i}\frac{\partial}{\partial t} - \mathcal{H}_{\text{red}\,2}\right)\Omega = -\mathcal{H}_{\text{red}\,2}\Omega$$

The operator $\mathcal{H}_{\text{red}\,2}$ is fourth order in a and a^*, so

$$\mathcal{H}_{\text{red}\,2}\Omega = (X_0, X_1, X_2, X_3, X_4, 0, \cdots). \qquad (1)$$

Want: $U_{\text{red}\,2}\Omega$ to be close to Ω, or $\mathcal{H}_{\text{red}\,2}\Omega$ to be close to 0

Motivated by this, the new, coupled equations for ϕ and k that we introduce in 2013 can be written abstractly as

$$X_1 = 0 \quad \text{and } X_2 = 0. \tag{2}$$

These equations are Euler-Lagrange equations for the Lagrangian $\int X_0$, and conserve the number of particles and the energy. These equations can be written down, but their analysis is difficult. 2013 version of the equations:

$$\frac{1}{i}\partial_t\phi(t,x) - \Delta\phi + \int v_N(x-y)\Lambda(t,x,y)\overline{\phi}(t,y)dy$$
$$+\frac{1}{N}(v_N * Tr(\mathsf{sh}(k)\circ\overline{\mathsf{sh}(k)}))(t,x)\phi(t,x)$$
$$+\frac{1}{N}\int v_N(x-y)(\mathsf{sh}(k)\circ\overline{\mathsf{sh}(k)})(t,x,y)\phi(t,y)dy = 0$$

Here $Tr(\mathsf{sh}(k)\circ\overline{\mathsf{sh}(k)})(t,x) = (\mathsf{sh}(k)\circ\overline{\mathsf{sh}(k)})(t,x,x)$ denotes the trace density.

$$\tilde{\mathbf{S}}\,(\mathsf{sh}(2k)) + (v_N\Lambda)\circ\mathsf{ch}(2k) + \overline{\mathsf{ch}(2k)}\circ(v_N\Lambda) = 0$$
$$\tilde{\mathbf{W}}\left(\overline{\mathsf{ch}(2k)}\right) + (v_N\Lambda)\circ\overline{\mathsf{sh}(2k)} - \mathsf{sh}(2k)\circ(\overline{v_N\Lambda}) = 0$$

Λ, Γ defined on the next slide. Notice the delta-like singularity in the forcing term $v_N(x-y)\Lambda = N^{3\beta}v(N^{\beta}(x-y))\Lambda(t,x,y)$

In their most elegant form (2015), these equations are expressed in terms of the "generalized marginal density matrices"

$$\mathcal{L}_{m,n}(t, y_1, \ldots, y_m; x_1, \ldots, x_n) :=$$
$$C_N \left\langle a_{y_1} \cdots a_{y_m} e^{-\sqrt{N}\mathcal{A}} e^{-\mathcal{B}} \Omega,\, a_{x_1} \cdots a_{x_n} e^{-\sqrt{N}\mathcal{A}} e^{-\mathcal{B}} \Omega \right\rangle$$

Also, it turns out that

$$\mathcal{L}_{0,1}(t,x) = \phi(t,x)$$
$$\mathcal{L}_{1,1}(t,x,y) = \overline{\phi}(t,x)\phi(t,y) + \frac{1}{N}(\overline{\mathsf{sh}(k)} \circ \mathsf{sh}(k))(t,x,y)$$
$$:= \Gamma(t,x,y)$$
$$\mathcal{L}_{0,2}(t,x,y) = \phi(t,x)\phi(t,y) + \frac{1}{2N}\mathsf{sh}(2k)(t,x,y)$$
$$:= \Lambda(t,x,y)$$

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

The 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!)

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

Very recently we learned that, independently and in a different framework, Bach, Breteaux, T. Chen, Fröhlich and Sigal derived equations closely related to the equations these. Those equations become equivalent to the previous equations in the case of pure states.

(Thomas Chen's talk)

We need good estimates, uniform in N, for solutions to these coupled equations. Model case:

$$\mathbf{S}\phi(t,x) = -\Lambda(t,x,x)\bar{\phi}(t,x)$$

$$\left(\mathbf{S} + \frac{1}{N}v_N(x-y)\right)\Lambda(t,x,y)$$
$$= -\Lambda(t,x,x)\bar{\phi}(t,x)\phi(t,y) - \Lambda(t,y,y)\bar{\phi}(t,y)\phi(t,x)$$

where

$$\mathbf{S} = \frac{1}{i}\frac{\partial}{\partial t} - \Delta$$

in $3+1$ or $6+1$ dimensions.

One ingredient: $\mathbf{S}\Lambda = 0$ then

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

(improvement over the trace theorem, which follows from Strichartz if $\Lambda(t,x,y) = \phi(t,x)\phi(t,y)$). This also holds if $\nabla|_x^{1/2}|\nabla|_y^{1/2}\Lambda \in X^{0,1/2+}$ and, ignoring the potential, the RHS of the equation (previous slide) satisfies

$$\nabla_x^{1/2}\left(\Lambda(t,x,x)\bar{\phi}(t,x)\right)\nabla_y^{1/2}\phi(t,y)$$
$$\in L^2(dt)L^{6/5}(dx)L^2(dy)$$
$$\subset X^{-1/2-}$$

(such spaces and inclusions were used by X. Chen and Holmer).

As long as $\beta < 2/3$ the potential can be treated as a perturbation using Strichartz, etc. and

A theorem:

Theorem 1. *Let* $\frac{1}{3} < \beta < \frac{2}{3}$ *, and let the interaction potential* $v \in \mathcal{S}$ *with some additional technical assumptions. Let* ϕ*,* k *be solutions to the above equations with* $\phi(0,\cdot)$ *and* $k(0,\cdot)$ *regular (unif. in* N*), but not too regular, so*

$$\frac{\partial}{\partial t}\phi(t,x)\Big|_{t=0}, \frac{\partial}{\partial t}\Lambda(t,x,y)\Big|_{t=0} \text{ and}$$
$$\frac{\partial}{\partial t}\Gamma(t,x,y)\Big|_{t=0} \text{ are sufficiently regular.}$$

Then for some real function $\chi(t) = \chi_N(t)$ *and* $T_0 > 0$ *small such that*

$$\|e^{it\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(\phi_0)}e^{-\mathcal{B}(k(0))}\Omega -$$
$$e^{i\chi(t)}e^{-\sqrt{N}\mathcal{A}(\phi(t))}e^{-\mathcal{B}(k(t))}\Omega\|_{\mathcal{F}}$$
$$\leq \frac{C}{N^{1/6}}$$

for $0 \leq t \leq T_0$*.*

The analysis of the coupled PDEs, for $\beta > 2/3$, is very interesting and challenging.

The condition $\frac{\partial}{\partial t}\Lambda(t,x,y)\Big|_{t=0}$ smooth is not as innocent as it looks, since it rules out $\Lambda(0,x,y)$ smooth:

$$\frac{\partial}{\partial t}\Lambda(t,x,y) = \left(\Delta - \frac{1}{N}v_N(x-y)\right)\Lambda(t,x,y)$$
$$+ \text{smoother terms}$$

This is very natural, is compatible with the expected form of the ground state

$$\Lambda(0,x,y) = \phi(0,x)\phi(0,y)(1 - N^{\beta-1}w(N^{\beta}(x-y))$$

where

$$\left(-\Delta_{x,y} + \frac{1}{N}v_N(x-y)\right)(1 - N^{\beta-1}w(N^{\beta}(x-y)) = 0$$

The proof is, essentially, a local existence theorem with initial conditions such that

$$\| < \nabla_x >^{\frac{1}{2}+\epsilon} < \nabla_y >^{\frac{1}{2}+\epsilon} \Lambda(0,\cdot)\|_{L^2} \leq C$$
$$\| < \nabla_x >^{\frac{1}{2}+\epsilon} < \nabla_y >^{\frac{1}{2}+\epsilon} \Gamma(0,\cdot)\|_{L^2} \leq C$$
$$\| < \nabla_x >^{\frac{1}{2}+\epsilon} \phi(0,\cdot)\|_{L^2} \leq C$$

in other words, $\frac{1}{2}+\epsilon$ derivatives/particle, unlike the Gross-Pitaevskii hierarchy for which all known results in 3+1 dimensions, including Erdös-Schlein-Yau, Klainerman-Machedon, Kirkpatrick-Schlein-Staffilani, T. Chen-Pavlovic, T. Chen-Hainzl-Pavlovic-Seiringer require one derivative per particle.

The proof uses $X^{s,b}$ spaces, as in the work of X. Chen and Holmer.

One can show, based on the conservation of energy and number of particles

$$\| < \nabla_x >^{\frac{1}{2}+\epsilon} < \nabla_y >^{\frac{1}{2}+\epsilon} \Lambda(t,\cdot)\|_{L^2} \leq C(t)$$
$$\| < \nabla_x >^{\frac{1}{2}+\epsilon} < \nabla_y >^{\frac{1}{2}+\epsilon} \Gamma(t,\cdot)\|_{L^2} \leq C$$
$$\| < \nabla_x >^{\frac{1}{2}+\epsilon} \phi(t,\cdot)\|_{L^2} \leq C$$

uniformly in N. This makes it likely that the previous Theorem extends globally in time with some constant $C = C(t)$ depending on t. We do not yet know how $C(t)$ will depend on t as $t \to \infty$.

This is currently being investigated by Jacky Chong.