Quantum Dynamics of Many-Body systems, the Hartree equation, and Beyond.

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BACKGROUND

N quantum mechanical bosons described by a state function $\Psi_N(t, X_N) \in L^2(\mathbb{R}^{3N+1})$, symmetric in all space variables $(x_1, x_2, \dots x_N) := X_N$, and verifying

$$i\partial_t \Psi_N = H_N \Psi_N, \quad \|\Psi_N(t)\|_{L^2(\mathbb{R}^{3N})} = 1,$$

with Hamiltonian

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

$N \to \infty$

with $v \geq 0$, $v \in C_0^\infty$ and $0 < \beta \leq 1$

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

or else $\beta = 0$, $v_N = v$.

The ground state of H_N is, asymptotically, a tensor product. Is this preserved by the evolution?

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

where

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

for some constant $c > 0$ if $0 < \beta \leq 1$

c related to the scattering length of v if $b = 1$, $c = \int v$ if $0 < \beta < 1$.

while if $\beta = 0$, ϕ satisfies the Hartree equation

$$i\partial_t \phi + \Delta\phi - (v * |\phi|^2)\phi = 0$$

What does it mean for

$$\psi(t, x_1, \cdots, x_N) \backsimeq \psi'(t, x_1, \cdots, x_N)$$

$N \to \infty$? If

$$\psi(t, x_1, \cdots, x_N) = \phi(t, x_1)\phi(t, x_2) \cdots \phi(t, x_N)$$

and

$$\psi'(t, x_1, \cdots, x_N) = \phi'(t, x_1)\phi'(t, x_2) \cdots \phi'(t, x_N)$$

then

$$\|\psi - \psi'\|^2_{L^2(\mathbb{R}^{3N})} = 2 - 2\Re\left(\int \phi\overline{\phi'}\right)^N \to 2$$

as $N \to \infty$ if $\phi \neq \phi'$ so tensor products don't want to be close to each other in $L^2(\mathbb{R}^{3N})$. One way around this :marginal densities, as used by Erdös, Schelin and Yau.
(Another way: our new approach).

Original approach of Erdös, Schelin and Yau:

construct the orthogonal projection kernels

$$\gamma_N(\psi_N)(t, \mathbf{x}_N, \mathbf{x}'_N) = \psi_N(t, \mathbf{x}_N)\bar{\psi}_N(t, \mathbf{x}'_N)$$

and the **k-particle marginal density**:

$$\gamma_N^{(k)}(\psi_N)(t, \mathbf{x}_k, \mathbf{x}'_k)$$
$$= \int \gamma_N(t, \mathbf{x}_k, \mathbf{x}_{N-k}, \mathbf{x}'_k, \mathbf{x}_{N-k})\, d\mathbf{x}_{N-k}$$

Here, $\mathbf{x}_k$ represents the first k variables, and $\mathbf{x}_{N-k}$ represents the last $N-k$ variables. Their results are that

$$\gamma_N^{(1)}(t, x_1, x'_1) \to \phi(t, x_1)\overline{\phi}(t, x'_1)$$

in the trace norm, as $N \to \infty$. Improvement due to Rodnianski and Schlein: rate of convergence.

Contribution of Grillakis, M, Margetis: Can one relate $\psi(t, x_1, \cdots, x_N)$ to $\phi(t, x_1) \cdots \phi(t, x_N)$ without averaging out most variables?

Different approach, based on the second quantization:

Symmetric Fock space $\mathbf{F}$ over $L^2(\mathbf{R}^3)$: The elements of $\mathbf{F}$ are vectors of the form $\psi = (\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \cdots)$ 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 $\mathbf{F}$ is given by $(\phi, \psi) = \sum_n \int \phi_n \overline{\psi_n} dx$.

For $f \in L^2(\mathbf{R}^3)$ the (unbounded, closed, densely defined) creation operator $a^*(f) : \mathbf{F} \to \mathbf{F}$ and annihilation $a(\bar{f}) : \mathbf{F} \to \mathbf{F}$ 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

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

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

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

$$[a_x, a_y] = [a_x^*, a_y^*] = 0$$

For instance, a_x lowers the number of variables by one while a_x^* raises it:

$$\left(a_x \psi_{\text{n variables}}\right)(x_1, \cdots x_{n-1})$$
$$= \sqrt{n}\psi(x, x_1, \cdots x_{n-1})$$

$$\left(a_x^* \psi_{\text{n-1 variables}}\right)(x_1, x_2, \cdots, x_n)$$
$$= \sqrt{n}\delta(x - x_1)\psi(x_2, \cdots, x_n) \text{ symmetrized}$$

and

$$\left(a_x^* a_x \psi_{\text{n variables}}\right)(x_1, \cdots x_n)$$
$$= n\delta(x - x_1)\psi(x, x_2, \cdots x_n) \text{ symmetrized}$$

and

$$\left(\int a_x^* a_x dx\right) \psi_{\text{n variables}} = n\psi_{\text{n variables}}$$

In the same spirit

$$\left(\int a_x^* \Delta a_x dx\right) \psi(x_1, x_2, \cdots, x_n)$$
$$= \Delta_{x_1}\psi(x_1, x_2, \cdots, x_n) + \cdots + \Delta_{x_n}\psi(x_1, x_2, \cdots, x_n)$$
$$\left(\int v(x - y) a_x^* a_y^* a_x a_y \, dx \, dy\right) \psi(x_1, x_2, \cdots, x_n)$$
$$= \sum_{i \neq j} v(x_i - x_j)\psi(x_1, x_2, \cdots, x_n)$$

Let N be a fixed integer, $v(x)$ an even potential and consider the Fock space Hamiltonian $H : \mathbf{F} \to \mathbf{F}$ defined by

$$
\begin{aligned}
H_N &= \int a_x^* \Delta a_x dx - \frac{1}{2N} \int v(x-y) a_x^* a_y^* a_x a_y dx dy \\
&:= H_0 - \frac{1}{N} V
\end{aligned}
$$

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

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

When $n = N$ this is the mean field Hamiltonian corresponding to $\beta = 0$.

Alternative approach, due to Hepp, Ginibre and Velo, and, most recently, Rodnianski and Schlein, to study the Fock space evolution

$e^{itH_N}\psi_0$

where the initial data is a coherent state

$$\psi_0 = (c_0, c_1\phi_0(x_1), c_2\phi_0(x_1)\phi_0(x_2), \cdots)$$

The evolution of just one component can then be extracted as a "Fourier coefficient" from the Fock space evolution. If v is Coulomb and $\beta = 0$ Rodnianski and Schlein used this approach to prove strong convergence in the trace norm at the level of the density matrices $\gamma_1^{(N)}$.

$$\|\gamma_1^{(N)}(t,x,x') - \phi(t,x)\overline{\phi}(t,x')\|_{Tr} \leq \frac{e^{ct}}{\sqrt{N}}$$

Consider $\phi(t,x)$ to be determined later (as the solution of a Hartree equation). Define the skew-Hermitian closed unbounded operator

$$A(t) = a(\overline{\phi}) - a^*(\phi)$$

Let $\Omega = (1,0,0,\cdots) \in \mathbf{F}$ and define

$$W(\phi) = e^{-\sqrt{N}A(\phi)}$$

This is the Weyl operator (a unitary representation of the infinite dimensional Heisenberg group $= L^2(\mathbb{R}^3) \times \mathbb{R}$ with multiplication $(\phi,t)(\psi,s) = (\phi+\psi, t+s-\Im\int \phi\overline{\psi}\ )$, and

$$\psi_0 = e^{-\sqrt{N}A(\phi_0)}\Omega$$
$$= e^{-N/2}\left(1,\cdots,\left(\frac{N^n}{n!}\right)^{1/2}\phi_0(x_1)\cdots\phi_0(x_n),\cdots\right)$$

is a coherent state (initial data). $\Omega = (1,0,0,\cdots)$.

and

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

is a first candidate for an approximation for $e^{itH_N}\psi_0$ which works from the point of view of marginal densities (Erdös, Schlein, Yau; Rodnianski and Schlein), but not in the Fock space norm. Grillakis-M-Margetis: to refine this to a Fock space approximation.

$$\|e^{-\sqrt{N}A(t)}e^{-B(t)}e^{-i\int_0^t N\chi(s)ds}\Omega - e^{itH_N}\psi_0\|_{\mathbf{F}}$$
$$\leq \frac{\int_0^t f(s)ds}{\sqrt{N}} + \frac{\int_0^t g(s)ds}{N}$$

$k(t, x, y) = k(t, y, x)$ is a function to be determined later, with $k(0, x, y) = 0$ and

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

Notice B is skew-Hermitian.

How far can one get with tensor products? Look at

$$\|e^{-\sqrt{N}A(t)}\Omega - e^{itH_N}e^{-\sqrt{N}A(0)}\Omega\|_{\mathbf{F}}$$
$$= \|e^{\sqrt{N}A(t)}e^{itH_N}e^{-\sqrt{N}A(0)}\Omega - \Omega\|_{\mathbf{F}}$$

This is 0 at $t = 0$ so we would like

$$\left(\frac{\partial}{\partial t} - iL\right)\left(e^{\sqrt{N}A(t)}e^{itH_N}e^{-\sqrt{N}A(0)}\Omega\right) = 0$$

for some L self-adjoint, with

$$\left(\frac{\partial}{\partial t} - iL\right)\Omega$$

to be small (and it won't be). Define $\Psi_1(t) = e^{\sqrt{N}A(t)}e^{itH}e^{-\sqrt{N}A(0)}\Omega$

We have the basic calculation in the spirit of Hepp , Ginibre-Velo , and Rodnianski-Schlein.

Recall the formulas

$$\left(\frac{\partial}{\partial t}e^{C(t)}\right)\left(e^{-C(t)}\right) = \dot{C} + \frac{1}{2!}[C, \dot{C}] + \frac{1}{3!}\Big[C, [C, \dot{C}]\Big] + \dots$$

and

$$e^C H e^{-C} = H + [C,H] + \frac{1}{2!}\Big[C,[C,H]\Big] + \dots\ .$$

We apply these relations to $C = \sqrt{N}A$. H is fourth order in a, a^* and A is first order. Each commutator with A lowers the degree by 1 (because $[a,a^*] = \delta$). Thus the series are actually finite. We have

$$\frac{1}{i}\frac{\partial}{\partial t}\psi_1(t) = L_1\psi_1\ , \qquad (1)$$

where

$$L_1 = \frac{1}{i}\left(\frac{\partial}{\partial t}e^{\sqrt{N}A(t)}\right)e^{-\sqrt{N}A(t)} + e^{\sqrt{N}A(t)}He^{-\sqrt{N}A(t)}$$

$$= \frac{1}{i}\left(N^{1/2}\dot{A} + \frac{N}{2}[A,\dot{A}]\right) + H + N^{1/2}[A,H_0]$$

$$+ N^{-1/2}[A,V] + \frac{N}{2}\Big[A,[A,H_0]\Big]$$

$$\frac{1}{2}\Big[A,[A,V]\Big] + \frac{N^{1/2}}{3!}\Big[A,\Big[A,[A,V]\Big]\Big]$$

$$+ \frac{N}{4!}\Big[A,\Big[A,\Big[A,[A,V]\Big]\Big]\Big]\ .$$

The worst terms, with a weight of N, are scalar, and contribute a harmless phase function. The next worst terms, with a weight $N^{1/2}$ are essentially a(Hartree ϕ). Make them zero! But the N^0 terms stay.

Eliminating the terms with a weight of $\sqrt{N}$, or setting

$$\frac{1}{i}\dot{A} + [A, H_0] + \frac{1}{3!}\Big[A, \big[A, [A, V]\big]\Big] = 0 \ , \qquad (2)$$

is equivalent to the Hartree equation. We are left with

$$\frac{1}{i}\frac{\partial}{\partial t}\psi_1(t) = \Bigg(H_0 + \frac{1}{2}[A, [A, V]]$$

$$+N^{-1/2}[A, V] + N^{-1}V - N\frac{1}{4!}\Big[A, \Big[A, \big[A, [A, V]\big]\Big]\Big]\Bigg)\psi_1 \ .$$

We would like Ω to satisfy the same type of equation modulo $O(N^{-1/2})$, and it doesn't, because of a^*a^* terms with a coefficient $O(1)$.

Introduce e^B to get rid of them. The end result is:

$$\|e^{-\sqrt{N}A(t)}e^{-B(t)}e^{-i\chi(t)}\Omega - e^{itH_N}\psi_0\|_{\mathbf{F}}$$
$$\leq \frac{\int_0^t f(s)ds}{\sqrt{N}} + \frac{\int_0^t g(s)ds}{N}.$$

where

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

and k satisfies the equation

$$(i\mathrm{sh}(k)_t - (\Delta_x + \Delta_y)\,\mathrm{sh}(k) - \mathrm{ch}(k)m + \cdots)$$
$$= (i\mathrm{ch}(k)_t - (\Delta_x - \Delta_y)\mathrm{ch}(k) + \mathrm{sh}(k)\overline{m} + \cdots)$$
$$\times\ (\mathrm{ch}(k))^{-1}\mathrm{sh}(k)$$

where

$$\mathrm{sh}(k) := k + \frac{1}{3!}k\overline{k}k + \cdots$$
$$\mathrm{ch}(k) = \delta + \frac{1}{2!}k\overline{k} + \cdots$$
$$m(t,x,y) := v(x-y)\overline{\phi}(t,x)\overline{\phi}(t,y).$$

where all products are interpreted as spacial compositions.

The upper bounds

$$f(t) := \|e^{B}[A, V]e^{-B}\Omega\|_{\mathbf{F}}$$
$$g(t) := \|e^{B}Ve^{-B}\Omega\|_{\mathbf{F}}$$

can be easily computed.

Idea of the proof: just as before to estimate

$$\|e^{-\sqrt{N}A(t)}e^{-B(t)}\Omega - e^{itH_N}e^{-\sqrt{N}A(0)}\Omega\|_{\mathbf{F}}$$

it suffices to estimate

$$\|\Omega - e^{B(t)}e^{\sqrt{N}A(t)}e^{itH_N}e^{-\sqrt{N}A(0)}\Omega\|_{\mathbf{F}}$$

and in turn it suffices to arrange

$$\left(\frac{\partial}{\partial t} - iL\right)\left(e^{B(t)}e^{\sqrt{N}A(t)}e^{itH_N}e^{-\sqrt{N}A(0)}\Omega\right) = 0$$

with

$$\left(\frac{\partial}{\partial t} - iL\right)\Omega$$

small. The trouble comes from just one type of term in

$$\frac{\partial}{\partial t}\left(e^{B(t)}e^{\sqrt{N}A(t)}e^{itH_N}e^{-\sqrt{N}A(0)}\right)$$

namely quadratics in a^*a^*. $a\Omega = 0$, but $a^*\Omega \neq 0$, The equation for k comes from eliminating the coefficient of a^*a^*. Inspired (but essentially different from) work of Wu.

Computing

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

and

$$e^{B}He^{-B} = H + [B, H] + \frac{1}{2!}\Big[C, [C, H]\Big] + \dots \ .$$

is much harder for B than for A, because the series are truly infinite and there is no obvious elementary way to sum them.

Fortunately, the Segal-Shale-Weil representation is just the right tool.

It is a representation of the real symplectic group, which was worked out in the infinite dimensional case by Shale. Consider d, $k = k^T$, $l = l^T$ Hilbert-Schmidt (or $L^2(dxdy)$) kernels. (We work in a basis with respect to which these are complex). The Lie algebra (infinitesimal) Segal-Shale-Weil isomorphism from $sp(\mathbb{C})$ to operators is

$$\begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} \to \mathbf{I}\begin{pmatrix} d & k \\ l & -d^T \end{pmatrix}$$
$$= -\int d(x,y)\frac{a_x a_y^* + a_y^* a_x}{2}\ dx\,dy$$
$$+ \frac{1}{2}\int k(x,y) a_x a_y\ dx\,dy$$
$$- \frac{1}{2}\int l(x,y) a_x^* a_y^*\ dx\,dy$$

Under this isomorphism $B = \mathbf{I}(K)$ for

$$K = \begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix}$$

and, for instance,

$$\left(\frac{\partial}{\partial t} e^{B(t)}\right)\left(e^{-B(t)}\right) = \mathbf{I}\left(\frac{\partial}{\partial t} e^{K(t)}\right)\left(e^{-K(t)}\right)$$

which is elementary to compute.

Back to our new PDE

$$\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right) \mathsf{sh}(k)(t,x,y)$$
$$= i\left(\frac{\partial}{\partial t} - \Delta_x + \Delta_y\right) \mathsf{ch}(k)(t,x,y)$$
$$+ m + \cdots$$

where

$$m = v(x-y)\overline{\phi}(t,x)\overline{\phi}(t,y)$$

is actually linear if $v = 0$!

If

$$\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right) k = 0$$

then

$$\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right) \mathrm{sh}(k)$$

$$= Sk + \frac{1}{3!}\Big((Sk)\overline{k}k - k\overline{(Sk)}k + k\overline{k}(Sk)\Big) + \cdots = 0$$

and

$$\left(i\frac{\partial}{\partial t} - \Delta_x + \Delta_y\right) \mathrm{ch}(k)$$
$$+ (Sk)\overline{k} - k\overline{S(k)} + \cdots = 0$$

However, k picks up the singularity of v from the inhomogeneity m.
This is seen even in the crudest linearization:

$$\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right) k = m$$

Our complete equation is locally well posed (written up) and globally well-posed (work in progress) provided one controls $\|\phi\|_{L^2(L^4)}$ (and one does, for nice solutions of the Hartree equation).