Rigorous Derivation of the Gross-Pitaevskii Equation

Peter Pickl
Institut für Theoretische Physik
Universität Wien

We are interested in the scattering behavior of N interacting particles in 3d for large N.

Assume that the interaction potential v_N is positive and scales with N like

$$v_N(\mathbf{x}) := N^2 v(N\mathbf{x}) \geq 0$$

with v compactly supported.

Furthermore we shall allow a fixed external potential A acting on all the particles.

The respective Hamiltonian reads

$$H = \sum_{j=1}^{N} (-\Delta_j + A(x_j)) + \sum_{j<k} v_N(x_j - x_k) \ .$$

And we wish to estimate the solutions of the differential equation

$$\partial_t \Psi_t = H \Psi_t \quad \text{with } \Psi_0(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{j=1}^{N} \phi(x_j)$$

for some $\phi \in L^2(\mathbb{R}^3, \mathbb{C})$ in the limit $N \to \infty$.

Idea: Generalized Eigenfunction expansion.

How do the generalized eigenfunctions (roughly) look like?

Microscopic structure: (comes from the interaction potential)

$F(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ is the Zero energy scattering state of the interacting potential:

$$\left(\sum_{j=1}^{N} -\Delta_j + \sum_{j<k} v_N(x_j - x_k) \right) F(\mathbf{x}_1, \ldots, \mathbf{x}_N) = 0; .$$

Macroscopic structure:

$$\overline{\Psi}_t := \Psi_t / F \ . \tag{1}$$

Mean field: Given the microscopic structure it is clear how to “average out” the potential.

$$\overline{V}_0 = a|\phi_0|^2$$

where a is the scattering length of v.

Using the Ansatz (1) it follows that $\overline{\Psi}_t$ solves

$$\partial_t \overline{\Psi}_t = \sum_{j=1}^{N} \left(-\Delta_j + A(x_j) + \overline{V}_t \right) \overline{\Psi}_t + \delta H \overline{\Psi}_t$$

with some “error” δH.

One expects that $\overline{\Psi}_t$ is in good approximation a product of solution of the Gross-Pitaevskii equation

$$\partial_t \phi_t^{GP} = \left(-\Delta + A + a|\phi_t^{GP}|^2\right) \phi_t^{GP}$$

with $\phi_0^{GP} = \phi$, i.e. that in some sense (see below)

$$\begin{aligned} \overline{\Psi}_t(\mathbf{x}_1, \ldots, \mathbf{x}_N) &\approx \Psi_t^{GP}(\mathbf{x}_1, \ldots, \mathbf{x}_N) \\ &:= \prod_{j=1}^{N} \phi_t^{GP}(\mathbf{x}_j) \ . \end{aligned}$$

Problem for $t = \mathcal{O}(1)$ we have in general no L^2-closeness of $\overline{\Psi}$ and Ψ^{GP}.

Example: Assume that for some t

$$\overline{\Psi}_t = \left(\phi^{\perp}(\mathbf{x}_1) \prod_{j=2}^{N} \phi_t^{GP}(\mathbf{x}_j) \right)_{sym}$$

for some $\phi^{\perp} \perp \phi_t^{GP}$. Then obviously $\overline{\Psi}_t \perp \Psi^{GP}$.

For the problem at hand one can proof convergence of the one particle marginal density against $|\phi_t^{GP}\rangle\langle\phi_t^{GP}|$. This was done by Erdös, Schlein, Yau (Inv. Math. 2007) using BBGKY hierarchy. They need a sufficiently small a to have a convergent hierarchy.

Alternative Method

Let for any $t \in \mathbb{R}$ the $p_t : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ be the projector onto ϕ_t^{GP}, let $p_t^\perp := 1 - p_t$.

Define for any $M < N$ the projector $P_t^M : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$ via

$$P_t^M := \left(\prod_{j=1}^{M} p_t(x_j) \prod_{j=M+1}^{N} p_t^\perp(x_j) \right)_{sym} .$$

Let $D_t := \sum_{M=0}^{N} \frac{M}{N} P_t^M$.

Theorem. *(Pickl 2008) For any $t > 0$, "nice" ϕ_0, v and A*

$$\lim_{N\to\infty} \langle \overline{\Psi}_t, D_t \overline{\Psi}_t \rangle = 1$$

Remark. *The theorem implies the convergence of the one particle marginal density of Ψ_t against $|\phi_t^{GP}\rangle\langle\phi_t^{GP}|$. For our example above one gets easily*

$$\langle \overline{\Psi}_t, D_t \overline{\Psi}_t \rangle = \frac{N-1}{N} \langle \overline{\Psi}_t, \overline{\Psi}_t \rangle$$

Proof:

Using that $\partial_t p_t = [H^{GP}, p_t]$ and $\sum_{L=0}^{N} P_t^L = 1$we get that

$$\begin{aligned}
\partial_t \langle \overline{\Psi}_t, D_t \overline{\Psi}_t \rangle &= \langle \overline{\Psi}_t, [\delta H, D_t] \overline{\Psi}_t \rangle \\
&= \sum_{M,L=0}^{N} \frac{M}{N} \langle \overline{\Psi}_t, P_t^L \delta H P_t^M - P_t^M \delta H P_t^L \overline{\Psi}_t \rangle \\
&= \sum_{M,L=0}^{N} \frac{M-L}{N} \langle \overline{\Psi}_t, P_t^L \delta H P_t^M \overline{\Psi}_t \rangle \\
&\leq \sum_{M,L=0}^{N} \frac{3}{N} |\langle \overline{\Psi}_t, P_t^L \delta H P_t^M \overline{\Psi}_t \rangle| \\
&\sim \frac{3}{N} |\langle \overline{\Psi}_t, \delta H \overline{\Psi}_t \rangle|
\end{aligned}$$

Advantage: Proof needs no BBGKY hierarchy, since $\partial_t \langle \overline{\Psi}_t, D_t \overline{\Psi}_t \rangle$ can be controlled using the hamiltonian “directly”. Thus the proof is simpler and needs much weaker conditions on a.