A Better Derivation of the NLS (GP) Eq for a BEC

N-particle density matrix $\rho_N = |\Psi\rangle\langle\Psi|$

There is a unique ground state so it is a pure state.

$$i\hbar \frac{\partial \rho_N}{\partial t} = [H, \rho_N]$$

$$\rho_N(r_1 \cdots r_N | r_1' \cdots r_N') = \langle r_1 \cdots r_N | \rho_N | r_1' \cdots r_N' \rangle$$

$$H = \sum_i h_i + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} v_{ij}$$

$$h_i = \frac{p_i^2}{2m} + V_{trap}(\vec{r}_i) \qquad v_{ij} = V_{int}(|\vec{r}_i - \vec{r}_j|)$$

Reduced density matrices

$$\rho_1 = \mathrm{Tr}_{2\cdots N}\, \rho_N$$
$$= \int \rho_N(r_1\ r_2 \cdots r_N | r_1'\ r_2 \cdots r_N)\ dr_2 \cdots dr_N$$

$$\rho_2 = \mathrm{Tr}_{3\cdots N}\, \rho_N$$
$$= \int \rho_N(r_1, r_2\ \ r_3 \cdots r_N | r_1'\ r_2'\ \ r_3 \cdots r_N)\ dr_3 \cdots dr_N$$

Reduced density matrices obey a BBGKY heirarchy of eqns

evolution of ρ_1 depends on ρ_2
ρ_2 … ρ_3
ρ_3 … ρ_4

(Bogoliubov Born Green Kirkwood Yvon)

$$i\hbar \frac{d\rho_1}{dt} = i\hbar \frac{d}{dt} \mathop{Tr}_{2\cdots N} \rho_N$$

$$= \mathop{Tr}_{2\cdots N} [H_N, \rho_N]$$

One particle parts:

$$\left[\sum_i h(i), \rho_N\right]$$

$$PE_1 : \mathop{Tr}_{2\cdots N} \Big(v(r_1) \quad \rho(r_1 \; r_2 \cdots r_N | r_1' \; r_2 \cdots r_N)$$
$$- \rho(r_1 \; r_2 \cdots r_N | r_1' \; r_2 \cdots r_N) \; v(r_1') \Big)$$

$$= v(r_1)\, \rho_1(r_1, r_1') - \rho_1(r_1, r_1')\, v(r_1')$$
$$= \langle r_1 | \quad [v, \rho_1] \quad | r_1' \rangle$$

Another PE

$$\mathop{Tr}_{2\cdots N} \Big(v(r_2) \;\rho(1, 2\cdots N | 1'\, 2\cdots N) - \rho(1, 2\cdots N | 1', 2\cdots N) v(r_2) \Big)$$
$$= \mathop{Tr}_{2\cdots N} v(r_2) \Big(\rho(1, 2\cdots N | 1', 2\cdots N) - \rho(1, 2\cdots N | 1'\, 2\cdots N) \Big)$$

$$= \quad 0$$

$$KE_1 : \mathop{Tr}_{2\cdots N} \Big(-\frac{\hbar^2}{2m} \nabla_1^2 \quad \rho(r_1 \; r_2 \cdots r_N | r_1' \; r_2 \cdots r_N)$$
$$+ \rho(r_1 \; r_2 \cdots r_N | r_1' \; r_2 \cdots r_N) -\frac{\hbar^2}{2m} \nabla_{r_1'}^2 \Big)$$

$$= [KE_1, \rho_1]$$

KE_2 vanishes, along with all others

Interatomic Interaction

involving particle 1

$$\mathop{Tr}_{2\cdots N} \; v_{12} \; \rho(1, 2\cdots N | 1' 2\cdots N) \; (v_{12} - v_{1'2})$$

$$= \mathop{Tr}_{2} \left(v_{12} \, \rho_2(1\,2|1'2) - \rho_2(1\,2|1'2) \, v_{1'2} \right)$$

Including all interacting with 1

$$(N-1) \, Tr_2 \langle r_1 r_2 | [v, \rho_2] | r_1' \, r_2 \rangle$$

not involving particle 1

$$\text{eg} \; \mathop{Tr}_{2\cdots N} \left(v_{35} - v_{35} \right) \rho(1\,2 \;\; 3\cdots N | 1'\,2 \;\; 3\cdots N)$$

$$\boxed{i\hbar \frac{\partial \rho_1}{\partial t} = [h_1, \rho_1] + \underset{\Lambda}{\overset{(N-1)}{}} \mathop{Tr}_{2} [v, \rho_2]}$$

Similarly

$$i\hbar \frac{\partial \rho_2}{\partial t} = [(h_1 + h_2), \rho_2] + \underset{\Lambda}{\overset{\frac{(N-1)(N-2)}{2!}}{}} \mathop{Tr}_{3} [v_{13} + v_{23}, \rho_3]$$

$\rho_1 \leftarrow \rho_2$

$\rho_2 \leftarrow \rho_3$

$\rho_3 \leftarrow \rho_4$

etc.

Problem: Break the hierarchy.

Boltzmann: Assumption of "Molecular Chaos"

$$\rho_2(r_1 r_2 | r_1' r_2') \simeq \rho_1(r_1 | r_1') \; \rho_1(r_2 | r_2')$$

We will make a comparable assumption, but carefully examining the 2-scale picture of BEC's.

$$\rho_2(r_1 \; r_2 \,|\, r_1' \; r_2) \simeq \left[\psi_{trap}(r_1) \; \psi^*_{trap}(r_1') \right] \times \left[\psi_{scat}(\vec{r}_1 - \vec{r}_2) \; \psi^*_{scat}(\vec{r}_1{}' - \vec{r}_2) \right]$$

atomic scattering structure

1 unless $\vec{r}_1$ and/or $\vec{r}_1{}'$ is close to $\vec{r}_2$

Examine

$$\mathop{Tr}_2 \, [v, \rho_2] = \int \left\{ v(\vec{r}_1 - \vec{r}_2) \; \rho_2(\vec{r}_1 \; \vec{r}_2 \,|\, \vec{r}_1{}' \; \vec{r}_2) - \rho_2(\vec{r}_1 \; \vec{r}_2 \,|\, \vec{r}_1{}' \; \vec{r}_2) \, v(\vec{r}_1{}' - \vec{r}_2) \right\} d\vec{r}_2$$

Suppose $\vec{r}_1{}'$ is not too close to $\vec{r}_1$.

Then either coordinate 1 or coordinate 1' is close to $\vec{r}_2$. Consider the former. Then only the first term contributes

$$\int v(r_1 - r_2) \; \rho_2(r_1 \; r_2 \,|\, r_1' \; r_2) \; d\vec{r}_2$$

$$= \int v(\vec{r}_1 - \vec{r}_2) \; \underline{\psi_{trap}(\vec{r}_1)} \; \underline{\psi_{trap}(\vec{r}_1{}')} \; \underbrace{\psi_{scat}(\vec{r}_1 - \vec{r}_2)}_{\underline{\underline{|\psi_{trap}(\vec{r}_2)|^2}}} \; \underline{\underline{\underline{\psi^*_{scat}(\vec{r}_1{}' - \vec{r}_2)}}} \; d^3 r_2$$

— come out of integral

= slowly varying on scale in which v is significant. But v is significant only for $r_2 \sim r_1$.

≡ ~ 1

$$\int v(r)\, \psi_{scat}(r)\, d\vec{r} = \frac{4\pi\hbar^2}{m} a \qquad (\text{p ZES } 7)$$

$$\psi_{trap}(r_1) \quad \underbrace{\frac{4\pi\hbar^2}{m} a}_{g} \quad |\psi_{trap}(r_1)|^2 \qquad \psi^*_{trap}(r_1')$$

$$i\hbar \frac{\partial}{\partial t} \rho_1(r_1, r_1') = \left[-\frac{\hbar^2}{2m}\nabla_{r_1}^2 + V(r_1) + g\,|\psi_{trap}(r_1)|^2\right] \rho_1(\vec{r}_1, \vec{r}_1')$$
$$+ \left[\frac{\hbar^2}{2m}\nabla_{r_1'}^2 - V(r_1') - g|\psi_{trap}(r_1')|^2\right] \rho_1(\vec{r}_1, \vec{r}_1')$$

There exist separable solutions to this eq:

$$\rho(\vec{r}_1, \vec{r}_1') = \psi_{trap}(\vec{r}_1)\; \psi^*_{trap}(\vec{r}_1')$$

with

$$i\hbar \frac{\partial}{\partial t} \psi_{trap}(r_1) = \left[-\frac{\hbar^2}{2m}\nabla_{r_1}^2 + V(r_1) + g\,|\psi_{trap}(r_1)|^2\right] \psi_{trap}(r_1$$

with $g = \frac{4\pi\hbar^2}{m} a$

Notes:

- All particles have long-range attraction + short-range repulsion
- The scattering length is NOT a measure of the actual interaction between the particles
- As a fn of well depth, a varies rapidly from $-\infty$ to ∞.
- However, it has a collective effect, creating an average "attraction" ($a<0$) or "repulsion" ($a>0$) in the condensate as a whole.

This derivation leaves much uncertainty about the accuracy of GP. When are the assumptions valid?

Theorem 1: (Lieb, Seiringer + Yngvason) Statics

Consider the limit
$$N \to \infty$$
$$\text{"}a \to 0\text{"}$$
$$Na \text{ fixed}$$

volume "inside scat" → effective density → $a^3 \bar{\rho} \sim \frac{1}{N^2}$

$$N = \int |\psi(x)|^2 dx$$

$$\bar{\rho} = \frac{\int |\psi(\vec{r})|^4 d\vec{r}}{\int |\psi(\vec{r})|^2 d\vec{r}}$$

Density is high, but number of particles scattering is small.

In this limit:

The GP energy density approaches the exact energy density

Method: Find an upper + lower bound for the exact eigenvalue. Show that they approach each other in this limit. Show that GP eigenvalue lies between the

Theorem 2: (Erdős, Schlein, Yau) <u>Dynamics</u>

If at $t=0$ there is a condensate as in Thm 1 and H is allowed to change with time [the trap is suddenly turned off] then the GP density operator approaches the true one-particle density operator in the same limit:

$$i\hbar \frac{d}{dt} \rho^{1}_{true} = [h_1, \rho^{1}_{true}] + N\,\mathrm{Tr}_2\, [v_{12}, \rho^{2}_{true}]$$

$$i\hbar \frac{d}{dt} \rho_{GP} = \text{GP Eq.}$$

Then
$$\mathrm{Tr} \left| \rho_{GP} - \rho_{true} \right| \to 0 \quad \text{as } N \to \infty$$

Method: (Case I) Assume the presence of two-scale structure in the initial state. Then prove that 2-scale structure is preserved by showing that $\langle H \rangle$ and $\langle H^2 \rangle$ are conserved, and that this forces the 2-scale structure.

Notes on Limits

The "thermodynamic limit" was $(\hbar\omega/kT)$ small.
This was used to convert a sum to an integral.

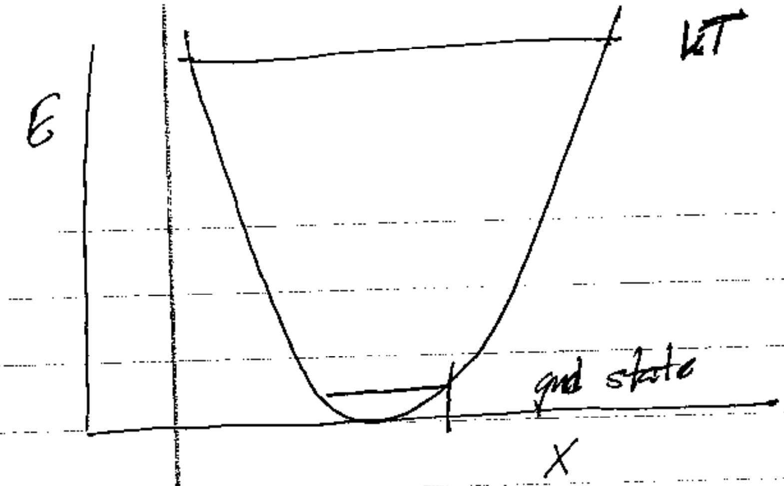
The transition temp is
$$k_B T_C = N^{1/3}\, \hbar\omega / [\zeta(3)]^{1/3}.$$
Thus as $N \to \infty$ we can have $(\hbar\omega/k_B T_C) \sim N^{-1/3}$ small

Size of condensate

Each atom is in ground state
$$\tfrac{1}{2}\hbar\omega = \tfrac{1}{2} k_{trap}\, x_{tp}^2 = \tfrac{1}{2} m\omega^2 x_{tp}^2$$
$$x_{tp}^0 \sim (\hbar/m\omega)^{1/2}$$

Volume of condensate $V_c = (\hbar/m\omega)^{3/2}$ indep of T, indep of N

Size of gas at any T:
$$\tfrac{1}{2} k_B T = \tfrac{1}{2} m\omega^2 x_{tp}^2$$
$$x_{tp}^{kT} = (k_B T/m\omega^2)^{1/2}$$
$$V_{gas} = \frac{(k_B T/m)^{3/2}}{\omega^3}$$
$$\frac{V_{gas}}{V_{cond}} = \frac{(k_B T/m)^{3/2}/\omega^3}{(\hbar/m\omega)^{3/2}} \sim \text{constants} \cdot \frac{T^{3/2}}{\omega^{3/2}}$$
indep of N



Fixing T,

~~As N~~ gets large,

$$\frac{N}{V_{condensate}} \to \infty$$

$$\frac{N}{V_{gas}} \to \infty$$

What is needed for GP eq to hold:

$$\frac{N}{V_{cond}} a^3 \text{ small}$$

scat length

Therefore the theorems proving validity of GP use a limit ω fixed, ($V_{condensate}$ fixed)

$$N \to \infty$$
$$a \to 0$$