Week 8

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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3.5 Quantum Field theory of Bose-Einstein Condensates

- – In section 3.4 we dealt with non-interacting quasi particles.
  – There also was no conversion from condensed to uncondensed component (heating).
- This section discusses one QFT method that can address both, and mentions few others.

3.5.1 Hartree-Fock Bogoliubov Method

We start again with the Heisenberg equation for the field operator (3.38).

$$i\hbar\dot{\hat{\psi}} = \hat{H}_0\hat{\psi} + U_0\hat{\psi}^\dagger\hat{\psi}\hat{\psi} \tag{3.82}$$

and take the expectation value, using $\hat{\psi}(\mathbf{x},t) = \phi(\mathbf{x},t) + \hat{\chi}(\mathbf{x},t)$, Eq. (3.60), assuming $\langle\hat{\chi}\rangle = 0$

$$\begin{aligned}\dot{\phi}(\mathbf{x},t) &= \hat{H}_0\phi(\mathbf{x},t) + U_0\langle(\phi^\star + \hat{\chi}^\dagger)(\phi+\hat{\chi})(\phi+\hat{\chi})\rangle \qquad (3.83)\\ &= \hat{H}_0\phi(\mathbf{x},t) + U_0[|\phi(\mathbf{x},t)|^2\phi(\mathbf{x},t) + 2\langle\hat{\chi}^\dagger\hat{\chi}\rangle\phi(\mathbf{x},t) + \langle\hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle + \langle\hat{\chi}\hat{\chi}\rangle\phi^*(\mathbf{x},t) + \langle\hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle]\end{aligned}$$

We in general do not know $\langle\hat{\chi}^\dagger\hat{\chi}\rangle$. Let us define

Normal correlation function:

$$G_N(\mathbf{x},\mathbf{x}') = \langle\hat{\chi}^\dagger(\mathbf{x}')\hat{\chi}(\mathbf{x})\rangle \tag{3.84}$$

Anomalous correlation function:

$$G_A(\mathbf{x},\mathbf{x}') = \langle\hat{\chi}(\mathbf{x}')\hat{\chi}(\mathbf{x})\rangle \tag{3.85}$$

- Now we see that we can express pieces of Eq. (3.83) using $G_N(\mathbf{x},\mathbf{x})$ and $G_A(\mathbf{x},\mathbf{x})$.
- For $\langle\hat{\chi}^\dagger\hat{\chi}^\dagger\hat{\chi}\rangle$ we use

Wick's Theorem For a Gaussian quantum state we have

$$\langle \hat{O}_1\hat{O}_2\hat{O}_3\rangle = \langle \hat{O}_1\hat{O}_2\rangle\langle \hat{O}_3\rangle + \langle \hat{O}_1\rangle\langle \hat{O}_2\hat{O}_3\rangle + \langle \hat{O}_1\hat{O}_3\rangle\langle \hat{O}_2\rangle - 2\langle \hat{O}_1\rangle\langle \hat{O}_2\rangle\langle \hat{O}_3\rangle \tag{3.86}$$
$$\langle \hat{O}_1\hat{O}_2\hat{O}_3\hat{O}_4\rangle = \underbracket{\hat{O}_1\hat{O}_2}\,\underbracket{\hat{O}_3\hat{O}_4} + \underbracket{\hat{O}_1\hat{O}_3}\,\underbracket{\hat{O}_2\hat{O}_4} + \underbracket{\hat{O}_1\hat{O}_4}\,\underbracket{\hat{O}_2\hat{O}_3} + \langle \hat{O}_1\rangle\langle \hat{O}_2\rangle\langle \hat{O}_3\rangle\langle \hat{O}_4\rangle$$

Here $\underbracket{\hat{O}_A\hat{O}_B} = \langle \hat{O}_A\hat{O}_B\rangle - \langle \hat{O}_A\rangle\langle \hat{O}_B\rangle$ is called a contraction.

• If the operators $\hat{O}_k$ are Fermionic, there are some additional minus signs. For each term on the rhs. of (3.86), first reorder the $\hat{O}_k$ by swapping neighbors such that those to be contracted are adjacent. For each swap, multiply a factor (-1).

BONUS MATERIAL, Gaussian quantum state:
Single mode example: $\rho = \mathcal{N}\exp(-\bar{n}\hat{a}^\dagger\hat{a} - \frac{1}{2}\bar{m}(\hat{a}^\dagger)^2 - \frac{1}{2}\bar{m}^*\hat{a}^2)$
e.g. a Coherent State or a thermal State: $\bar{m} = \bar{m}^* = 0, \bar{n} = -\beta(\epsilon - \mu)$ [See Eq. (3.4)]

Many mode generalisation:

$$\hat{\rho} = \mathcal{N}\exp(\sum_{i,j=1}^{2M} K_{ij}\hat{C}_i^\dagger\hat{C}_j) \quad \hat{C} = \begin{bmatrix} \hat{a}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{a}_M \\ \hat{a}_1^\dagger \\ \cdot \\ \cdot \\ \cdot \\ \hat{a}_M^\dagger \end{bmatrix} \tag{3.87}$$

- See e.g. Gardiner/ Zoller "Quantum Noise" 3rd ed. page 119

- See Blaizot and Ripka "Quantum theory of finite systems"(P. 93, Eq (4.47))
- Many variants of Wick's theorem exist all over QFT. They all express the final result of bringing operator products involving $\hat{a}, \hat{a}^\dagger$ into some default order.
- Using Wick's theorem in the form above, we see $\langle \hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle = 0$ since $\langle \hat{\chi}\rangle = 0$

We arrive at a

Modified GPE

$$i\hbar\frac{\partial\phi(\mathbf{x},t)}{\partial t} = \bar{H}_0\phi(\mathbf{x},t) + U_0|\phi(\mathbf{x},t)|^2\phi(\mathbf{x},t) + 2U_0\overbrace{G_N(\mathbf{x},\mathbf{x},t)}^{\equiv\bar{G}_N(\mathbf{x})}\phi(\mathbf{x},t) + U_0\overbrace{G_A(\mathbf{x},\mathbf{x},t)}^{\equiv\bar{G}_A(\mathbf{x})}\phi^*(\mathbf{x},t) \tag{3.88}$$

- We can see that $G_N(\mathbf{x},\mathbf{x}) = n_{\text{unc}}(\mathbf{x})$ is the density of uncondensed (thermal) atoms, by comparison with the discussion in section 3.4.4.
- The interpretation of the term $\sim G_N$, would thus be an interaction between condensed and un-condensed atoms.
- To make use of Eq. (3.88), we need to know $G_N(\mathbf{x},\mathbf{x},t)$ and $G_A(\mathbf{x},\mathbf{x},t)$

We can get those from the Heisenberg equation for $\hat{\chi}^\dagger(\mathbf{x}')\hat{\chi}(\mathbf{x})$ and $\hat{\chi}(\mathbf{x}')\hat{\chi}(\mathbf{x})$:

Hartree-Fock Bogulibov equations

$$\begin{aligned}
i\hbar\frac{\partial G_A(\mathbf{x},\mathbf{x}')}{\partial t} &= \langle[\hat{\chi}(\mathbf{x}')\hat{\chi}(\mathbf{x}),\hat{H}]\rangle \qquad (3.89)\\
&= [H_0(\mathbf{x}) + H_0(\mathbf{x}')]G_A(\mathbf{x},\mathbf{x}') + 2U_0\Big[|\phi(\mathbf{x})|^2 + |\phi(\mathbf{x}')|^2 + \bar{G}_N(\mathbf{x})\\
&\quad + \bar{G}_N(\mathbf{x}')\Big]G_A(\mathbf{x},\mathbf{x}') + U_0\Big[\phi(\mathbf{x})^2G_N^*(\mathbf{x},\mathbf{x}') + \phi(\mathbf{x}')^2G_N(\mathbf{x},\mathbf{x}')\\
&\quad + \bar{G}_A(\mathbf{x})G_N^*(\mathbf{x},\mathbf{x}') + \bar{G}_A(\mathbf{x}')G_N(\mathbf{x},\mathbf{x}')\Big] + U_0\Big[\phi(\mathbf{x})^2 + G_A(\mathbf{x},\mathbf{x})\Big]\delta^3(\mathbf{x}-\mathbf{x}')\\
i\hbar\frac{\partial G_N(\mathbf{x},\mathbf{x}')}{\partial t} &= [\hat{H}_0(\mathbf{x}) - \hat{H}_0(\mathbf{x}')]G_N(\mathbf{x},\mathbf{x}') + 2U_0\Big[|\phi(\mathbf{x})|^2 - |\phi(\mathbf{x}')|^2 + \bar{G}_N(\mathbf{x})\\
&\quad + \bar{G}_N(\mathbf{x}')\Big]G_N(\mathbf{x},\mathbf{x}') + U_0\Big[\bar{G}_A(\mathbf{x})G_A^*(\mathbf{x},\mathbf{x}') - \bar{G}_A(\mathbf{x}')G_A(\mathbf{x},\mathbf{x}')\Big]\\
&\quad + U_0\Big[\phi(\mathbf{x})^2G_A^*(\mathbf{x},\mathbf{x}') - \phi^*(\mathbf{x}')G_A(\mathbf{x},\mathbf{x}')\Big] \qquad (3.90)
\end{aligned}$$

- These form a coupled system of equations together with (3.88).
- We have again used Wick's theorem on terms like $\langle\hat{\chi}^\dagger\hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle$
- The general idea where
  1. equation for $\langle\hat{\psi}\rangle$ couples to
  2. $\langle\hat{\psi^\dagger}\hat{\psi}\rangle$ couples to
  3. $\langle\hat{\psi}^\dagger\hat{\psi}\hat{\psi}\rangle$

  is called cumulant expansion. It has to be truncated at some order, here this is done by using Wick's theorem.

We can define:

- Condensate density $|\phi(\mathbf{x})|^2$, and condensate number $N_{\mathrm{cond}} = \int |\phi|^2 dx$
- Thermal density $\bar{G}_N(\mathbf{x})$ and thermal number $N_{\mathrm{unc}} = \int \bar{G}_N(\mathbf{x}) dx$

- In the HFB equations (3.88) and (3.89), terms have the following interpretation (please see color file or printout)
  - $\cdots$ interactions between condensed and uncondensed atoms
  - $\cdots$ interactions of uncondensed atoms among each other
  - $\cdots$ conversion of condensed and uncondensed atoms (heating)

Example, Relation to Bogulibov equations (3.61): Let us consider $|\psi\rangle = 0$, the Bogulibov vacuum with zero quasiparticles in any mode, as our initial-state (eternal state in thre Heisenberg picture). Then we can see that

$$G_N(\mathbf{x}, \mathbf{x}') = \sum_n v_n(\mathbf{x}') v_n^*(\mathbf{x}), \tag{3.91}$$

$$G_A(\mathbf{x}, \mathbf{x}') = -\sum_n u_n(\mathbf{x}') v_n^*(\mathbf{x}). \tag{3.92}$$

For these G_A, G_N, a lengthy calculation gives from HFB equations Eq. (3.89):

$$i\hbar \dot{G}_N(\mathbf{x}, \mathbf{x}') = 0 \tag{3.93}$$

$$i\hbar \dot{G}_A(\mathbf{x}, \mathbf{x}') = -2\mu G_A(\mathbf{x}, \mathbf{x}') \to G_A(\mathbf{x}, \mathbf{x}', t) = e^{\frac{i2\mu t}{\hbar}} G_A(\mathbf{x}, \mathbf{x}', 0) \tag{3.94}$$

To reach this we ignore G relative to ϕ^2 (=fluctuations are small) and assume $\phi(t) = \phi_0(t=0)$
•Thus the Bogulibov vacuum is a steady state of the HFB-equations.

3.5.2 Depletion and Renormalisation

Let us further look at the density of uncondensed atoms $n_{\mathrm{unc}}(\mathbf{x}) = G_N(x, x)$ in the Bogoliubov vacuum $|\psi\rangle = |0\rangle$. Let us calculate $n_{\mathrm{unc}}(\mathbf{x})$ for a homogenous BEC, with constant density ρ, as used in section 3.4.1:

$$n_{\mathrm{unc}} = \sum_n |v_n(\mathbf{x})|^2 \to \frac{1}{\mathcal{V}} \sum_q v_q^2 \xrightarrow[3D]{} \frac{1}{\mathcal{V}} \int_{q=0}^{\infty} dq\, q^2 (4\pi) \underbrace{\overset{\text{(Density of states)}}{D}}_{=\frac{2\pi}{L}^3} v_q^2 \tag{3.95}$$

[We have converted sum $\to$ integral, using the density of states D for quantised particles in 3D box $(K_i = \frac{n\pi}{L})$ [But only one k_i per cell not two $(\pm|k_i|)$]]

$$= \frac{1}{2\pi^2} \int_0^{\infty} dq\, q^2 v_q^2 \overset{Eq. (3.71)}{=} \frac{8(mU_0\rho)^{\frac{3}{2}}}{3\hbar^3\pi^2}$$

Using also $U_0 = \frac{4\pi\hbar^2 a_s}{m}$, we find the

Condensate Depletion:

$$\frac{n_{\text{unc}}}{\rho} = \frac{8}{3\sqrt{\pi}}(\rho a_s^3)^{\frac{1}{2}} \tag{3.96}$$

- Depletion implies that, even though we are in the BdG vacuum with zero phonon excitations, interactions cause some atoms to remain outside of the condensate.
- Typical numbers: $a_s = 5.5nm$ for Rubidium, $\rho = 10^{19}/m^3 \implies \frac{n_{\text{unc}}}{\rho} = 0.2\%$ uncondensed density.

Let us also calculate

$$\bar{G}_A(\mathbf{x}) = G_A(x,x) = \sum_n u_n(\mathbf{x})v_m^*(\mathbf{x}) \overset{\text{trying as above}}{=} \infty \qquad \text{We have a divergent integral}$$

$$\overset{\text{cut-off integral at } K}{=} -\frac{4}{\pi^2}\int_0^K dq\, q^2 u_q v_q^* \overset{\text{large } K}{=} -\frac{4mU_0\rho K}{\pi^2\hbar^2} \equiv -\kappa U_0 \rho \tag{3.97}$$

This divergence has the same cause as in the other local quantum-field theories (e.g. particle physics): The implicit mathematical (but not physical) assumption that the theory is valid up to arbitrarily high energy scales. Solution: Renormalisation = we absorb "infinities" (in our case K) into parameters into the Hamiltonian (rather than having them in observables) and define the

Renormalised interaction U

$$U_0 = \frac{U}{1-\kappa U} \qquad \text{where } \kappa = \frac{4mK}{\pi^2\hbar^2} \tag{3.98}$$

- κ "infinite", $\underset{(\text{parameter in } \hat{H})}{U_0\text{"infinite"}}$, $\underset{(\text{observable quantity})}{\text{U "finite"}}$
- "Infinite" means ∞ in the limit $K \to \infty$
- To see that Eq. (3.98) makes sense, we can calculate e.g. the Born scattering amplitude from $\hat{H}$

Example, Renormalised mean-field interaction in modified GPE Eq. (3.88):

$$i\hbar\dot{\phi} = \hat{H}_0\phi + U_0|\phi|^2\phi + \overbrace{2U_0G_N\phi}^{\text{lets ignore } \bar{G}_N\text{, assuming small}} + U_0\bar{G}_A\phi_0^* \tag{3.99}$$

We now use Eq. (3.97) with the replacement $U_0 \to U$

$$\bar{G}_A = -\kappa U\rho \tag{3.100}$$

in (3.99) to replace $U_0 \to U$. Then

$$i\hbar\dot{\phi} = \hat{H}_0\phi + \underbrace{(U_0(1-\kappa U))}_{=U \text{ from Eq. (3.98) , which is finite}}|\phi|^2\phi + 2U\bar{G}_N\phi \tag{3.101}$$

(Steps in brown a is allowed because perturbations $\hat{\chi}$ (hence $G_N, G_A, \bar{G}_N, \bar{G}_A$) are "small")
• For numerical implementation : K frequently small enough that renormalisation can be ignored.

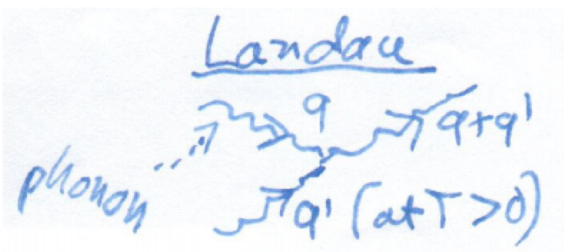
Appraisal of HFB:

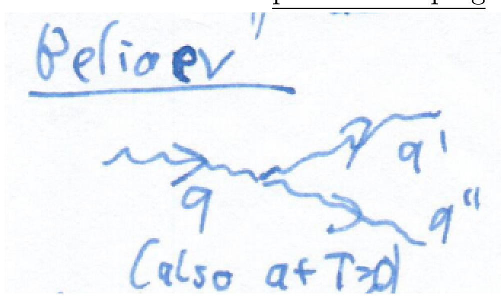
PROS:

- Seemingly straightforward implementation
- Easy implementation conceptually
- Includes repulsion between BEC and thermal cloud

CONS:

- Subtleties with renormalisation
- Excitations in this formalism have an energy gap, which means that $E_q \to$ nonzero for q$\to$ 0. However they should be gapless, according to a Hugenholtz-Pines theorem (related to the Goldstone theorem).
- Computationally hard in general 3D (in which case correlation functions G_A, G_N are 6D.
- No $\hat{\chi}^\dagger\hat{\chi}\hat{\chi}$ terms
  due to assumption of Gaussian state/ use of Wick theorem. $\implies$ Absence of phonon damping:





⇒ This led to the design of various "fixes" of HFB and alternatives. Some of those are listed below.

3.5.3 Other Bose-gas quantum field methods

HFB is straightforward to derive but has some issues listed on the previous page. Let us thus list some alternative methods to study quantum-field corrections beyond the GPE, or fully quantum models.

I: Truncated Wigner approximation:

- We write $W(\alpha, \alpha^*) = F[\hat{\Lambda}(\alpha, \alpha^*), \hat{\rho}(t)]$, where F denotes some functional, Λ is an operator basis and $\hat{\rho}$ the time evolving density matrix. In essence this is using the Wigner function (2.49) in a many-body setting.
- We next convert the time evolution equation for the density matrix into one for the Wigner function: $\dot{\hat{\rho}}=...\quad \rightarrow \dot{W} = ...$
- The result can be mapped to a set of stochastic differential equations $i\hbar\dot{\alpha}(\mathbf{x}) = ...$
- These take the same form as the GPE + random noise on the initial state.
- We can obtain all quantum observables, which are correlation functions such has $\langle\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x})\rangle$ from corresponding classical correlation functions over the noisy wave function, e.g. $\langle\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x})\rangle = \overline{\alpha^*(\mathbf{x}')\alpha(\mathbf{x})} - \frac{1}{2}$"$\delta(x - x')$".

II: t-DMRG:

This is short for **t**ime-dependent **d**ensity **m**atrix **r**enormalisation **g**roup. We discretise the full quantum many body problem (3.38) for example in the position basis: $\hat{\Psi}(\mathbf{x}) \rightarrow \hat{\Psi}(x_k)$, and then use an approximate method invented in the quantum information and condensed matter communities. It works well in 1D and if there is "not too much entanglement" in the system.

III: MCTDH(B):

Multi-**c**onfigurational **t**ime-**d**ependent **H**artree for **B**osons. Starts with a more complicated Ansatz than Eq. (3.27) into the many-body SE, that allows multiple strongly occupied states.

IV: Few exact solutions:

In some cases there are a few exact solutions of interesting many-body problems. One example is the exactly one dimensional system with Hamiltonian

$$\bar{H} = -\sum_{n=1}^{N} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_n^2} + \sum_{n,m=1}^{N} \frac{U_0}{2} \delta(x_n - x_m) \tag{3.102}$$

This is the first quantised Hamiltonian that we get for a bunch of Bosons in 1D, with no external potential $V(x) = 0$ and contact interactions U just as discussed in section 3.3.1. For the case

$U_0 < 0$ (attractive interactions), this is called Lieb-Liniger Hamiltonian, and has quantum soliton solutions:

$$\psi(x_1, ..., x_N) \sim e^{iKX_{CM}} \exp\left[-\frac{m|U_0|}{2\hbar}\sum_{i<j}|x_i - x_j|\right] \tag{3.103}$$

[Compare assignment 1, Q1(ii) and last page of week 7]