8 3.5. Quantum-field-theory of Bose-Einstein Condensates

- in 3.3: • Non-interacting quasiparticles
  • No conversion from condensed to uncondensed component (heating)
- this section discusses QFT methods that can rectify this

3.5.1. Hartree-Fock Bogoliubov method

We start again from Heisenberg eqn for field operator (3.26)

$$i\hbar \dot{\hat{\Psi}} = \hat{H}_0 \hat{\Psi} + U_0 \hat{\Psi}^+ \hat{\Psi} \hat{\Psi}$$

and take the expectation value, using $\hat{\Psi}(x,t) = \phi(x,t) + \hat{\chi}(x,t)$ (3.44)

We obtain and $\langle \hat{\chi} \rangle = 0$

(3.59)

$$i\hbar \dot{\phi}(x,t) = \hat{H}_0 \phi(x,t) + U_0 \langle (\phi^* + \hat{\chi}^+)(\phi + \hat{\chi})(\phi + \hat{\chi}) \rangle$$

$$= \hat{H}_0 \phi(x,t) + U_0 \Big[|\phi(x,t)|^2 \phi(x,t) + 2 \langle \hat{\chi}^+ \hat{\chi} \rangle \phi(x,t) + \langle \hat{\chi} \hat{\chi} \rangle \phi^* + \langle \hat{\chi}^+ \hat{\chi} \hat{\chi} \rangle$$

We in general don't know $\langle \hat{\chi}^+ \hat{\chi} \rangle$. Let us define

$$\boxed{\begin{array}{ll} \text{Normal correlation function} & G_N(x,x') = \langle \hat{\chi}^+(x') \hat{\chi}(x) \rangle \\ \text{anomalous correlation function} & G_A(x,x') = \langle \hat{\chi}(x') \hat{\chi}(x) \rangle \end{array}} \quad (3.60)$$

• We can write pieces of (3.45) as $G_N(x,x)$, $G_A(x,x)$

• For $\langle \hat{\chi}^+ \hat{\chi}^+ \hat{\chi} \rangle$ we use

got here

(3.61)

Wick's theorem: For a Gaussian quantum state

$$\langle \hat{O}_1 \hat{O}_2 \hat{O}_3 \rangle = \langle \hat{O}_1 \hat{O}_2 \rangle \langle \hat{O}_3 \rangle + \langle \hat{O}_1 \hat{O}_3 \rangle \langle \hat{O}_2 \rangle + \langle \hat{O}_1 \rangle \langle \hat{O}_2 \hat{O}_3 \rangle - 2 \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle \langle \hat{O}_3 \rangle$$

$$\langle \hat{O}_1 \hat{O}_2 \hat{O}_3 \hat{O}_4 \rangle = \underbrace{\hat{O}_1 \hat{O}_2}\, \underbrace{\hat{O}_3 \hat{O}_4} + \underbrace{\hat{O}_1 \hat{O}_3}\, \underbrace{\hat{O}_2 \hat{O}_4} + \underbrace{\hat{O}_1 \hat{O}_4}\, \hat{O}_2 \hat{O}_3 + \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle \langle \hat{O}_3 \rangle \langle \hat{O}_4 \rangle$$

(or treat as assumption)

$$\hat{O}_1 \hat{O}_2 = \langle \hat{O}_1 \hat{O}_2 \rangle - \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle$$

..ussian state:

Single mode example $\hat{\rho} = \mathcal{N} \exp\left(-\bar{n}\hat{a}^+\hat{a} - \frac{1}{2}\bar{m}\hat{a}^{+2} - \frac{1}{2}\bar{m}^*\hat{a}^2\right)$

Coherent state:

thermal state: $\bar{m} = \bar{m}^* = 0$, $\bar{n} = -\beta(\epsilon - \mu)$ [see Eq. (3.4) Grand Can.

Many mode generalisation:
(M-modes)

$$\hat{\rho} = N \exp\left(\sum_{i,j=1}^{2M} K_{ij}\, \hat{c}_i^+ \hat{c}_j\right) \qquad \{\hat{c}\} = \begin{pmatrix} \hat{a}_1 \\ \vdots \\ \hat{a}_M \\ \hat{a}^+_1 \\ \vdots \\ \hat{a}^+_M \end{pmatrix}$$

- Gardiner/Zoller "Quantum Noise" 3rd ed p. 119
- See Blaizot & Ripka "Quantum theory of finite systems" (p. 93, Eq. (4.47)
- [redacted] Many "variants" of Wick's theorem all over QFT, all express results of bringing a, a^+ into some default order.

- Using Wick's theorem, we see $\langle \hat{\chi}^+\hat{\chi}\hat{\chi}\rangle = 0$ since $\langle\hat{\chi}\rangle = 0$.

We arrive at a modified GPE

$$i\hbar\frac{\partial}{\partial t}\phi(x,t) = \hat{H}_0\,\phi(x,t) + U_0|\phi(x,t)|^2\phi(x,t) + 2U_0 \overbrace{G_N(x,x,t)}^{\equiv \bar{G}_N(x)}\phi(x,t) + U_0 \overbrace{G_A(x,x,t)}^{\equiv \bar{G}_A(x)}\phi^*(x,t) \qquad (3.62)$$

- $G_N(x,x) = n_{unc}(x) \equiv$ density of uncondensed (thermal) atoms [see p. 44 / 48]
- To make use of (3.62), we need to know $G_N(x,x,t)$, $G_A(x,x,t)$

We can get those from the Heisenberg equations for $\hat{\chi}^+(x)\hat{\chi}(x)$ and $\hat{\chi}(x')\hat{\chi}(x)$: Hartree-Fock Bogoliubov equations:

$$i\hbar\frac{\partial G_A(x,x')}{\partial t} = \left\langle\left[\hat{\chi}(x')\hat{\chi}(x), \hat{H}\right]\right\rangle = \left[\hat{H}_0(x) + \hat{H}_0(x')\right] G_A(x,x') \qquad (3.63)$$
$$+ 2U_0\left[|\phi(x)|^2 + |\phi(x')|^2 + \bar{G}_N(x) + \bar{G}_N(x')\right] G_A(x,x')$$
$$+ U_0\left[\phi(x)^2 G_N^*(x,x') + \phi(x')^2 G_N(x,x') + \bar{G}_A(x) G_N^*(x,x') + \bar{G}_A(x') G_N(x,x')\right]$$
$$+ U_0\left[\phi(x)^2 + G_A(x,x)\right]\delta^{(3)}(x-x')$$

$$i\hbar\frac{\partial}{\partial t}G_N(x,x') = \left[\hat{H}_0(x) - \hat{H}_0(x')\right]G_N(x,x') + 2U_0\left[|\phi(x)|^2 - |\phi(x')|^2 + \bar{G}_N(x) - \bar{G}_N(x')\right] G_N(x,x')$$
$$+ U_0\left[\bar{G}_A(x)\, G_A^*(x,x') - \bar{G}_A(x') G_A(x,x')\right]$$
$$+ U_0\left[\phi(x)^2 G_A^*(x,x') - \phi^*(x')^2 G_A(x,x')\right]$$

- We again used Wick's theorem on terms like $\langle \hat{\chi}^\dagger \hat{\chi}^\dagger \hat{\chi} \hat{\chi} \rangle$
- The general idea (i) equation for $\langle \hat{\Psi} \rangle$ couples to ↓
  (ii) $\langle \hat{\Psi}^\dagger \hat{\Psi} \rangle$ couples to ↓
  (iii) $\langle \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi} \rangle$

  is called <u>cumulant expansion</u>. It has to be truncated at some order, here using Wick's theorem

We can define:

$$\boxed{\begin{array}{llll} \text{Condensate density} & |\phi(x)|^2 , & \text{number} & N_{cond} = \int |\phi(x)|^2 dx \\ \text{thermal density} & \tilde{G}_N(x) , & \text{—''—} & N_{unc} = \int \tilde{G}_N(x)\, dx \end{array}} \quad (3.64)$$

- In HFB equations
  - green —— interactions between condensed & uncondensed atoms
  - brown —— —''— of uncondensed atoms among one another
  - yellow —— conversion between condensed & uncondensed atoms (heating)

<u>Example I</u> Relation to Bogoliubov equations (3.45)

Let us consider $|\Psi\rangle = |0\rangle$, the <u>Bogoliubov vacuum</u> with zero quasiparticles in any mode, as our initial-state (eternal state in Heisenberg picture)

Then $G_N(x,x') = \sum_n v_n(x) v_n^*(x')$ $\qquad G_A(x,x') = \sum_n -u_n(x') v_n^*(x)$

For those G_A, G_N a lengthy calculation gives from HFB equations (3.63):

$$i\hbar \dot{G}_N(x,x') = 0 \qquad i\hbar \dot{G}_A(x,x') = -2\mu\, G_A(x,x')$$

$$\hookrightarrow G_A(x,x',t) = e^{+i 2\mu t/\hbar} G_A(x,x',0)$$

For this we ignore G relative to ϕ^2 (= fluctuations small) and assume $\phi(t) = \phi_0(t=0)$

- Thus the Bogoliubov vacuum is a steady state of HFB-eqns

Depletion and renormalisation

In $|\psi\rangle = |0\rangle$ (BdG-vacuum) $n_{UNC}(x) = G_N(x,x)$ is the unconsensed density. For homogeneus BEC:

density of states

$$n_{UNC}(x) = \sum_n |v_n(x)|^2 = \frac{1}{\mathcal{V}} \sum_q v_q^2 \xrightarrow[3D]{} \frac{1}{\mathcal{V}} \int_{q=0}^{\infty} dq\, q^2 (4\pi) \underbrace{D}_{= (2\pi/L)^{-3}} v_q^2$$

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

$$= \frac{1}{2\pi^2} \int_0^{\infty} dq\, q^2 v_q^2 \overset{\text{Eq. (3.51)}}{=\!=} \frac{8 (m U_0 \varrho)^{3/2}}{3\hbar^3 \pi^2}$$

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

$$\boxed{\text{Condensate depletion:} \quad \frac{n_{unc}}{\varrho} = \frac{8}{3\sqrt{\pi}} (\varrho a_0^3)^{\frac{1}{2}} \qquad (3.65)}$$

- Typical numbers: $a_s = 5.5$ nm (Rb), $\varrho = 10^{19}/m^3$

  $\Rightarrow \frac{n_{unc}}{\varrho} = 0.2\%$ uncondensed density due to vacuum fluctuations.

Let us also calculate

$$\bar{G}_A(x) = G_A(x,x) = -\sum_n u_n(x) v_n^*(x) \overset{\text{as}}{\underset{\text{above}}{=\!=}} \infty \quad \text{↯ divergent integral.} \qquad (3.66)$$

$$\overset{\text{cut-off}}{\underset{\text{integral}}{=\!=}} -\frac{4}{\pi^2} \int_0^{K} dq\, q^2 u_q v_q^* \overset{K \gg \infty}{=\!=} -\frac{4 m U_0 \varrho K}{\pi^2 \hbar^2} \equiv -\varkappa U_0 \varrho$$

This divergence has the same cause as in other local quantum-field theories (e.g. particle physics): The implicit mathematical (but not physical) assumption that the theory is valid to arbitrarily high energy scales.

Solution: Renormalisation = we absorb "infinities" (here K) into parameters in the Hamiltonian.

~~Renormalis~~

Renormalised interaction U

?

$$U_0 = \frac{U}{1-\varkappa U} \qquad \varkappa = \frac{4mK}{2\pi^2\hbar^2} \tag{3.67}$$

- $\varkappa$ "infinite", U_0 "infinite" (parameter in $\hat{H}$), U "finite" ($\uparrow$ observable quantity)
- "infinite" means ∞ in the limit $K \to \infty$
- To see (3.67) can calc. e.g. Born scattering from $\hat{H}$

Example here: Renormalised mean-field interaction in modified GPE (3.62)

Ok, ignore, say $\bar{G}_N$ small

can't ignore if $\to\infty$

$$i\hbar\dot{\phi} = \hat{H}_0\phi + U_0|\phi|^2\phi \left(+ 2\underset{\downarrow\ \boxed{U}}{U_0}\bar{G}_N\phi \right) + U_0\bar{G}_A\phi^*$$

Would need BdG with $|\phi| + G_N$ for this (self consistent eqn)

Use $\bar{G}_A = -\varkappa \underline{U}\rho$ (from (3.66))

$\boxed{\text{Replacing } U_0 \to U \text{ in BdG equations}}$ (derived fr. already renormalized GPE)

Then

$$i\hbar\dot{\phi} = \hat{H}_0\phi + \underbrace{\left(U_0(1-\varkappa U)\right)}_{=U,\ \text{finite},\ \text{fr. } (3.53)}|\phi|^2\phi + 2U\bar{G}_N\phi \tag{3.68}$$

(steps in brown are allowed because perturbations $\hat{\chi}$ (hence $G_N, G_A, \bar{G}_N, \bar{G}_A$) are "small")

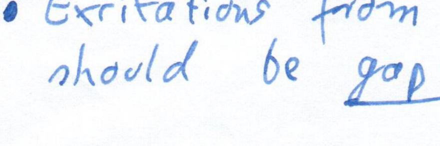
- For numerical implementation: K frequently small enough that renormalisation can be ignored

Appraisal of HFB:

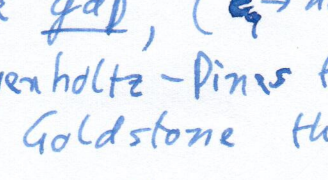
PRO
- Seemingly straightforward implementation
- Easy implementation conceptually
- Includes repulsion between BEC & thermal cloud
- Includes conversion —〃— (heating)

CON
- Subtleties with renormalisation, pdg
  ↳ self-consistent
- Excitations from (3.48) have <u>gap</u>, ($\epsilon_q \to$ nonzero for $q \to 0$) should be <u>gapless</u> (Hugenholtz–Pines theorem & Goldstone theorem)
- Computationally hard in general 3D case ($\Rightarrow$ 6D G_A, G_N)
- No $\hat{\chi}^\dagger \hat{\chi} \hat{\chi}$ terms $\Rightarrow$ Absence of <u>phonon damping</u>

<u>Landau</u>



<u>Beliaev</u>



⇨ Various "fixes" of HFB & Alternatives (see next page)

3.5.2. Other Bose-gas QFTs

- HFB straightforward to derive, but issues listed on previous page

Alternative methods to study <u>quantum-field corrections</u> beyond the GPE, or fully quantum models

① → FPI

Truncated Wigner approximation:

(see p. 246 for single mode example)

- review
- + single mode laser review

- Write $W(\alpha, \alpha^*) = F[\hat{\Lambda}(\alpha, \alpha^*), \hat{\rho}]$

  Wigner function; ℂ here, not operators; functional; operator basis; density matrix

- Convert $\dot{\hat{\rho}} = \ldots \longrightarrow \dot{W} = \ldots$
- Map to <u>stochastic differential equation</u> $i\hbar\dot{\alpha}(x) = \ldots$
- Looks like GPE + random noise
- Get e.g. $\langle \hat{\Psi}^\dagger(x') \hat{\Psi}(x) \rangle = \overline{\alpha^*(x')\alpha(x)} - \text{"}\frac{1}{2}\delta(x-x')\text{"}$

  renormalisation issues again

② **tDMRG:** time dependent density matrix renormalisation group

$\hat{\Psi}(x) \rightarrow \hat{\Psi}(x_k)$ solve all of (3.26) HE .. (Heisenberg eqn)

- Works well in 1D for not "too much entanglement"

③ **MCTDH(B)** Multi-configurational time-dependent Hartree for Bosons.

- Starts with a more complicated Ansatz than (3.16) $\left[\Psi = \prod_i \phi_i\right]$ into the many-body ~~...~~SE, that allows <u>multiple</u> strongly occupied states.

  $\prod_i \phi(x_i)$

  Now $\left(\prod_i^{N/2} \phi(x_i) + \prod_i^{N/2} \varphi(x_i)\right)$

④ **Few exact solutions:** 1D, $U_0 < 0$ (attractive)

<u>Lieb-Liniger Hamiltonian:</u>

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

(see Eq. (2.23), $V=0$, U_0 from (3.17)) (First quant A).

Soliton solution

$$\Psi(x_1, \ldots, x_N) \sim e^{iKX_{cm}} \exp\left[-\frac{m|U_0|}{2\hbar^2} \sum_{i<j} |x_i - x_j|\right]$$