# Week 7

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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### 3.4 Quasiparticles/quantized excitations

In section 3.3 we had assumed the gas is fully condensed and thus effectively replaced

$$\underbrace{\hat{\psi}(\mathbf{x})}_{\text{operator}} \rightarrow \underbrace{\phi(\mathbf{x})}_{\text{complex function}}, \text{ completely.}$$

Let us now retain some possibly non-condensed atoms, by writing the

**Field operator with fluctuations** (c.f. Eq. (3.58))

$$\hat{\psi}(\mathbf{x}) = \phi_0(\mathbf{x}) + \underbrace{\sum_n u_n(\mathbf{x})\hat{\alpha}_n - v_n^*(\mathbf{x})\hat{\alpha}_n^\dagger}_{\hat{\chi}(\mathbf{x})} \tag{3.60}$$

In this expression:

| | |
|---|---|
| $\hat{\psi}$ | Bose atomic field operator |
| $\langle\hat{\psi}\rangle = \phi_0$ | (still) condensate mean field |
| $u_n(\mathbf{x}), v_n(\mathbf{x})$ | Bogoliubov mode function |
| $\hat{\alpha}_n, \hat{\alpha}_n^\dagger$ | Bogoliubov creation and destruction operators (Bosonic) |
| $\hat{\chi}(\mathbf{x})$ | fluctuation operator, assumed small ($\mathcal{O}(\hat{\chi}^3) = 0$) |

We now insert (3.60) into Hamiltonian (3.37) and choose $u_n$, $v_n$ such that the Hamiltonian is diagonalized.

**Diagonalized:** in terms of Fock states for Bogoliubov operators means it takes the form

$$\hat{H} \approx \sum_n \varepsilon_n \hat{\alpha}_n^\dagger \hat{\alpha}_n$$

This is achieved when $u_n$ and $v_n$ fulfill the

**Bogoliubov-de-Gennes (BdG) equations**

$$\begin{aligned}\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + 2U_0|\phi_0(\mathbf{x})|^2 - \mu - \hbar\omega_n\right] u_n(\mathbf{x}) - U_0\phi_0(\mathbf{x})^2 v_n(\mathbf{x}) = 0 \\ \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + 2U_0|\phi_0(\mathbf{x})|^2 - \mu + \hbar\omega_n\right] v_n(\mathbf{x}) - U_0\phi_0^*(\mathbf{x})^2 u_n(\mathbf{x}) = 0\end{aligned} \tag{3.61}$$

and

**Orthonormality conditions**

$$\begin{aligned}\int d^3x \phi_0^*(\mathbf{x}) u_n(\mathbf{x}) = \int d^3x \phi_0^*(\mathbf{x}) v_n^*(\mathbf{x}) = 0 \quad \text{(modes are orthogonal to condensate)} \\ \int d^3x \left[u_n(\mathbf{x})u_m^*(\mathbf{x}) - v_n(\mathbf{x})v_m^*(\mathbf{x})\right] = \delta_{mn} \\ \int d^3x \left[u_n(\mathbf{x})v_m(\mathbf{x}) - v_n(\mathbf{x})u_m(\mathbf{x})\right] = 0\end{aligned} \tag{3.62}$$

Using (3.61) the Hamiltonian takes the form of a

**Quasi-particle Hamiltonian**

$$\hat{H} = E[\phi] + \sum_n (\mu + \hbar\omega_n)\hat{\alpha}_n^\dagger \hat{\alpha}_n \tag{3.63}$$

where we used the

$$E[\phi] = \underbrace{\int d^3x \ \phi^*(\mathbf{x}) \left[-\frac{\hbar^2}{2m}\nabla + V(\mathbf{x}) + U_0|\phi(\mathbf{x})|^2\phi(\mathbf{x})\right]}_{\text{Gross-Pitaevskii energy functional}} \tag{3.64}$$

- Eq. (3.63) takes the form of a Hamiltonian for non-interacting entities created by $\hat{\alpha}_n^\dagger$.
- For that reason $\hat{\alpha}_n, \hat{\alpha}_n^\dagger$ are called quasi-particle operators.
- Eq. (3.61) takes the same form as Eq. (3.59), which we got starting with a seemingly quite different question. We will comment on this later.
- Eq. (3.62) ensure that the quasi-particles are Bosons:

$$\begin{aligned}[\hat{\alpha}_n, \hat{\alpha}_m^\dagger] &= \int d^3\mathbf{x} \int d^3\mathbf{y} \Big( u_n^*(\mathbf{x}) u_m(\mathbf{y}) [\hat{\Psi}(\mathbf{x}), \hat{\Psi}^\dagger(\mathbf{y})] + v_n^*(\mathbf{x}) v_m(\mathbf{y}) [\hat{\Psi}^\dagger(\mathbf{x}), \hat{\Psi}(\mathbf{y})] \Big) \\ &= \int d^3\mathbf{x} \Big( u_n^*(\mathbf{x}) u_m(\mathbf{x}) - v_n^*(\mathbf{x}) v_m(\mathbf{x}) \Big) \overset{Eq.\ (3.62)}{=} \delta_{nm}.\end{aligned} \tag{3.65}$$

- Using (3.62), we can "invert" (3.60) [exercise] to find

$$
\begin{aligned}
\hat{\alpha}_n &= \int dx \left[u_m^*(\mathbf{x})\hat{\psi}(\mathbf{x}) + v_m^*(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\right] \\
\hat{\alpha}_n^\dagger &= \int dx \left[u_m(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}) + v_m(\mathbf{x})\hat{\psi}(\mathbf{x})\right]
\end{aligned}
\tag{3.66}
$$

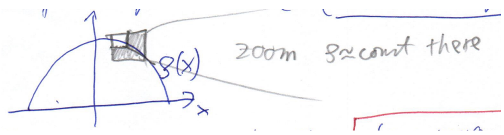
Hence we also call

$$
\begin{aligned}
u_m(\mathbf{x}) &- \underline{\text{particle amplitude}} \\
v_m(\mathbf{x}) &- \underline{\text{hole amplitude}}
\end{aligned}
$$

$\Longrightarrow$ A BdG excitation is a <u>superposition</u> of <u>added</u> & <u>subtracted</u> particles.

### 3.4.1 Phonons

Let us proceed to solve the BdG equations (3.61) for the simple case of a <u>homogenous, constant</u> condensate $\Longrightarrow \phi_0(\mathbf{x}) = \underset{\text{(indep of x)}}{\sqrt{\rho}}$ ; $\rho =$ atom density.




**left:** This can be realistic when concentrating on a small piece of a large BEC cloud. This would be called the <u>local density approximation</u> (LDA).

For this case, we make the

**<u>Plane-wave Ansatz</u>**

$$
u_q(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}\bar{u}_q e^{iqx} \qquad v_q(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}\bar{v}_q e^{iqx} \tag{3.67}
$$

- $\mathcal{V}$ is the quantisation volume
- q - wave number
- $\bar{u}_q$, $\bar{v}_q$ - are amplitudes, these are just complex numbers

Insert (3.67) into (3.61) and use $-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 u_q(\mathbf{x}) = \underbrace{\frac{\hbar^2 q^2}{2m}}_{\equiv E_q} u_q(\mathbf{x})$ etc., we can find the matrix equation

$$
\underbrace{\begin{pmatrix} E_q + 2U_0\rho - \mu - \hbar\omega_q & -U_0\rho \\ -U_0\rho & E_q + 2U_0\rho - \mu + \hbar\omega_q \end{pmatrix}}_{\equiv M} \begin{pmatrix} \bar{u}_q \\ \bar{v}_q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.68}
$$

For this to have any non-trivial solution, we need $\det(M) = 0$, hence

$$
\det(M) = -(\hbar\omega_q)^2 + (E_q + 2U_0\rho - \mu)^2 - U_0^2\rho^2 = 0. \tag{3.69}
$$

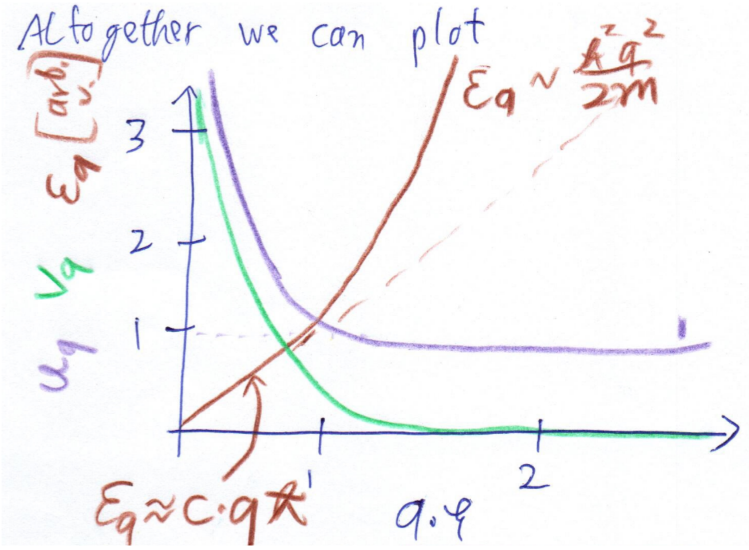
For a homogeneous condensate we know that $\mu = U_0\rho$, which follows from Eq. (3.45). Using that, we find for the excitations of the condensate the

**Bogoliubov dispersion relation**

$$\varepsilon_q \equiv \hbar\omega_q = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m} + 2U_0\rho\right)} \tag{3.70}$$

Using (3.62), (3.68) and (3.70) we can show, after defining the abbreviation $\zeta_q \equiv E_q + U_0\rho$, that

$$\bar{u}_q^2 = \frac{1}{2}\left(\frac{\zeta_q}{\varepsilon_q} + 1\right), \quad \bar{v}_q^2 = \frac{1}{2}\left(\frac{\zeta_q}{\varepsilon_q} - 1\right). \tag{3.71}$$




**left:** Combined plot of Bogoliubov energy $\varepsilon_q$ (3.70) (brown), particle amplitude $\bar{u}_q$ (violet) and hole amplitude $\bar{v}_q$ (green) (3.71).

In the figure we have used the definition of the

**Speed of sound**

$$c = \sqrt{\frac{U_0\rho}{m}} \tag{3.72}$$

Comments about Bogoliubov excitations:

- for $q \ll \zeta$, we have $\varepsilon_q \approx cq\hbar$ and $|\bar{u}_q|^2 + |v_q|^2 \gg 1$. $\varepsilon_q \approx cq\hbar$ is a linear dispersion relation as for sound-waves. $|\bar{u}_q|^2 + |v_q|^2 \approx N_{\text{atoms}}$, the number of atoms involved in an exciation (see yellow box * below). So long wavelength excitations with $q \ll \zeta$ are collective excitations/ sound-waves.

- for $q \gg \zeta$, we can approximate $\varepsilon_q \sim \frac{\hbar^2 q^2}{2m}$, which is the energy of a free particle. Also $|\bar{u}_q|^2 + |v_q|^2 \to 1$. This is a single-atom excitation ($\sim$ 1 atom got kicked so hard, it no longer feels the others).

**Number of excited atoms***: Let us consider the number of excited atoms

$$N_{\text{exc}} = \int \langle \hat{\chi}^\dagger \hat{\chi} \rangle dx \quad (\text{see}(3.60))$$

Let $|\,\psi\,\rangle = |\,N_1 N_2 ...\,\rangle$ be the Fock state for occupation of Bogoliubov excitations. $\Longrightarrow$

$$N_{\text{exc}} = \int_V dx \sum_{qq'} \Bigg( u_q^*(\mathbf{x}) u_{q'}(\mathbf{x}) \underbrace{\hat{\alpha}_q^\dagger \hat{\alpha}_{q'}}_{\sim \delta_{qq'} \text{ in state}|\,\psi\,\rangle} + v_q(\mathbf{x}) v_{q'}^*(\mathbf{x}) \underbrace{\hat{\alpha}_q \hat{\alpha}_{q'}^\dagger}_{= \hat{\alpha}_{q'}^\dagger \hat{\alpha}_q + \delta_{qq'}} \Bigg)$$
$$= \sum_q \left( |u_q|^2 + |v_q|^2 \right) N_q + \sum_q |v_q|^2. \tag{3.73}$$

Since $N_q$ here is the number of excitations, this motivates the allocation of $|\bar{u}_q|^2 + |\bar{v}_q|^2$ as "number of atoms within a single excitation".

### 3.4.2 Time-dependence

The overall time-dependence of the field operator in Eq. (3.60) is

**Time-dependence of BdG modes**

$$\hat{\psi}(x,t) = e^{-i\frac{\mu}{\hbar}t} \left[ \phi_0(\mathbf{x}) + \sum_n u_n(\mathbf{x}) \hat{\alpha}_n e^{-i\omega_n t} - v_n^*(\mathbf{x}) \hat{\alpha}_n^\dagger e^{i\omega_n t} \right] \tag{3.74}$$

- c.f. Eq. (3.58)
- to see this insert (3.60) into $\underset{\text{Heisenberg}}{Eq.}$ (3.38) using $\underset{\text{GPE}}{Eq.}$ (3.3.3) and $\underset{\text{BdG}}{Eq.}$ (3.61)

### 3.4.3 Coherent vs incoherent excitation

We have now addressed two seemingly different questions:

(A) In section 3.3.7: If we slightly perturb the GPE solution $\phi(x,t) = \phi_0(\mathbf{x}) + \delta\phi(x,t)$, how does the perturbation $\delta\phi$ evolve in time?

(B) In section 3.4: In a QFT problem, which fluctuation modes outside the BEC diagonalize the Hamiltonian?

Seemingly different questions give the same BdG equations for condensate excitations, compare (3.59) and (3.61).

The reason is that (A) is included in (B). Consider a single Bogoliubov mode only (say $n = 1$). Assume its quantum state is $|\,\psi\,\rangle = |\,\beta\,\rangle$ where $\beta \in \mathbb{C}$.
↓ coherent state

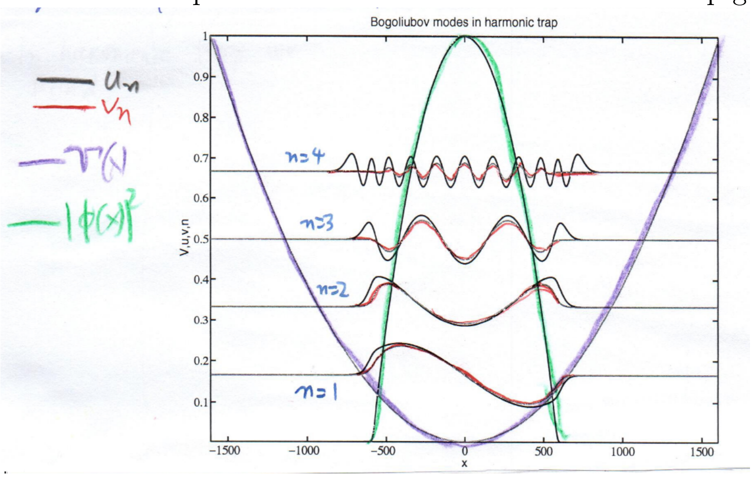
Then

$$\underbrace{\langle\hat{\psi}(x,t)\rangle}_{\text{Eq. (3.74)}} = e^{-i\frac{\mu}{\hbar}t}\left[\phi_0(\mathbf{x}) + u_1(\mathbf{x})\beta e^{-i\omega_1 t} - v_1^*(\mathbf{x})\beta^* e^{i\omega_1 t}\right]$$

which is a BEC mean field perturbation as in (3.59) (So here the population in mode number one has phase-coherence with the BEC). Had we used $\hat{\rho} = \sum_n p_n |\,n\,\rangle\langle\,n\,|$ for mode one, we keep $\langle\hat{\psi}\rangle = e^{-i\frac{\mu}{\hbar}t}\phi_0(\mathbf{x})$ with no perturbation of the mean field itself, so in that setting the $p_n$ correspond to incoherent thermal population.

### 3.4.4 The thermal cloud

In general (3.61) has to be solved numerically, but see Pethick & Smith for some analytical approximation techniques. The numerical solution in a 1D trap gives the following:




**left:** BdG modes in 1D trap (violet) are shown as black lines ($u_n$) and red lines ($v_n$). We also show the Thomas-Fermi shape of the condensate (green).

As $n \to \infty$, the modes approach the following

$$u_n \to \varphi_n \quad \text{(S.H.O states, see 1.9)}$$
$$v_n \to 0$$

As for the homogeneous case, we see that high energy BdG modes essentially become like single-particle excitations.

The modes now allow us to describe the "thermal cloud": BEC experiments never reach $T = 0$, hence we write

**Thermal cloud state**

$$\hat{\rho} = \sum_{\mathbf{N}} P_{\mathbf{N}} |\,\mathbf{N}\,\rangle\langle\,\mathbf{N}\,| \qquad P_{\mathbf{N}} - \text{see Eq. (3.5)} \tag{3.75}$$

for the state of thermal uncondensed atoms.

- We assume there is a (much larger) BEC component co-existing (not described by Eq. (3.75), but Eq. (3.60), in $\hat{\psi} = \phi + \hat{X}$).

  Let us now try to determine the total atom density

$$n(\mathbf{x}) = \langle\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\rangle = |\phi_0(\mathbf{x})|^2 + \underset{\text{Tr}[\hat{\rho}\hat{\alpha}]}{\underset{\downarrow}{0}} + \sum_{nn'} \text{Tr}\left[\hat{\rho}(u_n^*(\mathbf{x})\hat{\alpha}_n^\dagger - v_n(\mathbf{x})\hat{\alpha}_n)(u_{n'}(\mathbf{x})\hat{\alpha}_{n'} - v_{n'}^*(\mathbf{x})\hat{\alpha}_{n'}^\dagger)\right] \tag{3.76}$$

$$= |\phi_0(\mathbf{x})|^2 + \sum_n \text{Tr}\left[\hat{\rho}\left\{\left(|u_n(\mathbf{x})|^2 + |v_n(\mathbf{x})|^2\right)\hat{\alpha}_n^\dagger\hat{\alpha}_n + |v_n(\mathbf{x})|^2\right\}\right], \tag{3.77}$$

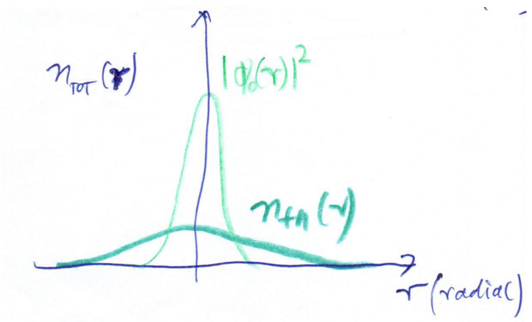
  where, to reach the second line, we have used that the expectation value of terms like $\alpha_n\alpha_{n'}^\dagger$ in the Fock states appearing in (3.75) is zero, unless $n = n'$. We thus have a total

**Atom density**

$$n_{\text{tot}}(\mathbf{x}) = \underbrace{|\phi_0(\mathbf{x})|^2}_{\text{BEC}} + \sum_n \left\{\underbrace{\left(|u_n(\mathbf{x})|^2 + |v_n(\mathbf{x})|^2\right)}_{\text{thermal cloud}} \underset{=\bar{m}_b,\ \text{see Eq. (3.12)}}{\underset{\downarrow}{n_{th}}} + \underbrace{|v_n(\mathbf{x})|^2}_{\text{quantum fluctuations}}\right\} \tag{3.78}$$

**Example:** Approximate $v \approx 0$, $u_n \to \varphi_n \implies$, then do some technical calculation to reach the thermal cloud shape:

$$n_{th}(\mathbf{x}) = \frac{N_{th}}{\pi^{3/2}R_xR_yR_z} e^{-\frac{x^2}{2R_x^2}} e^{-\frac{y^2}{2R_y^2}} e^{-\frac{z^2}{2R_z^2}}. \tag{3.79}$$




**left:** Thus the thermal cloud shape is Gaussian, with widths $R_i = \sqrt{\frac{2k_BT}{m\omega_i}}$, which depend on the temperature. Together with the condensate, we thus have a bi-modal density distribution, which can often be used to measure temperature $T$.

### 3.4.5 Superfluidity

We can give a phenomenological definition. A substance is a superfluid if it shows the following properties:

(i) flow without friction through small capillaries

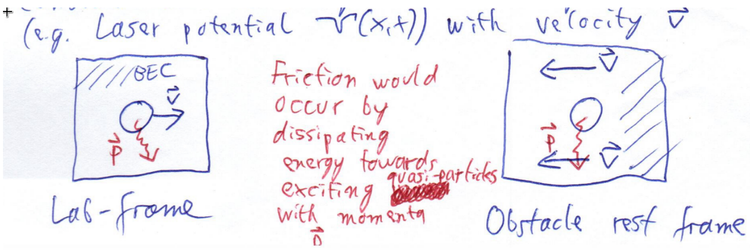
(ii) perfect heat conductivity (via convection)

(iii) rotation only via quantized vortices (see section 3.3.6)

Found e.g. in dilute gas BEC & cold liquid helium. How does it arise?

**Critical velocity:**

Consider a BEC through which we drag an obstacle (e.g. Laser potential $V(\mathbf{x}, t)$) with velocity $\mathbf{v}$.




**left:** Sketch of moving obstacle in BEC medium in the lab-frame versus obstacle rest frame.

Consider energy of gas in the two frames

| | Lab-frame | Rest frame |
|---|---|---|
| Ground-state (BEC only) | $E'$ (some internal energy) | $E' + \frac{1}{2} N m v^2$ ($N \to N_{\text{atoms}}$, $m \to$ mass of one atom) |
| Excited state (BEC plus one excitation $\mathbf{p}$) | $E' + \varepsilon_p$ ($\varepsilon_p \to$ see Eq. (3.70)); V(x,t), Hamiltonian time-dependent energy NOT CONSERVED | $E' + \varepsilon_p - \underbrace{\mathbf{p} \cdot \mathbf{v}}_{\text{Doppler shift}} + \frac{1}{2} N m v^2$; V(x), energy conserved, can only create excitation if $\Delta E$=0 |

**Energy needed to create excitation:**

$$\Delta E = \varepsilon_p - \mathbf{p} \cdot \mathbf{v} \tag{3.80}$$

Smallest gap at $\mathbf{p} \parallel \mathbf{v} \implies$ critical velocity for $\Delta E = 0 \implies 0 = \varepsilon_p - |\mathbf{p}||\mathbf{v}| \implies \mathrm{v}_{\text{crit}} = \underset{\mathbf{p}}{\text{Min}} \left[ \frac{\varepsilon_p}{|\mathbf{p}|} \right]$. If it moves slower than $\mathrm{v}_{\text{crit}}$, the obstacle cannot create any excitation. From Eq. (3.70) we then find

**Critical velocity:** below $v_{crit}$, there is superfluidity

$$v_{crit} = \operatorname*{Min}_{\mathbf{p}} \left[ \frac{\sqrt{\frac{p^2}{2m}\left(\frac{p^2}{2m} + 2U_o\rho\right)}}{p} \right] = \sqrt{\frac{\rho U_o}{m}} = c \quad \underline{\text{speed of sound}} \tag{3.81}$$

$(\mathbf{p} \leftrightarrow \hbar \mathbf{q})$

- In a usual fluid, there are single particle excitations $\varepsilon_p \sim \frac{p^2}{2m}$ for arbitrarily small $\mathbf{p}$ (unlike here) $\implies$ No superfluidity.
- Thus superfluidity relies on interactions.

### 3.4.6 Condensate stability

Lets return to Eq. (3.58) for perturbations of the mean field, the same conclusions can be found from Eq. (3.60).

$$\phi(x,t) = e^{-i\frac{\mu}{\hbar}t}\left[\phi_0(\mathbf{x}) + u(\mathbf{x})e^{-i\omega t} - v^*(\mathbf{x})e^{i\omega t}\right]$$

- Solutions to the BdG equations (3.61) do not have to have real frequencies $\omega \in \mathbb{R}$, the frequency can in general be complex $\omega \in \mathbb{C}$.

  **Example:** Homogeneous condensate with attractive interactions $U_0 < 0$

  $$\hbar\omega_q = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m} + U_0\rho\right)} \qquad \text{Im}(\hbar\omega_q) \neq 0 \text{ for } q < \frac{\sqrt{4|U_0|\rho m}}{\hbar}$$

- They also do not guarantee that $\text{Re}[\omega] > 0$, which would make sure that the excitation has in fact a higher energy than the BEC. For the following, let us write $\omega = \underset{\text{Re}}{\omega'} + i\underset{\text{Im}}{\omega''}$ for the real and imaginary parts of $\omega$.

We can classify results into three cases:

$\omega' > 0, \omega'' = 0$: Usual stable case, oscillatory modes

$\omega'' \neq 0$: The condensate is dynamically (modulationally) unstable. Small perturbations in Eq. (3.58) will grow exponentially with growth rate $\sim (\omega'')$

**Examples:**

homogeneous $U_0 \longrightarrow$ bright solitons

rotated BEC $\longrightarrow$ vortices

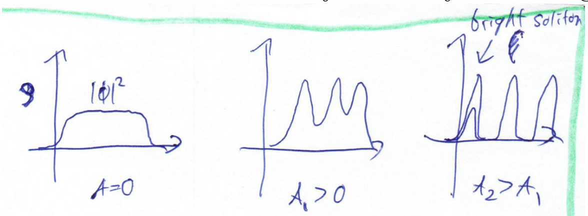
BEC $\underset{\text{Band-gap}}{U_0 > 0} \overset{\text{optical-lattice}}{\longrightarrow}$ gap-solitons

Usually the end-product of this instability is a new (stable) non-linear solution of TIGPE.

$\omega' < 0$: The condensate is energetically unstable

- All is fine in Eq. (3.58), which assumes unitary evolution, but $\phi_0(\mathbf{x})$ is NOT a local minimum of $E[\phi]$ Eq. (3.64). Hence any dissipation will destroy $\phi_0(\mathbf{x})$.

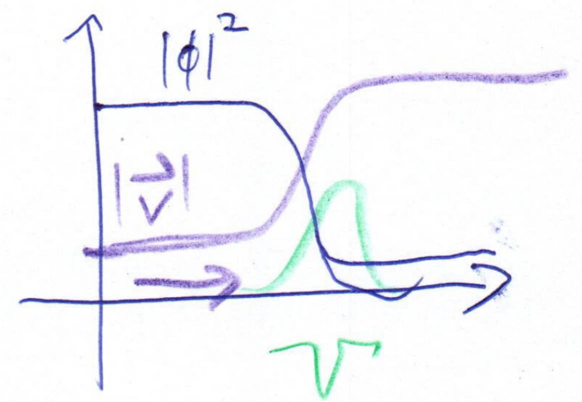
**Examples:** (i) Collapse of a homogenous BEC collapse with attractive interactions $U_0 < 0$. Here the initial state is dynamically and energetically unstable.




**left:** Density of initially almost homogenous BEC during dynamical instability. Unstable modes grow into bumps in time, the end-result is a train of bright solitons plus excess heating.

As an endproduct of the instability, we obtain Bright solitons: Non-linear solutions of TIGPE for $U_0 < 0$. Using $\phi_0 \sim \text{sech}(\mathbf{x})$ [soliton] in Eq. (3.61) instead of the initial homogenous state, all BdG modes are stable in the final state.

(ii) A partially supersonic ($v_{\text{flow}} > c$) flow of a BEC with repulsive interactions $U_0 > 0$ . This can be dynamically stable but is energetically unstable.




**left:** Sketch of condensate which makes a subsonic-supersonic transition when flowing over an external potential hump $V(x)$ (green). Density (blue), velocity $|\mathbf{v}|$ (violet) can be inferred from Eq. (3.54) and Eq. (3.55).

Again, we can use a Doppler shift argument as in section 3.4.5 $\hbar\omega' = \hbar\omega - vk \implies v_{crit}$ previous section = some phonons become energetically unstable.

We would reach similar conclusions looking at quantized, incoherent excitations.

How do they all (mean-field BEC, thermal & quantum excitations) play together in a time-dependent manner? $\longrightarrow$ Next chapter.