On the infimum of the excitation spectrum of a homogeneous Bose gas

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Homogeneous Bose gas

n bosons on $\mathbb{R}^d$ interacting with a 2-body potential v are described by the Hilbert space $L^2_{\mathrm{s}}\left((\mathbb{R}^d)^n\right)$ and the Hamiltonian

$$H^n \;=\; -\sum_{i=1} \frac{1}{2}\Delta_i + \sum_{1\leq i<j\leq n} v(\mathbf{x}_i - \mathbf{x}_j)$$

commuting with total momentum

$$P^n := \sum_{i=1}^{n} -\mathrm{i}\nabla_{\mathbf{x}_i}.$$

We assume that the potential v decays fast at infinity, $v(\mathbf{x}) = v(-\mathbf{x})$ and $\hat{v}(k) \geq 0$.

System in a box I

We are interested in the properties at fixed density ρ. Therefore, we enclose the system in $\Lambda = [0, L]^d$. We assume that the number of particles equals $n = \rho V$, where $V = L^d$ is the volume. The Hilbert space is $L^2_{\mathrm{s}}(\Lambda^n)$.

We replace the potential by its periodization

$$v^L(\mathbf{x}) = \frac{1}{V} \sum_{\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\, \hat{v}(\mathbf{k}).$$

System in a box II

The Hamiltonian, with periodic boundary conditions, equals

$$H^{L,n} = -\sum_{i=1}^{n} \frac{1}{2}\Delta_i^L + \sum_{1\leq i<j\leq n} v^L(\mathbf{x}_i - \mathbf{x}_j)$$

and has the ground state energy $E^{L,n} := \inf \mathrm{sp} H^{L,n}$.

The total momentum

$$P^{L,n} := \sum_{i=1}^{n} -\mathrm{i}\nabla_{\mathbf{x}_i}^L$$

has the spectrum $\mathrm{sp}P^{L,n} = \frac{2\pi}{L}\mathbb{Z}^d$.

Infimum of the excitation spectrum

For $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ we set

$$\epsilon^{L,n}(\mathbf{k}) := \inf \mathrm{sp} H^{L,n}(\mathbf{k}) - E^{L,n}.$$

Let $\mathbf{k} \in \mathbb{R}^d$. For $L \to \infty$, keeping $\frac{n}{V} = \rho > 0$, we set (informally)

$$\epsilon^{\rho}(\mathbf{k}) := \lim_{L\to\infty} \epsilon^{L,n}(\mathbf{k}).$$

Boost operator

Define the Boost operator in the direction of the first coordinate:

$$U_1 := \exp\left(\frac{\mathrm{i}2\pi}{L}\sum_{i=1}^{n}\mathbf{x}_{i,1}\right).$$

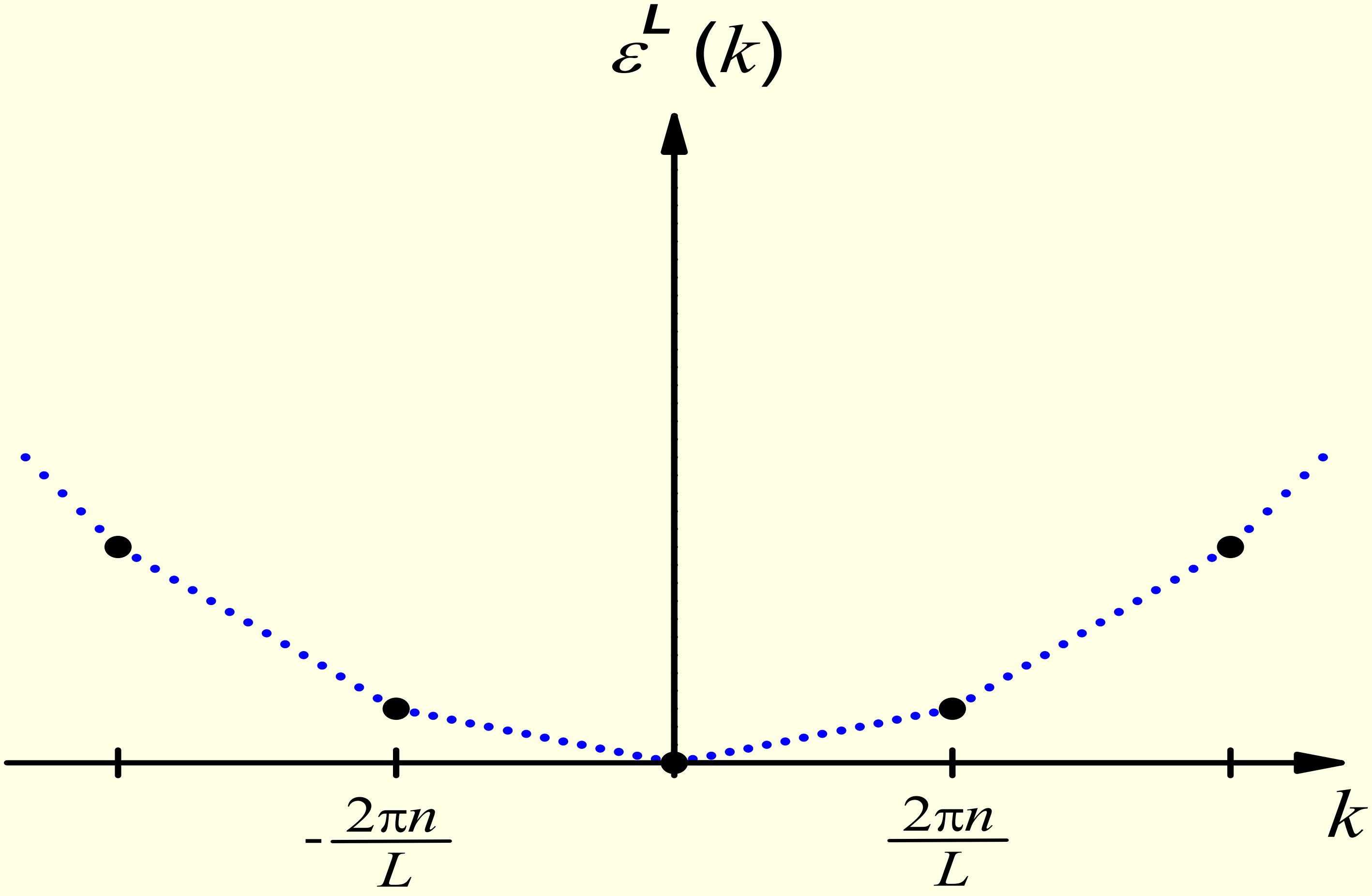
We easily compute

$$\begin{aligned} U_1^* P_1^{L,n} U_1 &= P_1^{L,n} + 2\pi\rho L^{d-1}, \\ U_1^*\left(H^{L,n} - \frac{1}{2\rho L^d}(P_1^{L,n})^2\right)U_1 &= H^{L,n} - \frac{1}{2\rho L^d}(P_1^{L,n})^2. \end{aligned}$$

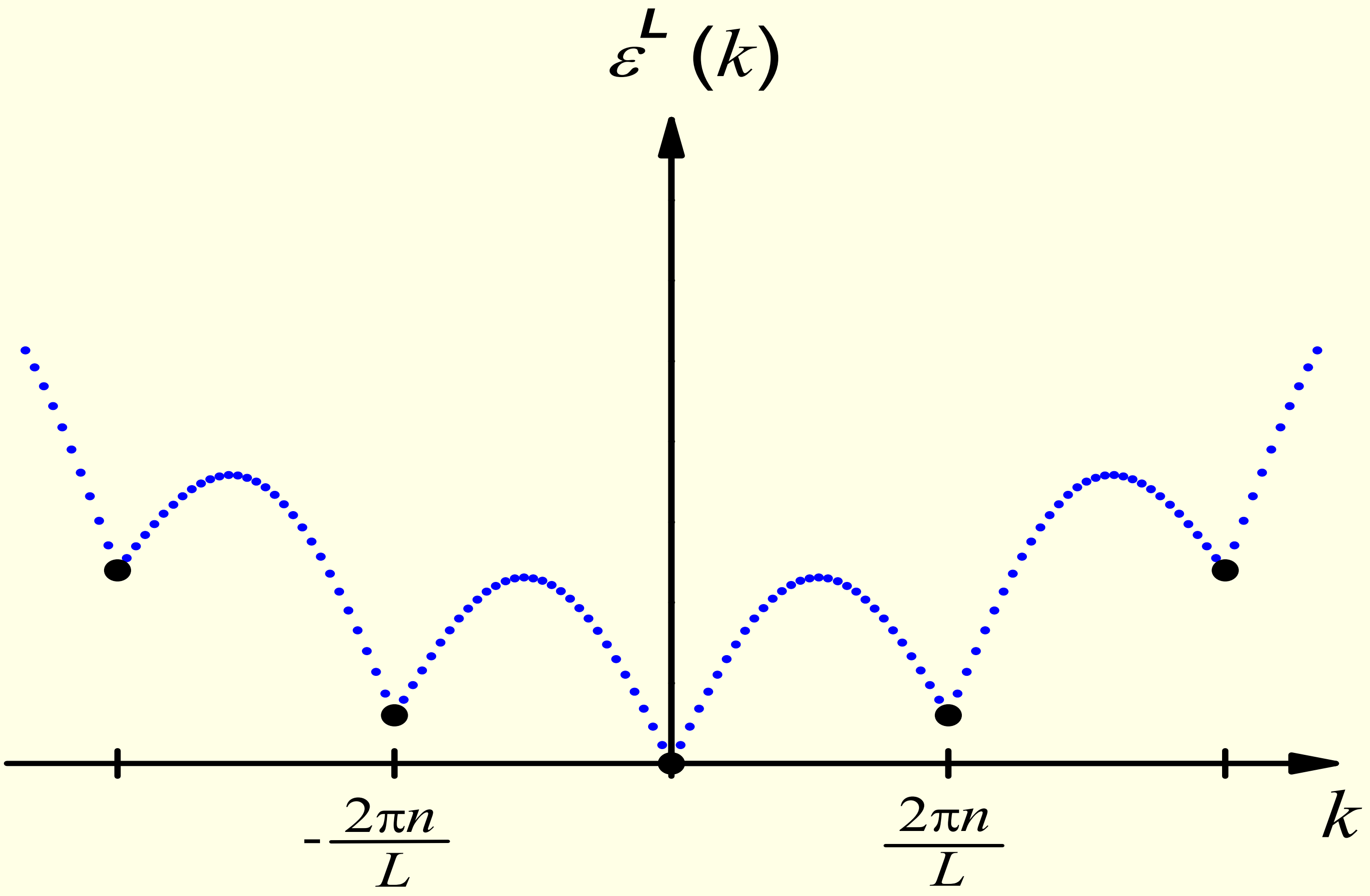
Therefore, in particular

$$\mathrm{sp}H^{L,n}(m2\pi\rho L^{d-1}\hat{e}_1) = \mathrm{sp}H^{L,n}(0) + \frac{m^2(2\pi)^2\rho L^{d-2}}{2}.$$

Excitation spectrum of free Bose gas in finite volume



Excitation spectrum of interacting Bose gas in finite volume



1-dimensional case

Theorem. In dimension $d = 1$ we have
$\epsilon(\mathbf{k} + 2\pi\rho) = \epsilon(\mathbf{k})$.

Proof. If Φ

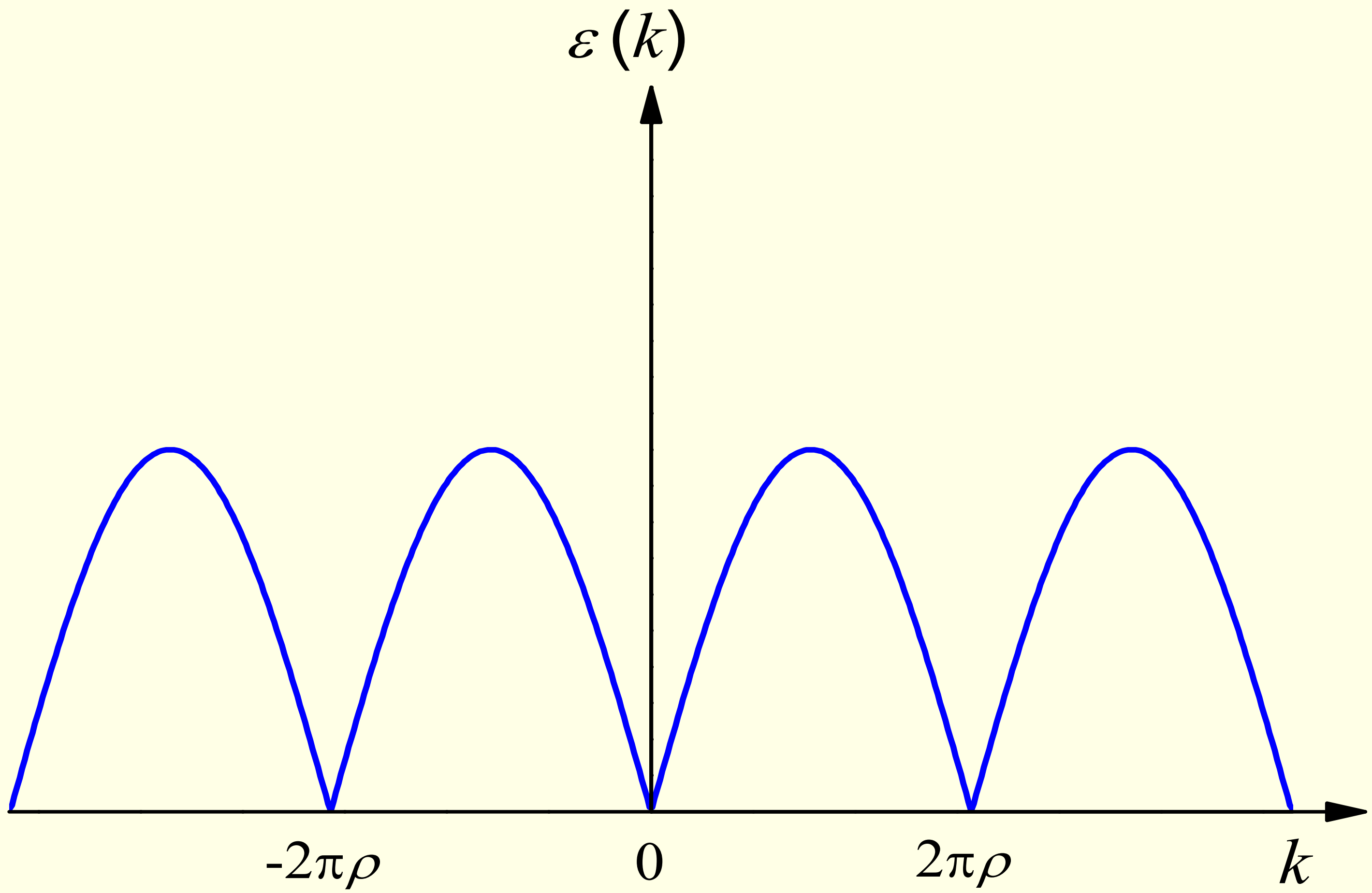
$$\begin{aligned}(H^{L,n} - E)\Phi &= 0, \\ (P^{L,n} - \mathbf{k})\Phi &= 0,\end{aligned}$$

then

$$\begin{aligned}(H^{L,n} - E)U\Phi &= \frac{1}{L}(2\pi\mathbf{k} + 2\pi^2\rho)U\Phi, \\ (P^{L,n} - \mathbf{k} - 2\pi\rho)U\Phi &= 0.\end{aligned}$$

Then we let $L \to \infty$.

Excitation spectrum of 1-dimensional interacting Bose gas



Conjecture about the infimum of the excitation spectrum

Conjecture.

(1) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon^\rho(\mathbf{k}) \in \mathbb{R}_+$ is continuous.

(2) Let $\mathbf{k} \in \mathbb{R}^d$. If $L_j \to \infty$, $\frac{n_j}{L_j^d} \to \rho$, $\mathbf{k}_s \in \frac{2\pi}{L_j}\mathbb{Z}^d$, then we have that $\epsilon^{L_j,n_j}(\mathbf{k}_j) \to \epsilon^\rho(\mathbf{k})$.

(3) If $d \geq 2$, then there exists $c_{\rm cr} > 0$ such that $\epsilon^\rho(\mathbf{k}) > c_{\rm cr}|\mathbf{k}|$.

(4) For some $c_{\rm ph} > 0$, $\epsilon^\rho(\mathbf{k}) \approx c_{\rm ph}|\mathbf{k}|$ for small $\mathbf{k}$.

(5) $\mathbf{k} \mapsto \epsilon^\rho(\mathbf{k})$ is subadditive, that is $\epsilon^\rho(\mathbf{k}_1) + \epsilon^\rho(\mathbf{k}_2) \geq \epsilon^\rho(\mathbf{k}_1 + \mathbf{k}_2)$.

(1) and (2) can be interpreted a kind of a spectral thermodynamic limit.

If (1) and (2) are true around $\mathbf{k} = 0$, then there is no gap in the excitation spectrum. (It is easy to show that $\epsilon(0) = 0$).

(3) implies the superfluidity of the Bose gas. More precisely, a drop of Bose gas will travel without friction as long as its speed is less than c_{cr}.

(4) suggests that speed of sound for at low energies is well defined and equals c_{ph}.

If one can superimpose (almost) independent elementary excitations, then (5) is true.

The above conjecture has important physical consequences.

In particular, it implies the superfluidity of the Bose gas at zero temperature.

The above conjecture seems plausible.

It is suggested by the arguments going back to Bogoliubov, Hugenholz, Pines, Bieliaev, as well as Bijls and Feynman.

Nobody has an idea how to prove it rigorously.

Subadditive functions

We say that $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon(\mathbf{k}) \in \mathbb{R}$ is subadditive iff

$$\epsilon(\mathbf{k}_1 + \mathbf{k}_2) \leq \epsilon(\mathbf{k}_1) + \epsilon(\mathbf{k}_2), \quad \mathbf{k}_1, \mathbf{k}_2 \in \mathbb{R}^d.$$

Let $\mathbb{R}^d \ni \mathbf{k} \mapsto \omega(\mathbf{k}) \in \mathbb{R}$ be another function. We define the subbadditive hull of ω to be

$$\epsilon(\mathbf{k}) := \inf\{\omega(\mathbf{k}_1)+\cdots+\omega(\mathbf{k}_n) \ : \ \mathbf{k}_1+\cdots+\mathbf{k}_n = \mathbf{k},\ n = 1, 2, \dots\}.$$

Clearly, the subadditive hull is always subadditive.

Quadratic Hamiltonians

Consider the Hamiltonian

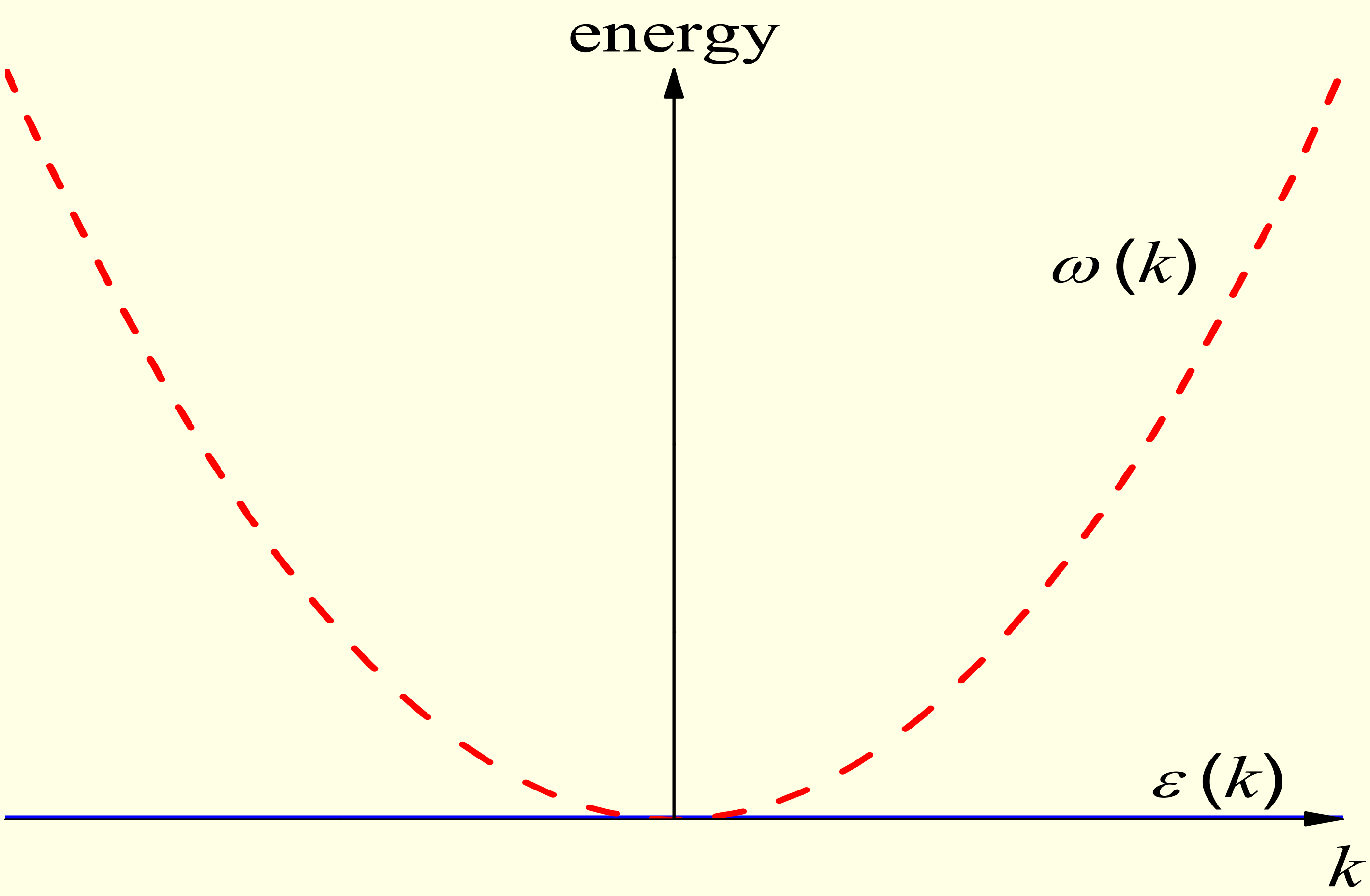
$$H = \int_{\mathbb{R}^d} \omega(\mathbf{k}) a^*_{\mathbf{k}} a_{\mathbf{k}} \mathrm{d}\mathbf{k},$$

and the total momentum

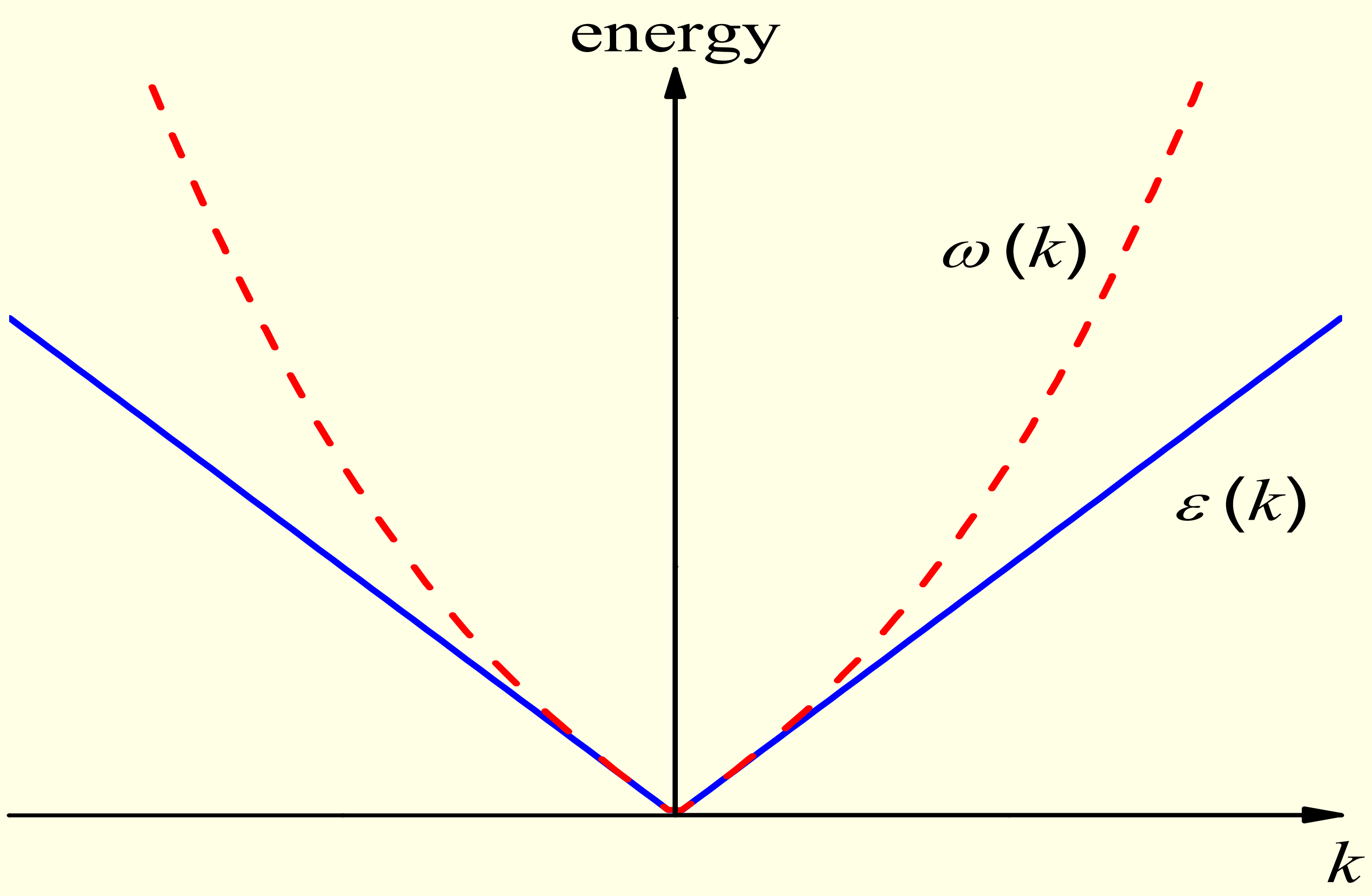
$$P = \int_{\mathbb{R}^d} \mathbf{k} a^*_{\mathbf{k}} a_{\mathbf{k}} \mathrm{d}\mathbf{k}.$$

We will call the function ω appearing in H the elementary excitation spectrum. Clearly, the infimum of the energy-momentum spectrum of H is equal to the subadditive hull of ω.

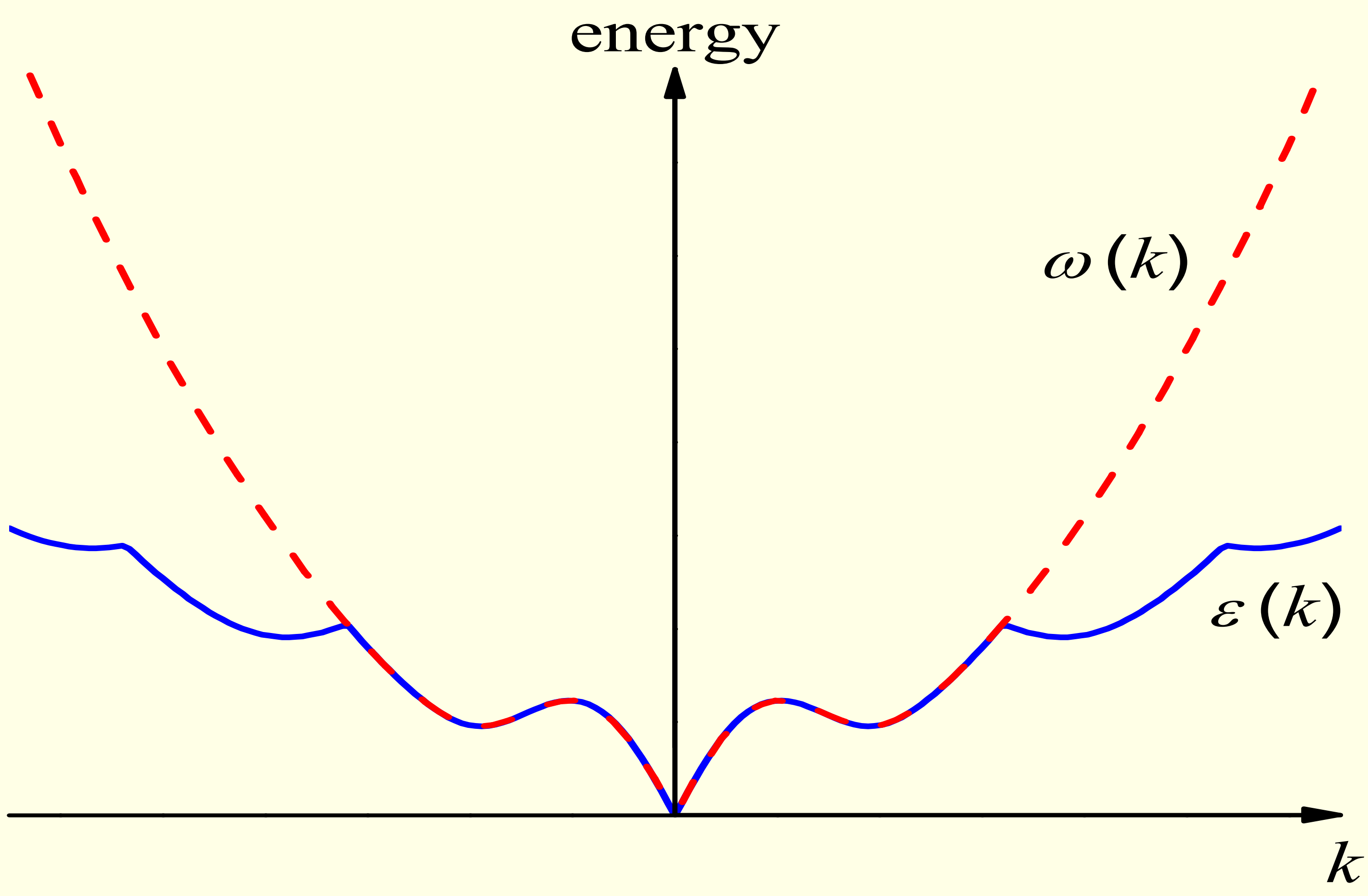
Excitation spectrum of free Bose gas



Hypothethic excitation spectrum of interacting Bose gas with no "rotons"



Hypothethic excitation spectrum of interacting Bose gas with "rotons"



Criterion for subadditivity

Theorem. (1) Let f be an increasing concave function with $f(0) \geq 0$. Then $f(|\mathbf{k}|)$ is subadditive.
(2) Let ϵ_0 be subadditive and $\epsilon_0 \leq \omega$. Let ϵ be the subadditive hull of ω. Then $\epsilon_0 \leq \epsilon$.

It often happens that the subadditive hull of a function is equal to zero everywhere. This is the case e.g. when $\omega(\mathbf{k}) = c\mathbf{k}^2$, which corresponds to the free Bose gas. But not for superfluid systems:

Subadditive hulls with phononic shape and positive critical velocity

Corollary. Suppose that $c_{\rm cr}, c_{\rm s} > 0$ and ω satisfies

1. $\omega(\mathbf{k}) \geq c_{\rm cr}|\mathbf{k}|$;
2. $\lim_{\mathbf{k}\to 0} \frac{\omega(\mathbf{k})}{|\mathbf{k}|} = c_{\rm s}$.

Let ϵ be the subadditive hull of ω. Then ϵ also satisfies

1. $\epsilon(\mathbf{k}) \geq c_{\rm cr}|\mathbf{k}|$;
2. $\lim_{\mathbf{k}\to 0} \frac{\epsilon(\mathbf{k})}{|\mathbf{k}|} = c_{\rm s}$.

Landau's argument for the superfluidity I

We add to H the perturbation u travelling at a speed w:

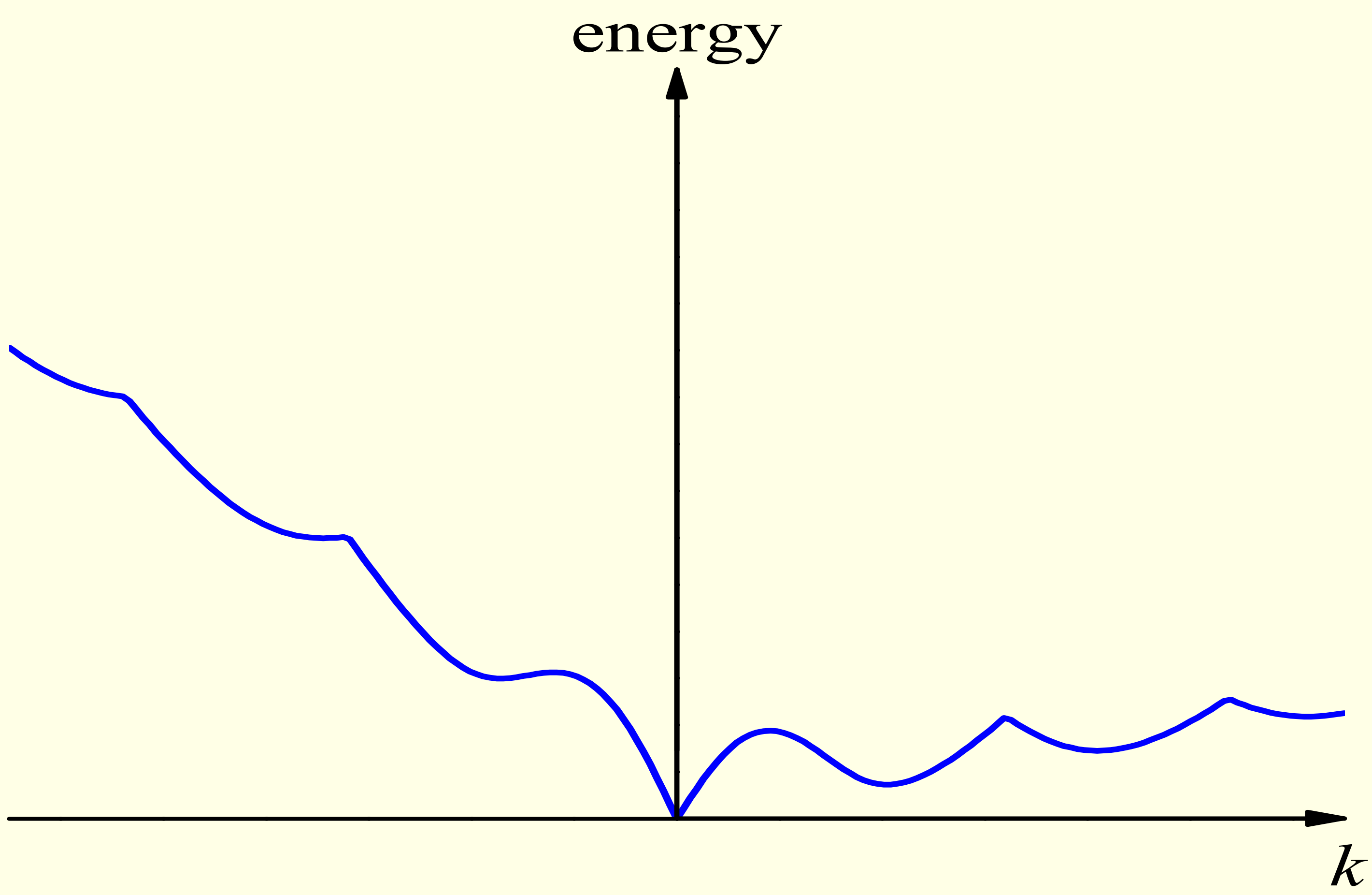
$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Psi_t = \Big(H + \lambda\sum_{i=1}^{n} u(x_i - \mathrm{w}t)\Big)\Psi_t.$$

We go to the moving frame:
$\Psi_t^{\mathrm{w}}(x_1, \dots, x_n) := \Psi_t(x_1 - \mathrm{w}t, \dots, x_n - \mathrm{w}t)$.
We obtain a Schrödinger equation with a time-independent Hamiltonian

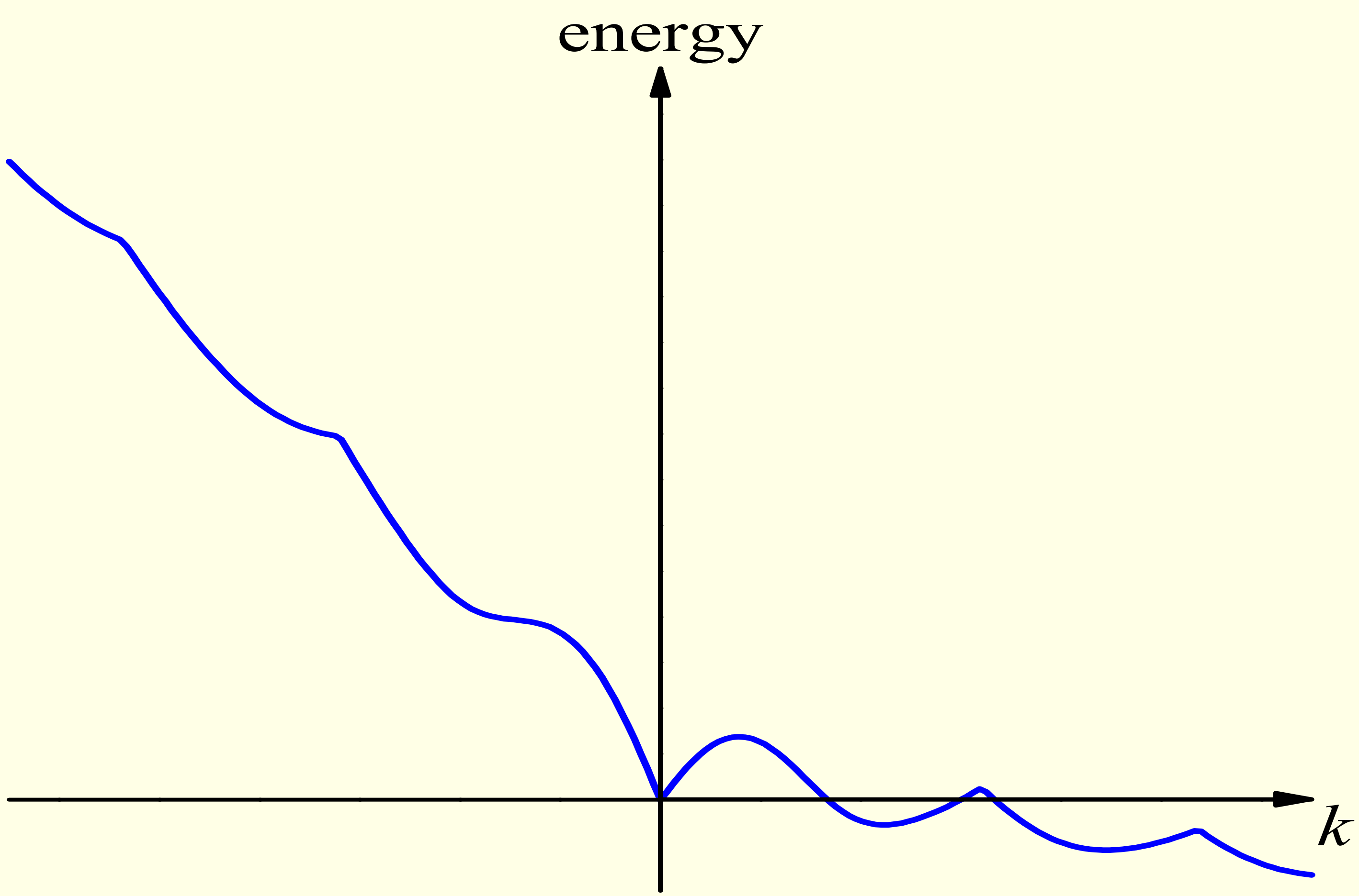
$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Psi_t^{\mathrm{w}} = \Big(H - \mathrm{w}P + \lambda\sum_{i=1}^{n} u(x_i)\Big)\Psi_t^{\mathrm{w}}.$$

Is the ground state $H\Psi_{\mathrm{gr}} = E\Psi_{\mathrm{gr}}$ stable against the travelling perturbation?

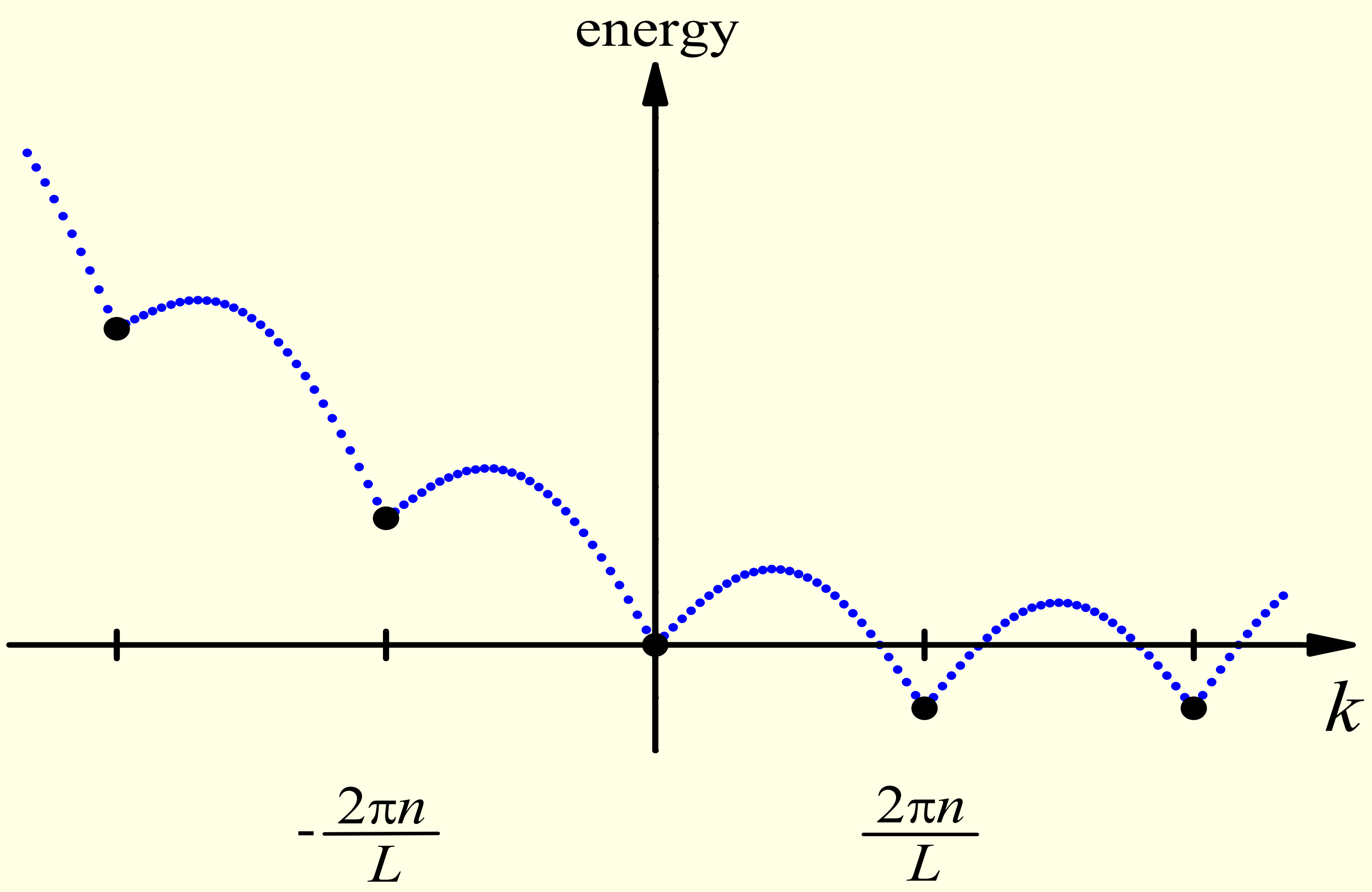
Bose gas travelling slower than critical velocity



Bose gas travelling faster than critical velocity



Travelling Bose gas in finite volume



Stability

Define the global critical velocity

$$c_{\mathrm{cr}}^{L,n} := \inf_{|\mathbf{k}|} \frac{\epsilon^{L,n}(\mathbf{k})}{|\mathbf{k}|}$$

If $|w| < c_{\mathrm{cr}}^{L,n}$, then the ground state of $H^{L,n}$ remains the ground state of the "tilted Hamiltonian", hence it is stable.

For the free Bose gas we have $c_{\mathrm{cr}}^{L,n} = \frac{\pi}{L} > 0$. In general, $c_{\mathrm{cr}}^{L,n} \le \frac{\pi}{L}$. Hence the global critical velocity is very small and vanishes in the thermodynamic limit.

Metastability

Define the restricted critical velocity below the momentum R as

$$c^{L,n}_{\mathrm{cr},R} := \inf \left\{ \frac{\epsilon^{L,n}(\mathbf{k})}{|\mathbf{k}|} \quad \mathbf{k} \neq 0, \quad |\mathbf{k}| < R \right\}.$$

We expect that for repulsive potentials

$$c^{\rho}_{\mathrm{cr},R} := \lim_{L \to \infty} c^{L,n}_{\mathrm{cr},R}, \quad \frac{n}{V} = \rho,$$

exists and, in dimension $d \geq 2$,

$$\liminf_{R \to \infty} c^{\rho}_{\mathrm{cr},R} > 0.$$

We expect metastability against a travelling perturbation travelling at a smaller speed.

2nd quantized grand-canonical approach I

Consider the symmetric Fock space $\Gamma_{\mathrm{s}}(L^2(\Lambda))$. For a chemical potential $\mu > 0$, we define the grand-canonical Hamiltonian

$$
\begin{aligned}
H^L &= \int a_{\mathbf{x}}^* (-\frac{1}{2}\Delta_{\mathbf{x}} - \mu) a_{\mathbf{x}} \mathrm{d}\mathbf{x} \\
&\quad + \frac{1}{2} \int \int a_{\mathbf{x}}^* a_{\mathbf{y}}^* v^L(\mathbf{x} - \mathbf{y}) a_{\mathbf{y}} a_{\mathbf{x}} \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{y}, \\
&= \oplus_{n=0}^{\infty} (H^{n,L} - \mu n).
\end{aligned}
$$

2nd quantized grand-canonical approach II

In the momentum representation it equals

$$H^L = \sum_{\mathbf{k}} (\frac{1}{2}\mathbf{k}^2 - \mu) a_{\mathbf{k}}^* a_{\mathbf{k}}$$

$$+ \frac{1}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \hat{v}(\mathbf{k}_2 - \mathbf{k}_3) a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}.$$

The momentum operator equals $P^L := \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}}$.
If E^L is the ground state energy of H^L, then one can get the corresponding density by

$$\partial_\mu E^L \;=\; -V\rho.$$

Infimum of the excitation spectrum – a rigorous definition I

We define

the ground state energy in the box

$$E^L = \inf \mathrm{sp} H^L.$$

For $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$, we define

the infimum of the excitation spectrum in the box

$$\epsilon^L(\mathbf{k}) := \inf \mathrm{sp} H^L(\mathbf{k}) - E^L.$$

Infimum of the excitation spectrum
– a rigorous definition II

For $\mathbf{k} \in \mathbb{R}^d$ we define
the infimum of the excitation spectrum in the thermodynamic limit

$$\epsilon(\mathbf{k}) := \sup_{\delta>0} \left(\liminf_{L\to\infty} \left(\inf_{\mathbf{k}'_L \in \frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k}-\mathbf{k}'_L|<\delta} \epsilon^L(\mathbf{k}'_L) \right) \right).$$

Proposition. At zero total momentum, the excitation spectrum has a global minimum where it equals zero: $\epsilon^L(0) = \epsilon(0) = 0$.

Conjecture about the infimum of the excitation spectrum

Conjecture.

(1) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon(\mathbf{k}) \in \mathbb{R}_+$ is continuous.

(2) Let $\mathbf{k} \in \mathbb{R}^d$. If $L_j \to \infty$, $\mathbf{k}_j \in \frac{2\pi}{L_j}\mathbb{Z}^d$, $\mathbf{k}_j \to \mathbf{k}$, then $\epsilon^{L_j}(\mathbf{k}_j) \to \epsilon(\mathbf{k})$.

(3) If $d \geq 2$, then there exists $c_{\mathrm{cr}} > 0$ such that $\epsilon(\mathbf{k}) > c_{\mathrm{cr}}|\mathbf{k}|$.

(4) For some $c_{\mathrm{ph}} > 0$ such that $\epsilon(\mathbf{k}) \approx c_{\mathrm{ph}}|\mathbf{k}|$ for small $\mathbf{k}$.

(5) $\mathbf{k} \mapsto \epsilon(\mathbf{k})$ is subadditive.

Minimization among coherent states

For $\alpha \in \mathbb{C}$, we define the displacement or Weyl operator of the zeroth mode: $W_\alpha := \mathrm{e}^{-\alpha a_0^* + \overline{\alpha} a_0}$. Set $\Omega_\alpha := W_\alpha \Omega$. Note that $P^L \Omega_\alpha = 0$. The expectation of the Hamiltonian in those coherent states equals

$$(\Omega_\alpha | H^L \Omega_\alpha) = -\mu |\alpha|^2 + \frac{\hat{v}(0)}{2V} |\alpha|^4,$$

and is minimized for $\alpha = \mathrm{e}^{\mathrm{i}\tau} \frac{\sqrt{V\mu}}{\sqrt{\hat{v}(0)}}$.

Translation of the zero mode

We apply the Bogoliubov translation to the zero mode of H^L by $W(\alpha)$. This means making the substitution

$$a_0 = \tilde{a}_0 + \alpha, \quad a_0^* = \tilde{a}_0^* + \overline{\alpha},$$
$$a_{\mathbf{k}} = \tilde{a}_{\mathbf{k}}, \qquad a_{\mathbf{k}}^* = \tilde{a}_{\mathbf{k}}^*, \qquad \mathbf{k} \neq 0.$$

Note that

$$\tilde{a}_{\mathbf{k}} = W_\alpha^* a_{\mathbf{k}} W_\alpha, \quad \tilde{a}_{\mathbf{k}}^* = W_\alpha^* a_{\mathbf{k}}^* W_\alpha,$$

and thus the operators with and without tildes satisfy the same commutation relations. We drop the tildes.

Translated Hamiltonian

$$
\begin{aligned}
H^L \quad := \quad & -V\frac{\mu^2}{2\hat{v}(0)} \\
& +\sum_{\mathbf{k}}\left(\frac{1}{2}\mathbf{k}^2+\hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(0)}\right)a_{\mathbf{k}}^*a_{\mathbf{k}} \\
& +\sum_{\mathbf{k}}\hat{v}(\mathbf{k})\frac{\mu}{2\hat{v}(0)}\left(\mathrm{e}^{-\mathrm{i}2\tau}\,a_{\mathbf{k}}a_{-\mathbf{k}}+\mathrm{e}^{\mathrm{i}2\tau}\,a_{\mathbf{k}}^*a_{-\mathbf{k}}^*\right) \\
& +\sum_{\mathbf{k},\mathbf{k}'}\frac{\hat{v}(\mathbf{k})\sqrt{\mu}}{\sqrt{\hat{v}(0)V}}\left(\overline{\mathrm{e}}^{\mathrm{i}\tau}a_{\mathbf{k}+\mathbf{k}'}^*a_{\mathbf{k}}a_{\mathbf{k}'}+\mathrm{e}^{\mathrm{i}\tau}\,a_{\mathbf{k}}^*a_{\mathbf{k}'}^*a_{\mathbf{k}+\mathbf{k}'}\right) \\
& +\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\frac{\hat{v}(\mathbf{k}_2-\mathbf{k}_3)}{2V}a_{\mathbf{k}_1}^*a_{\mathbf{k}_2}^*a_{\mathbf{k}_3}a_{\mathbf{k}_4}.
\end{aligned}
$$

Let H_{bg}^L denote the first 3 lines of the above expression.

Translated Hamiltonian with a coupling constant

If we (temporarily) replace the potential $v(\mathbf{x})$ with $\lambda v(\mathbf{x})$, where λ is a (small) positive constant, the translated Hamiltonian can be rewritten as

$$H^{\lambda,L} = \lambda^{-1} H^L_{-1} + H^L_0 + \sqrt{\lambda} H^L_{\frac{1}{2}} + \lambda H^L_1,$$

Thus the 3rd and 4th terms are in some sense small, which suggests dropping them.

Bogoliubov rotation

We want to analyze H^L_{bg}. To this end, for nonzero $\mathbf{k}$ we substitute

$$a^*_{\mathbf{k}} = c_{\mathbf{k}} b^*_{\mathbf{k}} - s_{\mathbf{k}} b_{-\mathbf{k}}, \quad a_{\mathbf{k}} = c_{\mathbf{k}} b_{\mathbf{k}} - \overline{s}_{\mathbf{k}} b^*_{-\mathbf{k}},$$

with $c_{\mathbf{k}} = \sqrt{1 + |s_{\mathbf{k}}|^2}$, so that

$$[b_{\mathbf{k}}, b^*_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}, \quad [b_{\mathbf{k}}, b_{\mathbf{k}'}] = 0.$$

For the zero mode we introduce $p_0 = \frac{1}{\sqrt{2}}(a^*_0 + a_0)$ and $x_0 = \frac{\mathrm{i}}{\sqrt{2}}(a_0 - a^*_0)$.

Bogoliubov Hamiltonian after rotation

$$H^L_{\rm bg} \;=\; \mu p_0^2 + {\sum_{\mathbf{k}}}' \omega_{\rm bg}(\mathbf{k}) b^*_{\mathbf{k}} b_{\mathbf{k}} + E^L_{\rm bg},$$

where the elementary excitation spectrum of $H^L_{\rm bg}$ is

$$\omega_{\rm bg}(\mathbf{k}) = \sqrt{\frac{1}{2}\mathbf{k}^2(\frac{1}{2}\mathbf{k}^2 + 2\mu\frac{\hat{v}(\mathbf{k})}{\hat{v}(0)})},$$

and its ground state energy equals

$$E^L_{\rm bg} \;=\; -\mu^2\frac{V}{2\hat{v}(0)} - \sum_{\mathbf{k}}\frac{1}{2}\left((\frac{1}{2}\mathbf{k}^2 + \mu\frac{\hat{v}(\mathbf{k})}{\hat{v}(0)}) - \omega_{\rm bg}(\mathbf{k})\right).$$

Zeroth mode

The number α has an arbitrary phase. Thus we broke the symmetry when translating the Hamiltonian. This is related to the fact that the zero mode is not a harmonic oscillator – it has continuous spectrum. The zeroth mode can be interpreted as a kind of a Goldstone boson.

Infimum of excitation spectrum in the Bogoliubov approximation I

The infimum of the excitation spectrum of H_{bg}^{L} is given by

$$\begin{aligned}\epsilon_{\mathrm{bg}}(\mathbf{k}) \;\; := \;\; & \inf\{\omega_{\mathrm{bg}}(\mathbf{k}_1)+\cdots+\omega_{\mathrm{bg}}(\mathbf{k}_n) \;: \\ & \qquad \mathbf{k}_1+\cdots+\mathbf{k}_n=\mathbf{k}, \;\; n=1,2,\ldots\}.\end{aligned}$$

$\omega_{\mathrm{bg}}(\mathbf{k})$ and $\epsilon_{\mathrm{bg}}(\mathbf{k})$ have a phononic shape and a positive critical velocity.

Infimum of excitation spectrum in the Bogoliubov approximation II

Replace the potential $v(x)$ with $\lambda v(x)$, where $\lambda > 0$. Let $\epsilon^\lambda(\mathbf{k})$ be the grand-canonical IES for the potential λv.

Conjecture. Let $d \geq 2$. Then for a large class of repulsive potentials the Bogoliubov method gives the correct IES in the weak coupling limit:

$$\lim_{\lambda \searrow 0} \epsilon^\lambda(\mathbf{k}) = \epsilon_{\mathrm{bg}}(\mathbf{k}).$$

Bogoliubov transformations commuting with momentum

Let $\alpha \in \mathbb{C}$ and $\frac{2\pi}{L}\mathbb{Z}^d \ni \mathbf{k} \mapsto \theta_{\mathbf{k}} \in \mathbb{C}$ be a sequence with $\theta_{\mathbf{k}} = \theta_{-\mathbf{k}}$. Set

$$U_\theta := \prod_{\mathbf{k}} \mathrm{e}^{-\frac{1}{2}\theta_{\mathbf{k}} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + \frac{1}{2}\overline{\theta}_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}}$$

Then $U_{\alpha,\theta} := U_\theta W_\alpha$ is the general form of a Bogoliubov transformation commuting with P.

Improving the Bogoliubov method I

Let Ω denote the vacuum vector. $\Psi_{\alpha,\theta} := U^*_{\alpha,\theta}\Omega$ is the general form of a squeezed vector of zero momentum.

Vectors $\Psi_{\alpha,\theta,\mathbf{k}} := U^*_{\alpha,\theta}a^*_{\mathbf{k}}\Omega$ have momentum $\mathbf{k}$, that means

$$(P^L - \mathbf{k})\Psi_{\alpha,\theta,\mathbf{k}} = 0.$$

Clearly we have bounds

$$\begin{aligned} E^L &\leq (\Psi_{\alpha,\theta}|H^L\Psi_{\alpha,\theta}) \\ E^L + \epsilon^L(\mathbf{k}) &\leq (\Psi_{\alpha,\theta,\mathbf{k}}|H^L\Psi_{\alpha,\theta,\mathbf{k}}) \end{aligned}$$

Improving the Bogoliubov method II

After the translation, for all $\mathbf{k}$ we make the substitution

$$a_{\mathbf{k}}^* = c_{\mathbf{k}} b_{\mathbf{k}}^* - \overline{s}_{\mathbf{k}} b_{-\mathbf{k}}, \quad a_{\mathbf{k}} = c_{\mathbf{k}} b_{\mathbf{k}} - s_{\mathbf{k}} b_{-\mathbf{k}}^*,$$

where

$$c_{\mathbf{k}} := \cosh|\theta_{\mathbf{k}}|, \quad s_{\mathbf{k}} := -\frac{\theta_{\mathbf{k}}}{|\theta_{\mathbf{k}}|} \sinh|\theta_{\mathbf{k}}|.$$

Note that

$$U_\theta^* a_{\mathbf{k}} U_\theta = b_{\mathbf{k}}, \quad U_\theta^* a_{\mathbf{k}}^* U_\theta = b_{\mathbf{k}}^*,$$

Improving the Bogoliubov method III

$$H^L = B^L + C^L b_0^* + \overline{C}^L b_0$$
$$+ \frac{1}{2}\sum_{\mathbf{k}} O^L(\mathbf{k}) b_{\mathbf{k}}^* b_{-\mathbf{k}}^* + \frac{1}{2}\sum_{\mathbf{k}} \overline{O}^L(\mathbf{k}) b_{\mathbf{k}} b_{-\mathbf{k}} + \sum_{\mathbf{k}} D^L(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}}$$
$$+ \text{terms higher order in } b\text{'s.}$$

Then

$$(\Psi_{\alpha,\theta}|H^L\Psi_{\alpha,\theta}) = B^L, \qquad (\Psi_{\alpha,\theta,\mathbf{k}_L}|H^L\Psi_{\alpha,\theta,\mathbf{k}}) = B^L + D^L(\mathbf{k}).$$

Minimizing the energy in squeezed states I

We look for the infimum of the Hamiltonian among the states $\Psi_{\alpha,\theta}$. This means that B attains a minimum.

Computing the derivatives with respect to α and $\overline{\alpha}$ we obtain

$$C = c_0 \partial_{\overline{\alpha}} B - s_0 \partial_\alpha B$$

so that the condition:

$$\partial_{\overline{\alpha}} B = \partial_\alpha B = 0$$

entails $C = 0$.

Minimizing the energy in squeezed states II

Computing the derivatives with respect to s and $\overline{s}$ we obtain

$$O(\mathbf{k}) = \left(-2c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{c_{\mathbf{k}}}\right)\partial_{\overline{s}_{\mathbf{k}}}B - \frac{s_{\mathbf{k}}^2}{c_{\mathbf{k}}}\partial_{s_{\mathbf{k}}}B.$$

Thus $\partial_{s_{\mathbf{k}}}B = \partial_{\overline{s}_{\mathbf{k}}}B = 0$ entails $O(\mathbf{k}) = 0$.

Fixed point equation I

Instead of $s_{\mathbf{k}}$, $c_{\mathbf{k}}$, it is more convenient to use functions

$$S_{\mathbf{k}} := 2 s_{\mathbf{k}} c_{\mathbf{k}},$$
$$C_{\mathbf{k}} := c_{\mathbf{k}}^2 + |s_{\mathbf{k}}|^2.$$

We will keep $\alpha = |\alpha| \, \mathrm{e}^{\mathrm{i}\tau}$ instead of μ as the parameter of the theory. We can later on express μ in terms of α^2:

$$\mu = \frac{\hat{v}(0)}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(0) + \hat{v}(\mathbf{k}')}{2V}(C_{\mathbf{k}'} - 1) - \mathrm{e}^{\mathrm{i}2\tau} \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{2V} \overline{S}_{\mathbf{k}'},$$

$$\rho = \frac{|\alpha|^2 + \sum_{\mathbf{k}} |s_{\mathbf{k}}|^2}{V}.$$

Fixed point equation II

$$
\begin{aligned}
D(\mathbf{k}) &= \sqrt{f_{\mathbf{k}}^2 - |g_{\mathbf{k}}|^2}, \\
S_{\mathbf{k}} &= \frac{g_{\mathbf{k}}}{D(\mathbf{k})}, \\
C_{\mathbf{k}} &= \frac{f_{\mathbf{k}}}{D_{\mathbf{k}}}, \\
f_{\mathbf{k}} : &= \frac{\mathbf{k}^2}{2} + |\alpha|^2 \frac{\hat{v}(\mathbf{k})}{V} \\
& + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}' - \mathbf{k}) - \hat{v}(\mathbf{k}')}{2V} (C_{\mathbf{k}'} - 1) + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{2V} \, \mathrm{e}^{\mathrm{i}2\tau} \, \overline{S}_{\mathbf{k}'}, \\
g_{\mathbf{k}} : &= |\alpha|^2 \, \mathrm{e}^{\mathrm{i}2\tau} \, \frac{\hat{v}(\mathbf{k})}{V} - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}' - \mathbf{k})}{2V} S_{\mathbf{k}'}.
\end{aligned}
$$

Limit $L \to \infty$

In the thermodynamic limit one should take $\alpha = \sqrt{V\kappa}$, where κ has the interpretation of the density of the condensate. Then one could expect that $S_{\mathbf{k}}$ will converge to a function depending on $\mathbf{k} \in \mathbb{R}^d$ in a reasonable class and we can replace $\frac{1}{V}\sum\limits_{\mathbf{k}}$ by $\frac{1}{(2\pi)^d}\int \mathrm{d}\mathbf{k}$.

In particular,

$$D(0) = \sqrt{\frac{\hat{v}(0)}{2V}\alpha^2 \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{V}\overline{S}_{\mathbf{k}}} \to \sqrt{\frac{\hat{v}(0)\kappa}{2(2\pi)^d}\int \hat{v}(\mathbf{k})\overline{S}_{\mathbf{k}}\mathrm{d}\mathbf{k}}.$$

Thus it seems to imply $D(0) > 0$, which would mean that we have an energy gap in this approximation.

Perturbative approach based on the original Bogoliubov method

Recall that if we replace the potential $v(\mathbf{x})$ with $\lambda v(\mathbf{x})$, the Hamiltonian, after applying the original Bogoliubov method can be rewritten as

$$H^{\lambda,L} = \lambda^{-1} H^L_{-1} + H^L_0 + \sqrt{\lambda} H^L_{\frac{1}{2}} + \lambda H^L_1,$$

Unfortunately, perturbation theory is problematic in this set-up becaus of a serious infra-red problem: the unperturbed operator has no ground state.

Perturbative approach based on the improved Bogoliubov method I

After soving the fixed point equation we can write

$$H^{\lambda,L} = \lambda^{-1} H_{-1}^{\lambda,L} + H_0^{\lambda,L} + \sqrt{\lambda} H_{\frac{1}{2}}^{\lambda,L} + \lambda H_1^{\lambda,L},$$

where $\lambda^{-1} H_{-1}^{\lambda,L} = B^{\lambda,L}$ is the constant term,
$H_1^{\lambda,L} = \sum_{\mathbf{k}} D^{\lambda,L}(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}}$ is the quadratic term,
$H_{\frac{1}{2}}^{\lambda,L}$ and $H_1^{\lambda,L}$ are respectively the third and fourth order parts of H in operators $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^*$.

Perturbative approach based on the improved Bogoliubov method II

Consider the Hamiltonian

$$H^{\lambda,\delta,L} := \delta^{-1} H_{-1}^{\lambda,L} + H_0^{\lambda,L} + \sqrt{\delta} H_{\frac{1}{2}}^{\lambda,L} + \delta H_1^{\lambda,L},$$

where δ is an additional parameter introduced for bookkeeping reasons, that we use to produce the perturbation expansion. At the end we set $\delta = \lambda$.

Perturbative approach of the old literature I

1. Replace the zeroth mode operator a_0 with a c-number α, obtaining the Hamiltonian $H^{\lambda,L}(\alpha)$.
2. Substitute $\alpha = \sqrt{\lambda^{-1}\kappa V}$ and split the Hamiltonian as

$$H^{\lambda,L}(\alpha) = \lambda^{-1} H^{\kappa,L}_{-1} + H^{\kappa,L}_{0} + \sqrt{\lambda} H^{\kappa,L}_{\frac{1}{2}} + \lambda H^{\kappa,L}_{1}.$$

3. Compute perturbatively the ground state energy: $E^{\lambda,\kappa,L} = \sum_n \lambda^n E^{\kappa,L}_n$.
4. Compute the desired quantity.
5. Minimize (up to the desired order in λ) $E^{\kappa,L}$, obtaining $\kappa^{\lambda,L}$ as a function of λ, L.
6. Substitute $\kappa^{\lambda,L}$ into expression for desired quantity.

Perturbative approach of the old literature II

This approach was used e.g. by Bogoliubov, Beliaev, Hugenholz-Pines, Gavoret-Nozieres.

It is OK if we compute intensive quantities. E.g. it gives the correct energy density, as proven by Lieb, Seiringer, Yngvason.

It is dubious for finer quantities, such as the infimum excitation spectrum, since we modify the Hamiltonian.

Various limits

Low density limit. (Rigorous results by Lieb, Seiringer, Yngvason). Fix the potential v, fix the density ρ, go to themodynamic limit $L \to \infty$, consider the leading behavior of the desired quantity for small ρ.

Gross-Pitaevski limit. (Rigorous results by Lieb, Seiringer, Yngvason). Fix the potential v, fix n/L, go to themodynamic limit $L \to \infty$. (Very low density).

Weak coupling limit. (Adapted to the Bogoliubov method, implicit in Bogoliubov, Hugenholz-Pines, Gavoret-Nozieres, etc.) Fix μ, consider the potential λv, go to themodynamic limit $L \to \infty$ with a small λ. (Very high density).