FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

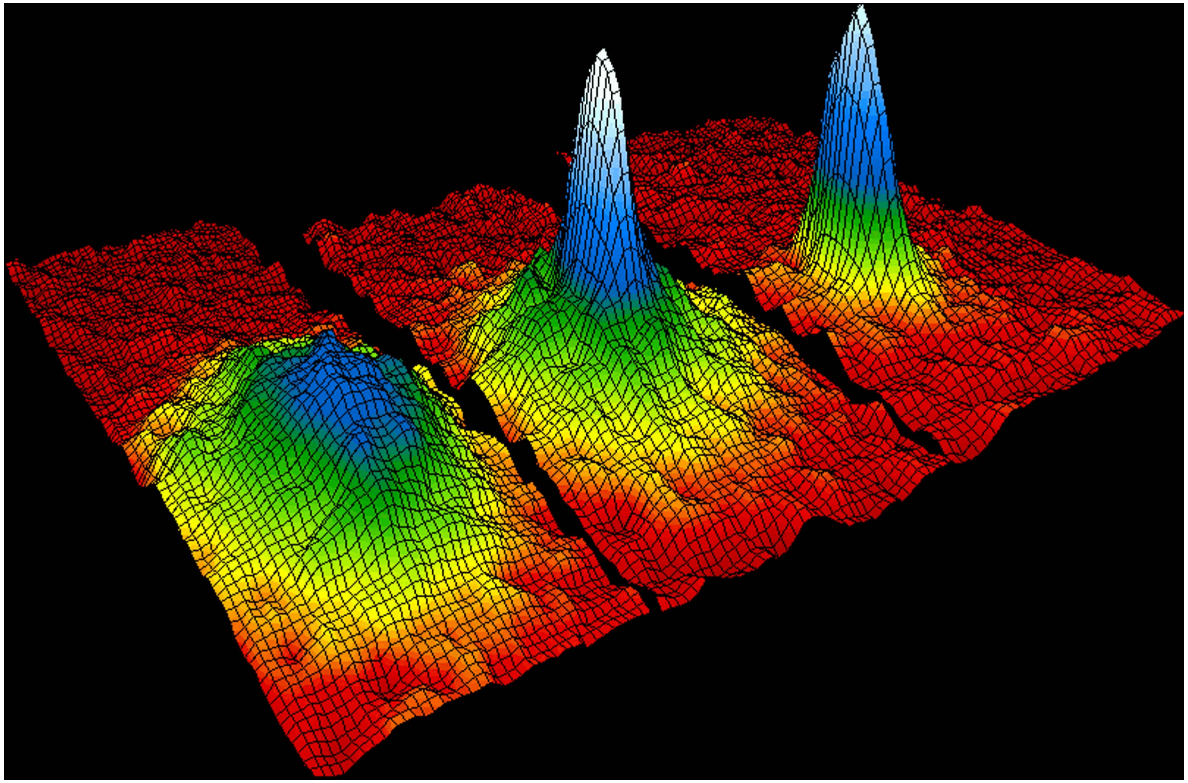
2º Semestre de 2023

10/08/2023

Aula 4

O gás diluído de bósons com interação de curto alcance

- ^{4}He (mas muito denso)
- Átomos frios bosônicos:
  - condensação de Bose-Einstein, Nobel de 2001 para E. A. Cornell, C. E. Wieman, W. Ketterle



Hamiltoniano

$$H_{GB} = \sum_{\mathbf{k}} \frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U(\mathbf{q})\, a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}}$$

$$U(\mathbf{q}) = \int d^3 r e^{i\mathbf{q}\cdot\mathbf{r}} U(\mathbf{r})$$

ÁLGEBRA BOSÔNICA:

$$[a_{\vec{k}}, a_{\vec{k}'}] = [a^\dagger_{\vec{k}}, a^\dagger_{\vec{k}'}] = 0$$

$$[a_{\vec{k}}, a^\dagger_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$$

O caso não interagente

EST. FUNDAMENTAL: TODAS AS PARTÍCULAS NO ESTADO DE PARTÍCULA ÚNICA DE MENOR ENERGIA: $\vec{k}=0$

$$|\Phi_0(N)\rangle = |N,0,0,0,0,\ldots\rangle = \frac{(a^{+}_{\vec{k}=0})^N}{\sqrt{N!}}|0\rangle$$

A ATUAÇÃO DO a_0, a_0^{+} EM $|\Phi_0(N)\rangle$ É TAL QUE:

$$a_0^{+}|\Phi_0(N)\rangle = \sqrt{N+1}\,|\Phi_0(N+1)\rangle \qquad N \sim 10^{23}$$

$$a_0|\Phi_0(N)\rangle = \sqrt{N}\,|\Phi_0(N-1)\rangle$$

$$a^{+}_{\vec{k}\neq 0}|\Phi_0(N)\rangle = |N,0,0,0,1,000\rangle$$

$$a_{\vec{k}\neq 0}|\Phi_0(N)\rangle = 0$$

$$\xi_0 = \frac{a_0}{\sqrt{V}} \qquad \xi_0^+ = \frac{a_0^+}{\sqrt{V}}$$

$$\xi_0^+ |\Phi_0(N)\rangle = \left(\frac{N+1}{V}\right)^{1/2} |\Phi_0(N+1)\rangle$$

$$\xi_0 |\Phi_0(N)\rangle = \left(\frac{N}{V}\right)^{1/2} |\Phi_0(N-1)\rangle$$

$$[\xi_0, \xi_0^+] = \frac{1}{V}[a_0, a_0^+] = \frac{1}{V} \longrightarrow 0$$

PARA EST. FUND. E ESTADOS FRACAMENTE EXCITADOS, ξ_0 E ξ_0^+ EFETIVAMENTE COMUTAM E SE COMPORTAM COMO <u>VARIÁVEIS CLÁSSICAS</u>

ISSO SUGERE TRATÁ-LAS COMO NÚMEROS.

OS OUTROS $a_{\vec{k}\neq 0}$, $a_{\vec{k}\neq 0}^+$ CONTINUAM SENDO TRATADOS QUANTICAMENTE.

O caso interagente:
o método de Bogolyubov

SEPARAR a_0, a_0^+ DOS OUTROS E TRATÁ-LOS COMO NÚMEROS: $a_0 \to \sqrt{N_0}$ $a_0^+ \to \sqrt{N_0}$

$N_0 \neq N$ MAS $N_0 \sim 10^{23}$

N_0 = OCUPAÇÃO DO CONDENSADO

$$\frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U(\mathbf{q})\, a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}}$$

A) $\vec{k} = \vec{k}' = \vec{q} = 0$: $\frac{1}{2V} U(0)\left(\sqrt{N_0}\right)^4 = \frac{U_0}{2V} N_0^2 \sim O(nN_0)$

B) $\vec{k} = 0$, $\vec{k}' = 0$ $\vec{k}' - \vec{q} = 0 \Rightarrow \vec{q} = 0$ E RECAÍMOS NO CASO $\underline{A}$

E TODOS OS OUTROS CANDIDATOS A TERMOS DE ORDEM $\left(\sqrt{N_0}\right)^3$ RECAEM NO CASO $\underline{A}$.

$$-\frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U(\mathbf{q})\, a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}}$$

c) $O\left(\sqrt{N_0}\right)^2$:

$$\left.\begin{array}{l}\vec{k}=0\\ \vec{k}'=0\\ \vec{q}\neq 0\end{array}\right\} \quad \frac{N_0}{2V}\sum_{\vec{q}}{}' U(\vec{q})\, a^+_{\vec{q}}\, a^+_{-\vec{q}} \sim O(\mu)$$

$$\sum' \to \sum_{\vec{q}\neq 0}$$

$$\left.\begin{array}{l}\vec{k}+\vec{q}=0\\ \vec{k}'-\vec{q}=0\\ \hline \vec{k}+\vec{k}'=0\end{array}\right\} \quad \frac{N_0}{2V}\sum_{\vec{k},\vec{q}} U(\vec{q})\, a_{-\vec{k}}\, a_{\vec{k}} = \frac{N_0}{2V}\sum_{\vec{k}}{}' U(-\vec{k})\, a_{-\vec{k}}\, a_{\vec{k}}$$

$$= \frac{N_0}{2V}\sum_{\vec{q}}{}' U(\vec{q})\, a_{\vec{q}}\, a_{-\vec{q}}$$

$$\Rightarrow 2\vec{q}+\vec{k}-\vec{k}'=0$$

$$\vec{q}=\frac{\vec{k}'-\vec{k}}{2}=-\vec{k}$$

LEMBRANDO QUE $U^*(\vec{q})=U(-\vec{q})$, UM É O HERMITIANO CONJUGADO DO OUTRO.

ANALOGAMENTE:

$$4 \times \frac{N_0}{2V} \sum_{\vec{k}}' U(\vec{k})\, a_k^{+} a_k$$

ASSIM COMO NO CASO FERMIÔNICO, AS BAIXAS EXCITAÇÕES ENVOLVEM MOMENTOS PEQUENOS E FAREMOS: $U(\vec{q}) \rightarrow U(\vec{0})$

$D)\ O(\sqrt{N_0})$ DESPREZAREMOS TODOS ESSES TERMOS NO LIMITE DILUÍDO: $\frac{N_0}{V} \sim \frac{N}{V} << 1$

$$H_{int} = \frac{U(0) N_0^2}{2V} + \frac{N_0 U(0)}{2V} \left[\sum_{\vec{k}}' \left(a_{\vec{k}}^{+} a_{-\vec{k}}^{+} + h.c. \right) + 4 \sum_{\vec{k}}' a_{\vec{k}}^{+} a_{\vec{k}} \right]$$

NÚMERO TOTAL DE PARTÍCULAS:

$$N = \sum_{\vec{k}} a_{\vec{k}}^{+} a_{\vec{k}} = N_0 + \sum_{\vec{k}}' a_{\vec{k}}^{+} a_{\vec{k}}$$

$$N_0 = N - \sum_{\vec{k}}' a_{\vec{k}}^{+} a_{\vec{k}}$$

LEVANDO NO PRIMEIRO TERMO DE H_{int}:

$$\frac{U(0)}{2V}\left[N - {\sum_{\vec{k}}}' a^{+}_{\vec{k}} a_{\vec{k}}\right]^2 = \frac{U(0)N^2}{2V} - \frac{U(0)N}{2V}\left[2{\sum_{\vec{k}}}' a^{+}_{\vec{k}} a_{\vec{k}}\right] + O(a^4)$$

E FAZENDO $N_0 = N + O(a^2)$ NO 2º TERMO:

$$H_{int} = \frac{U(0)N^2}{2V} + \frac{U(0)N}{2V}\left[{\sum_{\vec{k}}}'(a^{+}_{k} a^{+}_{-\vec{k}} + h.c.) + 2{\sum_{\vec{k}}}' a^{+}_{\vec{k}} a_{\vec{k}}\right]$$

Resumo

$$H_B = \frac{U(0)N^2}{2V} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{U(0)N}{2V}\left[2\sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}\neq 0}\left(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}}\right)\right]$$

$$H_B = N\lambda + \sum_{\mathbf{k}\neq 0}\left[(\epsilon_{\mathbf{k}} + 2\lambda) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \lambda\left(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}}\right)\right] \qquad \boxed{\lambda = \frac{U(0)N}{2V}}$$

O HAMILTONIANO É QUADRÁTICO, MAS NÃO ESTÁ NA FORMA DIAGONAL. ELE PODE SER RESOLUIDO ATRAVÉS DA TRANSF. DE BOGOLYUBOV.

RE-ESCREVENDO EM TERMOS DO COMPRIMENTO DE ESPALHAMENTO $\underline{a}$:

$$\frac{4\pi a}{m} = U(0) - \frac{m}{V} U(0) \sum_{\vec{k}}{}' \frac{1}{|\vec{k}|^2} \Rightarrow U(0) = \frac{4\pi a}{m}\left[1 + \frac{4\pi a}{V}\sum_{\vec{k}}{}' \frac{1}{k^2}\right]$$

$$\frac{U(0)N^2}{2V} = \frac{N^2}{V}\frac{2\pi a}{m}\left[1 + \frac{4\pi a}{V}\sum_{\vec{k}}{}'\frac{1}{k^2}\right]$$

NO 2º TERMO:

$U(0) \rightarrow \frac{4\pi a}{m}$

A transformação de Bogolyubov

$$a_{\vec{k}} = u_{\vec{k}} b_{\vec{k}} + v_{\vec{k}} b^{\dagger}_{-\vec{k}} \qquad b_{\vec{k}} = u_k a_{\vec{k}} - v_k a^{\dagger}_{-\vec{k}}$$

$$a^{\dagger}_{\vec{k}} = u_{\vec{k}} b^{\dagger}_{\vec{k}} + v_{\vec{k}} b_{-\vec{k}} \qquad b^{\dagger}_{\vec{k}} = u_k a^{\dagger}_{\vec{k}} - v_k a_{-\vec{k}}$$

$(u_k, v_k \in \mathbb{R})$

A TRANSF É CANÔNICA, OU SEJA,

$[b_{\vec{k}}, b_{\vec{k}'}] = [b^{\dagger}_{\vec{k}}, b^{\dagger}_{\vec{k}'}] = 0$ E $[b_{\vec{k}}, b^{\dagger}_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$

SE: $\boxed{u_k^2 - v_k^2 = 1}$

O VÍNCULO PODE SER AUTOMATICAMENTE SATISFEITO FAZENDO:

$$u_k = \cosh \varphi_k$$

$$v_k = \sinh \varphi_k$$

LEVANDO OS $a_{\vec{k}}$'s EM TERMOS DOS $b_{\vec{k}}$'s NO HAMILTONIANO:

$$H_{int} = \sum_{\vec{k}}{}' \Big\{ (\epsilon_{\vec{k}} + 2\lambda)\left[u_k^2\, b_k^\dagger b_k + v_k^2 \underbrace{b_{-k} b_{-k}^\dagger}_{b_{-k}^\dagger b_{-k} + 1} \right] + 2\lambda u_k v_k \left(b_k^\dagger b_k + \underbrace{b_{-k} b_{-k}^\dagger}_{b_{-k}^\dagger b_{-k} + 1} \right)$$

$$+ (\epsilon_k + 2\lambda) u_k v_k \left(b_k^\dagger b_{-k}^\dagger + h.c. \right) + \lambda (u_k^2 + v_k^2)\left(b_k^\dagger b_{-k}^\dagger + h.c. \right) \Big\}$$

ESCOLHO φ_k TAL QUE:

$$(\epsilon_k + 2\lambda) u_k v_k + \lambda (u_k^2 + v_k^2) = 0$$

$$2 u_k v_k = 2 \sinh\varphi_k \cosh\varphi_k = \sinh(2\varphi_k)$$

$$u_k^2 + v_k^2 = \cosh^2\varphi_k + \sinh^2\varphi_k = \cosh(2\varphi_k)$$

$$\Rightarrow \frac{(\epsilon_k + 2\lambda)}{2} \sinh(2\varphi_k) + \lambda \cosh(2\varphi_k) = 0$$

$$\Rightarrow \boxed{\tanh(2\varphi_k) = -\frac{2\lambda}{\epsilon_k + 2\lambda}}$$

$$u_k^2 = \frac{1}{2}\left[\frac{\epsilon_k + 2\lambda}{E_k} + 1\right] \qquad (u_k > 0)$$

$$v_k^2 = \frac{1}{2}\left[\frac{\epsilon_k + 2\lambda}{E_k} - 1\right] \qquad (v_k < 0)$$

$$E_k = \sqrt{(\epsilon_k + 2\lambda)^2 - 4\lambda^2} > 0$$

A FORMA FINAL DE H É:

$$\boxed{H = N\lambda + \frac{1}{2}\sum_{\vec{k}}{}' \left[E_{\vec{k}} - \epsilon_{\vec{k}} - 2\lambda + \frac{4m\lambda^2}{k^2}\right] + \sum_{\vec{k}}{}' E_{\vec{k}}\, b_{\vec{k}}^\dagger b_{\vec{k}}}$$

H AGORA ESTÁ NA FORMA DIAGONAL:

$$b_k^\dagger b_k = 0, 1, 2, \ldots \qquad \text{PARA CADA } \vec{k} \neq 0$$

Transformação de Bogoliubov

$$a_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} + v_{\mathbf{k}} b^{\dagger}_{-\mathbf{k}} \qquad b_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a^{\dagger}_{-\mathbf{k}}$$

$$a^{\dagger}_{\mathbf{k}} = v_{\mathbf{k}} b_{-\mathbf{k}} + u_{\mathbf{k}} b_{-\mathbf{k}} \qquad b^{\dagger}_{\mathbf{k}} = -v_{\mathbf{k}} a_{-\mathbf{k}} + u_{\mathbf{k}} a_{\mathbf{k}}$$

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1 \Rightarrow \begin{cases} u_{\mathbf{k}} = \cosh\varphi_{\mathbf{k}} \equiv \mathrm{c} \\ v_{\mathbf{k}} = \sinh\varphi_{\mathbf{k}} \equiv \mathrm{s} \end{cases} \qquad \tanh(2\varphi_{\mathbf{k}}) = -\frac{2\lambda}{2\lambda + \epsilon_{\mathbf{k}}} \in (-1, 1)$$

$$\sinh\varphi_{\mathbf{k}} = -\frac{1}{\sqrt{2}}\sqrt{\frac{\epsilon_{\mathbf{k}} + 2\lambda}{E_{\mathbf{k}}} - 1} < 0 \qquad \sinh(2\varphi_{\mathbf{k}}) = -\frac{2\lambda}{E_{\mathbf{k}}}$$

$$\cosh\varphi_{\mathbf{k}} = \frac{1}{\sqrt{2}}\sqrt{\frac{\epsilon_{\mathbf{k}} + 2\lambda}{E_{\mathbf{k}}} + 1} > 1 \qquad \cosh(2\varphi_{\mathbf{k}}) = \frac{\epsilon_{\mathbf{k}} + 2\lambda}{E_{\mathbf{k}}}$$

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} + 2\lambda)^2 - 4\lambda^2}$$

$$\frac{4\lambda^2 m}{k^2}$$

$$\boxed{H_B = N\lambda + \frac{1}{2}\sum_{\mathbf{k}\neq 0}(E_{\mathbf{k}} - \epsilon_{\mathbf{k}} - 2\lambda) + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}} b^{\dagger}_{\mathbf{k}} b_{\mathbf{k}}}$$

O ESTADO FUNDAMENTAL INTERAGENTE CORRESPONDE A:

$$b^{\dagger}_{\vec{k}} b_{\vec{k}} = 0 \quad \forall \ \vec{k} \neq 0$$

ENERGIA DO ESTADO FUNDAMENTAL:

$$E_0 = N\lambda + \frac{1}{2} \sum_{\vec{k}}{}' \left[E_{\vec{k}} - \epsilon_{\vec{k}} - 2\lambda + \underbrace{\frac{4m\lambda^2}{k^2}}_{} \right]$$

NECESSÁRIO PARA TORNAR O RESULTADO CONVERGENTE:

$$E_0 = N\lambda + \frac{V}{2} \int \frac{d^3k}{(2\pi)^3} \left[E_{\vec{k}} - \epsilon_{\vec{k}} - 2\lambda + \frac{4m\lambda^2}{k^2} \right]$$

$$\frac{E_0}{N} = \frac{2\pi a n}{m} \left[1 + \frac{128}{15} \left(\frac{n a^3}{\pi} \right)^{1/2} \right] \qquad n = \frac{N}{V}$$

$$P = -\frac{\partial E_0}{\partial V} \implies P_B = \frac{2\pi \hbar^2}{m} a\, n^2 \quad \text{(BÓSONS)}$$

$$P_F = \frac{\hbar^2}{5m} (3\pi^2)^{2/3} n^{5/3} \quad \text{(FÉRMIONS)}$$

$$\frac{P_F}{P_B} = \frac{(3\pi^2)^{2/3}}{10\pi} \frac{1}{(na^3)^{1/3}} >> 1 \qquad \text{SE } na^3 << 1$$