FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

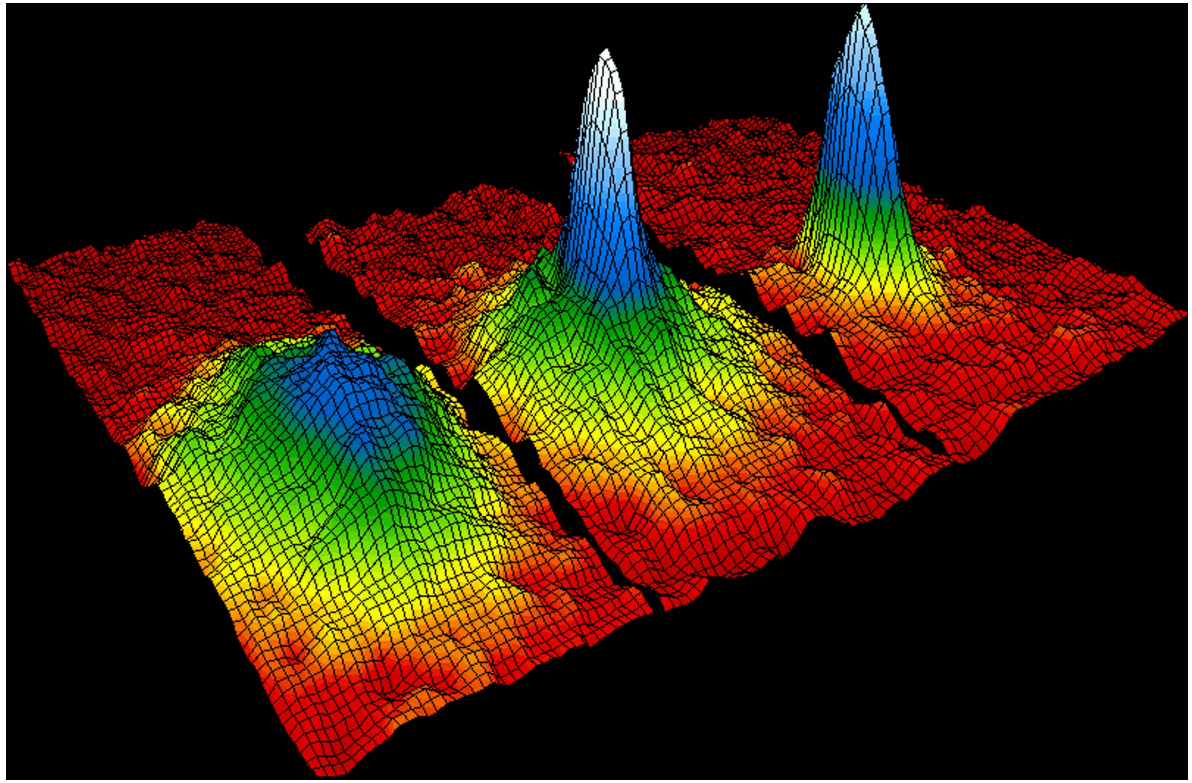
1º Semestre de 2025

11/03/2025

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

Bósons sem spin com interação de curto alcance:

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

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

Álgebra bosônica:

$$\left[a_{\mathbf{k}}, a_{\mathbf{k}'}\right] = \left[a^\dagger_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}\right] = 0$$

$$\left[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k},\mathbf{k}'}$$

Limite termodinâmico:

$$\begin{cases} N \to \infty \\ V \to \infty \\ \frac{N}{V} \to n = \text{const.} \end{cases}$$

O caso não interagente

$$H_0 = \sum_{\vec{k}} \frac{k^2}{2m} a^\dagger_{\vec{k}} a_{\vec{k}}$$

EST. FUND.: $|\Phi_0(N)\rangle = |N_{\vec{k}=0} = N, 0, 0, 0, \dots\rangle$

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

$$a_0^\dagger |\Phi_0(N)\rangle = \sqrt{N+1}\, |\Phi_0(N+1)\rangle$$

$$a^\dagger_{\vec{k}\neq 0} |\Phi_0(N)\rangle = |N_{\vec{k}=0} = N, 0, 0, \dots, 1, 0, 0, \dots\rangle$$

DEFINIMOS: $\xi_0 = \frac{a_0}{\sqrt{V}} \qquad \xi_0^\dagger = \frac{a_0^\dagger}{\sqrt{V}}$

$$\Rightarrow \xi_0 |\Phi_0(N)\rangle = \sqrt{\frac{N}{V}}\, |\Phi_0(N-1)\rangle$$

$$\xi_0^\dagger |\Phi_0(N)\rangle = \underbrace{\sqrt{\frac{N+1}{V}}}_{\sim\sqrt{n}}\, |\Phi_0(N+1)\rangle$$

$$[\xi_0, \xi_0^\dagger] = \frac{1}{V}[a_0, a_0^\dagger] = \frac{1}{V} \xrightarrow[V\to\infty]{} 0$$

NO LIMITE TERMODINÂMICO ESSES OPERADORES SÃO (QUASE-)CLÁSSICOS.

$a_0 \sim \sqrt{N_0}$ $\quad a_0^\dagger \sim \sqrt{N_0}$

$\vec{k} \neq 0$

$$\hat{N} = \sum_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} = a_0^\dagger a_0 + \sum_{\vec{k}}{}' a^\dagger_{\vec{k}} a_{\vec{k}} \sim N_0 + \sum_{\vec{k}}{}' a^\dagger_{\vec{k}} a_{\vec{k}}$$

O caso interagente: o método de Bogolyubov

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

$$\simeq \sum_{\vec{k}} \frac{\vec{k}^2}{2m} a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{U(0)}{2V} \sum_{\vec{k},\vec{k}',\vec{q}} a^\dagger_{\vec{k}+\vec{q}} a^\dagger_{\vec{k}'-\vec{q}} a_{\vec{k}'} a_{\vec{k}}$$

ASSUMINDO QUE, EM BAIXAS ENERGIAS, APENAS VALORES DE $|\vec{k}| \sim 0$ SÃO ACESSADOS.

(i) SE $\vec{k} = \vec{k}' = \vec{q} = 0 \Rightarrow \frac{U(0)}{2V} (a^\dagger_0)^2 (a_0)^2 \to \frac{U(0) N_0^2}{2V} = \text{CONST.}$

(ii) $\left.\begin{array}{l} \vec{k}+\vec{q}=0 \\ \vec{k}'-\vec{q}=0 \\ \vec{k}'=0 \end{array}\right\} \left.\begin{array}{l} \vec{k}+\vec{k}'=0 \\ \vec{k}=-\vec{k}'=0 \end{array}\right\} \to$ NÃO EXISTE TERMO $\sim (\sqrt{N_0})^3$

$$\frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \overbrace{U(\mathbf{q})}^{U(0)}\, a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}}$$

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

h.c.

$\vec{k}=0=\vec{k}' \Rightarrow \frac{U(0)}{2V} N_0 \sum_{\vec{q}}{}' a^\dagger_{\vec{q}} a^\dagger_{-\vec{q}} = \frac{U(0) N_0}{2V} \sum_{\vec{k}}{}' a^\dagger_{\vec{k}} a^\dagger_{-\vec{k}}$

$\vec{k}=0$
$\vec{k}'-\vec{q}=0 \Rightarrow \vec{k}'=\vec{q} \Rightarrow \frac{U(0) N_0}{2V} \sum_{\vec{q}}{}' a^\dagger_{\vec{q}} a_{\vec{q}} = \frac{U(0) N_0}{2V} \sum_{\vec{k}}{}' a^\dagger_{\vec{k}} a_{\vec{k}}$

E MAIS 3 TERMOS IGUAIS, EM ORDEM N_0

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

E DESPREZAMOS TERMOS DE ORDEM $\frac{U(0)}{2V}\sqrt{N_0}$ E MAIORES

TANTO POR CAUSA DE EXCITAÇÕES TÉRMICAS QUANTO POR EFEITO DAS INTERAÇÕES $N_0 \neq N$

$$\hat{N} \to N = N_0 + \sum_{k}{}' a^{+}_{k} a_{k} \Rightarrow N_0 = N - \sum_{k}{}' a^{+}_{k} a_{k}$$

LEVO N_0 NOS 2 TERMOS DE H

$$(i)\ \frac{U(0)}{2V} N_0^2 = \frac{U(0)}{2V}\left[N - \sum_{k}{}' a^{+}_{k} a_{k}\right]^2$$

$$= \frac{U(0)N^2}{2V} - \frac{U(0)N}{2V} 2\sum_{k}{}' a^{+}_{k} a_{k} + O(a^2 a^{+2})$$

$$(ii)\ \frac{U(0)}{2V} N_0 [\ \ ] \simeq \frac{U(0)N}{2V} [\ \ ]$$

ONDE DESPREZAMOS SEMPRE TERMOS QUÁRTICOS

Resumo

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

$$\frac{N}{2V}\left(\frac{4\pi a}{m}\right) = \frac{2\pi a N}{mV}$$

Em termos do comprimento de espalhamento

Segunda aproximação de Born: $$\frac{4\pi a}{m} = U(0) - \frac{mU^2(0)}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{|\mathbf{k}|^2}$$

$$\frac{4\pi a}{m} \to a$$
$$U(0) \to u$$
$$\frac{m}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{|\mathbf{k}|^2} \to b$$

$$a = u - bu^2$$

$$u = \alpha a + \beta a^2 \Rightarrow a = \alpha a + \beta a^2 - b\left(\alpha a + \beta a^2\right)^2 \approx \alpha a + \underbrace{\beta a^2 - b\alpha^2 a^2}_{(\beta - b\alpha^2)a^2}$$

$$\Rightarrow \begin{cases} \alpha = 1 \\ \beta = b\alpha^2 = b \end{cases} \Rightarrow u = a + ba^2$$

$$U(0) = \frac{4\pi a}{m} + \left(\frac{4\pi a}{m}\right)^2 \frac{m}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{|\mathbf{k}|^2} = \frac{4\pi a}{m}\left(1 + \frac{4\pi a}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{|\mathbf{k}|^2}\right)$$

$$\frac{U(0)N^2}{2V} = \frac{2\pi a N^2}{mV}\left(1 + \frac{4\pi a}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{|\mathbf{k}|^2}\right)$$

Resumo

$$H_B = \overbrace{\frac{2\pi a N^2}{mV}\left(1+\frac{4\pi a}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{|\mathbf{k}|^2}\right)}^{A_0} + \sum_{\mathbf{k}}\epsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{2\pi a N}{mV}\left[2\sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\boldsymbol{k}\neq 0}\left(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}}\right)\right]$$

$$H_B = A_0 + \sum_{\mathbf{k}\neq 0}\left[\left(\epsilon_{\mathbf{k}} + 2\lambda\right) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \lambda\left(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}}\right)\right]$$

$$\boxed{\lambda = \frac{2\pi a N}{mV}}$$

A transformação de Bogolyubov

$$① \begin{cases} a_{\vec{k}} = u_k b_{\vec{k}} + v_k b^\dagger_{-\vec{k}} \\ a^\dagger_k = u_k b^\dagger_{\vec{k}} + v_k b_{-\vec{k}} \end{cases} \qquad ② \begin{cases} b_{\vec{k}} = u_k a_{\vec{k}} - v_{\vec{k}} a^\dagger_{-\vec{k}} \\ b^\dagger_{\vec{k}} = u_k a^\dagger_{\vec{k}} - v_{\vec{k}} a_{-\vec{k}} \end{cases}$$

$u_k = u_{|\vec{k}|}$ $\qquad u_k, v_k \in \mathbb{R}$

$v_k = v_{|\vec{k}|}$

$[b_{\vec{k}}, b_{\vec{k}'}] = [b^\dagger_{\vec{k}}, b^\dagger_{\vec{k}'}] = 0 \qquad [b_{\vec{k}}, b^\dagger_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$

$$\Longrightarrow \boxed{u_k^2 - v_k^2 = 1} \Rightarrow \begin{array}{l} u_k = \cosh \varphi_k \\ v_k = \sinh \varphi_k \end{array}$$

LEVO (1) NO H_B E IMPÕE QUE OS TERMOS ANÔMALOS EM $b_{\vec{k}} b_{\vec{k}}$, $b^\dagger_{-\vec{k}} b^\dagger_{\vec{k}}$ TEM COEFICIENTES NULOS.

Transformação de Bogoliubov

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

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

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1 \Rightarrow \begin{cases} u_{\mathbf{k}} = \cosh\varphi_{\mathbf{k}} \equiv \mathrm{c} \\ v_{\mathbf{k}} = \sinh\varphi_{\mathbf{k}} \equiv \mathrm{s} \end{cases}$$

$$\tanh(2\varphi_{\mathbf{k}}) = -\frac{2\lambda}{2\lambda + \epsilon_{\mathbf{k}}} \in (-1, 1)$$

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

$$\sinh(2\varphi_{\mathbf{k}}) = -\frac{2\lambda}{E_{\mathbf{k}}}$$

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

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

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

$$\boxed{\lambda = \frac{2\pi a N}{mV}}$$

$$\boxed{H_B = N\lambda + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left(E_{\mathbf{k}} - \epsilon_{\mathbf{k}} - 2\lambda + \frac{4m\lambda^2}{k^2}\right) + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}} b^{\dagger}_{\mathbf{k}} b_{\mathbf{k}}}$$

A energia do estado fundamental

NO ESTADO FUNDAMENTAL $|0\rangle$, TEMOS:

$$b_{\vec{k}}|0\rangle = 0 \quad \forall \vec{k} \Rightarrow (u_k a_{\vec{k}} - v_k a^{\dagger}_{-k})|0\rangle = 0$$

$$\Rightarrow u_k a_{\vec{k}}|0\rangle = v_k a^{\dagger}_{\vec{k}}|0\rangle$$

E

$$\langle 0| b^{\dagger}_{\vec{k}} b_{\vec{k}} |0\rangle = 0 \quad \forall (\vec{k})$$

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

$$E_k = \sqrt{\epsilon_{\vec{k}} + 4\lambda\epsilon_{\vec{k}}} \qquad \sum_{\vec{k}} \Rightarrow V \int \frac{d^3k}{(2\pi)^3}$$

O TERMO EM $\frac{\lambda^2}{k^2}$ É NECESSÁRIO PARA GARANTIR A CONVERGÊNCIA DA INTEGRAL NO LIMITE $k \to \infty$

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

A pressão bosônica

$$P_0 = -\frac{\partial E_0}{\partial V}\Big|_N$$

$$P_0^B = \frac{2\pi\hbar^2 a}{m} n^2$$

DA AULA PASSADA: $P_0^F = \frac{\hbar^2}{5m}(3\pi^2)^{2/3} n^{5/3}$

RAZÃO: $\frac{P_0^F}{P_0^B} = \frac{(3\pi^2)^{2/3}}{10\,\pi}\frac{1}{(na^3)^{1/3}} \simeq \frac{0.30}{(na^3)^{1/3}}$

SE $na^3 \ll 1 \Rightarrow P_0^F \gg P_0^B$