统计物理
—(玻色系统、费米系统)

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Outline

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全同粒子

在量子力学中，把属于同一类的粒子称为全同粒子，也就是说固有性质 (质量、电荷、自旋、同位旋、宇称、奇异数等) 相同的粒子称为全同粒子。

- 总波函数对于任意两个粒子置换表现出对称性和反对称性

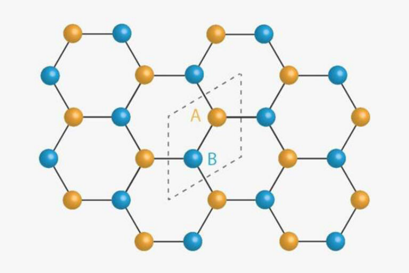
$$\psi(\ldots, x_i, \ldots, x_j, \ldots) = \pm\psi(\ldots, x_j, \ldots, x_i, \ldots)$$

- 光子，π 介子，α 粒子等具有整数自旋粒子服从对易规则—玻色子 (Boson)
- 电子、中子、质子等具有半整数自旋粒子服从反对易规则—费米子 (Fermion)

例：有 A 和 B 两个粒子占据两个简并态 $|0\rangle$ 和 $|1\rangle$，可能的微观状态和对应概率为

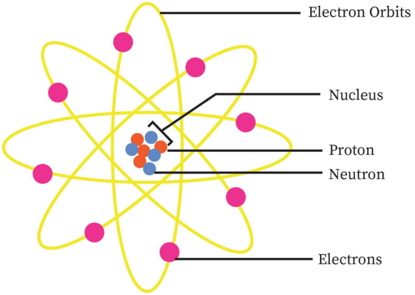
Particles	Both $|0\rangle$	Both $|1\rangle$	One $|0\rangle$ and one $|1\rangle$
Distinguishable	0.25	0.25	0.5
Bosons	0.33	0.33	0.33
Fermions	0	0	1

全同粒子



化学键长度的伸缩 → 原子振动 → 声子，也就是玻色子

全同粒子



玻色系统和费米系统的热力学函数

巨配分函数

$$Z(T,V) = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]$$

这里的求迹是对所有量子态空间下计算.

$$Z(T,V) = \sum_{n_l}\left[e^{-\sum_l \beta(\varepsilon-\mu)n_l}\right]$$

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对于费米气体，由于泡利不相容原理: $n_l = 0$ 或者 $n_l = 1$

$$\begin{aligned} Z_{FD}(T,V) &= \prod_l \left[\sum_{n_l=0}^{1} e^{-\beta n_l(\varepsilon_l-\mu)}\right] \\ &= \prod_l \left[1 + e^{-\beta(\varepsilon_l-\mu)}\right] \end{aligned}$$

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对于玻色气体: $n_l = 0 \sim \infty$

$$Z_{BE}(T,V) = \prod_l \left[\sum_{n_l=0}^{\infty} e^{-\beta n_l(\varepsilon_l-\mu)}\right]$$

$$= \prod_l \frac{1}{1-e^{-\beta(\varepsilon_l-\mu)}}$$

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对于玻色气体: $n_l = 0 \sim \infty$

$$\begin{aligned} Z_{BE}(T,V) &= \prod_l \left[\sum_{n_l=0}^{\infty} e^{-\beta n_l(\varepsilon_l-\mu)}\right] \\ &= \prod_n \left[\frac{1}{1-e^{-\beta(\varepsilon_n-\mu)}}\right]^{\omega_n} \end{aligned}$$

玻色系统和费米系统的热力学函数

巨势 (Grand potential)

$$\Omega = -k_B T \ln Z = \eta k_B T \sum_l \ln \left[1 - \eta \exp\left(\beta\mu - \beta\varepsilon_l\right)\right]$$

玻色子 $\eta = +1$; 费米子 $\eta = -1$

$$\Omega = -k_B T \ln Z_{BE}(T, V) = k_B T \sum_l \ln \left(1 - e^{-\beta(\varepsilon_l - \mu)}\right)$$

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粒子数

$$\bar{N} = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \sum_l \frac{1}{e^{\beta(\varepsilon_l - \mu)} - \eta}$$
$$= \sum_l \frac{e^{\beta\mu}}{e^{\beta\varepsilon_l} - \eta e^{\beta\mu}} \equiv \sum_l \frac{z}{e^{\beta\varepsilon_l} - \eta z}$$

内能

$$E_l = \sum_l \varepsilon_l n_l = \sum_l \frac{\varepsilon_l z}{e^{\beta\varepsilon_l} - \eta z}$$

量子气体

$$
\begin{aligned}
PV &= -\eta k_B T \sum_l \ln\left[1 - \eta z \exp\left(-\beta\varepsilon_l\right)\right] \\
&= -\eta k_B T \int \frac{\mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{p}}{h^3} \ln\left[1 - \eta z \exp\left(-\beta \frac{p^2}{2m}\right)\right] \\
&= -\eta k_B T V \frac{1}{h^3} \int_0^\infty 4\pi p^2 \ln\left[1 - \eta z \exp\left(-\beta \frac{p^2}{2m}\right)\right] \mathrm{d}p
\end{aligned}
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&\overset{x^2=\beta p^2/2m}{=\!=\!=} -\eta k_B T V \frac{1}{h^3} \int_0^\infty 4\pi \left(\frac{2m}{\beta}\right)^{3/2} x^2 \ln\left[1 - \eta z \exp\left(-x^2\right)\right] \mathrm{d}x \\
&= -\eta k_B T V \frac{4}{\sqrt{\pi}\lambda_T^3} \int_0^\infty \mathrm{d}x\, x^2 \ln\left[1 - \eta z \exp\left(-x^2\right)\right]
\end{aligned}
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&= -\eta k_B T V \frac{4}{\sqrt{\pi}\lambda_T^3}\int_0^\infty \mathrm{d}x\, x^2 \ln\left[1-\eta z \exp\left(-x^2\right)\right] \\
&= \eta k_B T V \frac{4}{\sqrt{\pi}\lambda_T^3}\int_0^\infty \mathrm{d}x \frac{x^3}{3}\frac{\eta z 2x e^{-x^2}}{1-\eta z e^{-x^2}} \qquad \text{(integration by parts)} \\
&= k_B T V \frac{1}{\lambda_T^3}\frac{4}{3\sqrt{\pi}}\int_0^\infty \mathrm{d}x \frac{2x^4}{z^{-1}e^{x^2}-\eta}
\end{aligned}
$$

量子气体

$$f_m^\eta(z) = \frac{1}{(m-1)!}\int_0^\infty \mathrm{d}x\,\frac{2x^{2m-1}}{z^{-1}e^{x^2}-\eta}$$

$$
\begin{aligned}
f_m^\eta(z) &= \frac{1}{(m-1)!}\int_0^\infty \mathrm{d}x\,\frac{2x^{2m-1}}{z^{-1}e^{x^2}-\eta} \\
&= \frac{1}{(m-1)!}\int_0^\infty \mathrm{d}y\,\frac{y^{m-1}}{z^{-1}e^{y}-\eta}, \qquad (\quad \text{set} \quad x=y^2) \\
&= \frac{1}{(m-1)!}\int_0^\infty \mathrm{d}y\, y^{m-1} z e^{-y}\frac{1}{1-\eta z e^{-y}} \\
&= \frac{1}{(m-1)!}\int_0^\infty \mathrm{d}y\, y^{m-1} z e^{-y}\sum_{n=0}\left(\eta z e^{-y}\right)^n \\
&= \frac{1}{(m-1)!}\sum_{n=0}^{\infty}\eta^n z^{n+1}\int_0^\infty \mathrm{d}y\, y^{m-1}e^{-(n+1)y}, \qquad (Gamma\ \ function) \\
&= \sum_{n=0}\eta^n z^{n+1}\frac{1}{(n+1)^m} \\
&= \sum_{n=1}\eta^{n+1}\frac{z^n}{n^m}
\end{aligned}
$$

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&= \sum_{n=1}\eta^{n+1}\frac{z^n}{n^m}
\end{aligned}
$$

- When $m = 5/2$, we have $(m-1)! = \left(\frac{3}{2}\right)! = \frac{3}{2}\cdot\frac{1}{2}! = \frac{3\sqrt{\pi}}{4}$

量子气体

得到量子气体方程 ($\lambda_T = \frac{h}{\sqrt{2\pi m k_B T}}$)

$$\beta P = \frac{1}{\lambda_T^3} f_{5/2}^{\eta}(z)$$

量子气体

得到量子气体方程 ($\lambda_T = \frac{h}{\sqrt{2\pi m k_B T}}$)

$$
\begin{aligned}
\beta P &= \frac{1}{\lambda_T^3} f_{5/2}^{\eta}(z) \\
n &= \frac{1}{\lambda_T^3} f_{3/2}^{\eta}(z) \\
\varepsilon &= \frac{3}{2} P
\end{aligned}
$$

量子气体

得到量子气体方程 ($\lambda_T = \frac{h}{\sqrt{2\pi m k_B T}}$)

$$\beta P = \frac{g}{\lambda_T^3} f_{5/2}^{\eta}(z)$$
$$n = \frac{g}{\lambda_T^3} f_{3/2}^{\eta}(z)$$
$$\varepsilon = \frac{3}{2} P$$

- g 为简并度

高温、低密度极限下

$$\begin{cases} \frac{n\lambda_T^3}{g} = f_{3/2}^{\eta}(z) = z + \eta\frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \dots \\ \frac{\beta P\lambda_T^3}{g} = f_{5/2}^{\eta}(z) = z + \eta\frac{z^2}{2^{5/2}} + \frac{z^3}{3^{5/2}} + \dots \end{cases}$$

微扰

$$\begin{aligned} z &= \frac{n\lambda_T^3}{g} - \eta\frac{z^2}{2^{3/2}} - \frac{z^3}{3^{3/2}} - \dots \\ &= \left(\frac{n\lambda_T^3}{g}\right) - \frac{\eta}{2^{3/2}}\left(\frac{n\lambda_T^3}{g}\right)^2 - \dots \\ &= \left(\frac{n\lambda_T^3}{g}\right) - \frac{\eta}{2^{3/2}}\left(\frac{n\lambda_T^3}{g}\right)^2 + \left(\frac{1}{4} - \frac{1}{3^{3/2}}\right)\left(\frac{n\lambda_T^3}{g}\right)^3 - \dots \end{aligned}$$

代入 P 的方程

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把微扰的解 z 代入 P 的方程：

$$\begin{aligned} \frac{\beta P\lambda_T^3}{g} = &\left(\frac{n\lambda_T^3}{g}\right) - \frac{\eta}{2^{3/2}}\left(\frac{n\lambda_T^3}{g}\right)^2 + \left(\frac{1}{4} - \frac{1}{3^{3/2}}\right)\left(\frac{n\lambda_T^3}{g}\right)^3 \\ &+ \frac{\eta}{2^{5/2}}\left(\frac{n\lambda_T^3}{g}\right)^2 - \frac{1}{8}\left(\frac{n\lambda_T^3}{g}\right)^3 + \frac{1}{3^{5/2}}\left(\frac{n\lambda_T^3}{g}\right)^3 + \dots \end{aligned}$$

量子气体

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$$\begin{cases} \frac{n\lambda_T^3}{g} = f_{3/2}^{\eta}(z) = z + \eta \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \dots \\ \frac{\beta P \lambda_T^3}{g} = f_{5/2}^{\eta}(z) = z + \eta \frac{z^2}{2^{5/2}} + \frac{z^3}{3^{5/2}} + \dots \end{cases}$$

$$p = nk_B T \left[1 - \frac{\eta}{2^{5/2}} \left(\frac{n\lambda_T^3}{g} \right) + \left(\frac{1}{8} - \frac{2}{3^{5/2}} \right) \left(\frac{n\lambda_T^3}{g} \right)^2 + \dots \right]$$

- $n\lambda_T^3 \geq g$: quantum degenerate limit
- 第二位力系数 $B_2 = -\eta\lambda^3/(2^{5/2}g)$
- 经典统计中，第二位力系数通过粒子与粒子之间的相互作用得到
- 高温（低密度）极限中，量子统计的结果等效于引入粒子的相互作用：对于玻色子，是吸引相互作用；对于费米子，是排斥相互作用
- 相互作用有效长度为 λ_T

弱简并理想玻色气体气体

分布函数

$$a_l = \frac{\omega_l}{\frac{1}{z}e^{\beta\varepsilon_l} - 1}$$

- $z = e^{-\alpha} = e^{\beta\mu}$ 称为逸度 (fugacity)，描述粒子全同性原理引起的量子效应的重要性
- 若只考虑 $\varepsilon_l \geq 0$，有 $e^{\beta\varepsilon_l} \geq 1$，逸度必须满足

$$0 \leq z \leq 1$$

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$$0 \leq z \leq 1$$

- 若 $z \ll 1$，粒子全同性引起的量子效应可以忽略，玻色分布和费米分布都过渡到玻尔兹曼分布

$$\frac{\omega_l}{\frac{1}{z}e^{\beta\varepsilon_l} - 1} \approx \frac{1}{\frac{1}{z}e^{\beta\varepsilon_l}} = e^{-\alpha+\beta\varepsilon_l} \rightarrow \quad \text{Boltzmann distribution}$$

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- 若 $z \to 1$?

Outline

玻色-爱因斯坦凝聚 (Bose-Einstein condensate, BEC)

考虑自由气体放在一个正方体容器中，并假设具有周期性边界条件

$$H = \frac{\mathbf{p}^2}{2m}, \quad \mathbf{p} = \hbar\left(\frac{2\pi}{L} l_x, \frac{2\pi}{L} l_y, \frac{2\pi}{L} l_z\right) = \frac{2\pi\hbar}{L}\mathbf{l}$$

粒子数

$$\begin{aligned}
\bar{N} &= \sum_{l_x, l_y, l_z=-\infty}^{\infty} \frac{z}{\exp\left[\beta(p_x^2+p_y^2+p_z^2)/2m\right]-z} \\
&= \int \mathrm{d}\mathbf{l} \, \frac{z}{\exp\left[\beta(p_x^2+p_y^2+p_z^2)/2m\right]-z} \\
&= \frac{V}{(2\pi\hbar)^3}\int_S \mathrm{d}\mathbf{p} \, \frac{z}{\exp\left[\beta(p_x^2+p_y^2+p_z^2)/2m\right]-z} \\
&= \frac{4\pi V}{(2\pi\hbar)^3}\int_{2\pi\hbar/L}^{\infty} p^2 \, \mathrm{d}p \, \frac{z}{\exp\left[\beta p^2/2m\right]-z}
\end{aligned}$$

玻色-爱因斯坦凝聚 (Bose-Einstein condensate, BEC)

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\bar{N} &= \sum_{l_x,l_y,l_z=-\infty}^{\infty} \frac{z}{\exp\left[\beta(p_x^2+p_y^2+p_z^2)/2m\right]-z} \\
&= \int \mathrm{d}\mathbf{l}\, \frac{z}{\exp\left[\beta(p_x^2+p_y^2+p_z^2)/2m\right]-z} + \frac{z}{1-z} \\
&= \frac{V}{(2\pi\hbar)^3}\int_S \mathrm{d}\mathbf{p}\, \frac{z}{\exp\left[\beta(p_x^2+p_y^2+p_z^2)/2m\right]-z} + \frac{z}{1-z} \\
&= \frac{4\pi V}{(2\pi\hbar)^3}\int_{2\pi\hbar/L}^{\infty} p^2\,\mathrm{d}p\, \frac{z}{\exp\left[\beta p^2/2m\right]-z} + \frac{z}{1-z}
\end{aligned}$$

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巨势

$$\begin{aligned}
\Omega_{\mathrm{BE}}(T,V,\mu) &= k_B T \sum_l \ln\left[1 - e^{-\beta(\varepsilon_l - \mu)}\right] \\
&= k_B T \ln(1-z) + \frac{4\pi V k_B T}{(2\pi\hbar)^3}\int_{2\pi\hbar/L}^{\infty} p^2\,\mathrm{d}p \ln\left[1 - z\exp\left(-\beta p^2/2m\right)\right] \\
&= k_B T \ln(1-z) - \frac{4\pi V k_B T}{(2\pi\hbar)^3}\int_{2\pi\hbar/L}^{\infty} p^2\,\mathrm{d}p \sum_n \frac{z^n}{n} e^{-n\beta p^2/2m} \\
&= k_B T \ln(1-z) - \frac{k_B T V}{\lambda_T^3}\sum_{n=1}^{\infty}\frac{z^n}{n^{5/2}} \\
&= k_B T \ln(1-z) - \frac{k_B T V}{\lambda_T^3} g_{5/2}(z)
\end{aligned}$$

其中

多重对数函数 $g_{5/2}(z) = \sum_{\alpha=1}^{\infty}\frac{z^\alpha}{\alpha^{5/2}}$， 热波长 $\lambda_T = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{1/2} = \frac{h}{\sqrt{2\pi m k_B T}}$

玻色-爱因斯坦凝聚

$$\bar{N} = \frac{4\pi V}{(2\pi\hbar)^3}\int_{2\pi\hbar/L} p^2\,\mathrm{d}p\,\frac{z}{\exp\left[\beta p^2/2m\right]-z} + \frac{z}{1-z}$$

变量代换 $x^2 = \beta p^2/2m$,

$$\begin{aligned}\bar{N} &= \frac{z}{1-z} + \frac{4V}{\lambda_T^3\sqrt{\pi}}\int_{\lambda_T\sqrt{\pi}/L}^{\infty}\mathrm{d}x\,\frac{x^2 z}{e^{x^2}-z}\\ &= \frac{z}{1-z} + \frac{4V}{\lambda_T^3\sqrt{\pi}}\int_{\lambda_T\sqrt{\pi}/L}^{\infty}\mathrm{d}x\,\sum_{n=1}^{\infty}x^2 e^{-nx^2}z^n\\ &= \frac{z}{1-z} + \frac{4V}{\lambda_T^3\sqrt{\pi}}\sum_{n=1}^{\infty}\frac{\sqrt{\pi}z^n}{4n^{3/2}}\\ &= \frac{z}{1-z} + \frac{V}{\lambda_T^3}g_{3/2}(z)\end{aligned}$$

其中

多重对数函数 $g_{3/2}(z) = \frac{4}{\sqrt{\pi}}\int_0^{\infty}\mathrm{d}x\,\frac{x^2 z}{e^{x^2}-z} = \sum_{\alpha=1}^{\infty}\frac{z^\alpha}{\alpha^{3/2}}$

用到了高斯积分 $\int_0^{\infty} e^{-ax^2} = \frac{1}{2}\sqrt{\frac{\pi}{a}}$

玻色-爱因斯坦凝聚

$$\langle n \rangle = \frac{1}{V}\frac{z}{1-z} + \frac{1}{\lambda_T^3} g_{3/2}(z)$$

$$P = -\frac{\Omega_{BE}}{V} = -\frac{k_B T}{V}\ln(1-z) + \frac{k_B T}{\lambda_T^3} g_{5/2}(z)$$

固定 $\langle n \rangle$ 和 T，让 $V \to \infty$ 和 $z \to 1$，由于 $g_{3/2}(1)$ 有限，则

$$z = 1 - \frac{1}{n_0 V}$$

玻色-爱因斯坦凝聚

$$\langle n\rangle = \frac{1}{V}\frac{z}{1-z} + \frac{1}{\lambda_T^3}g_{3/2}(z)$$

$$P = -\frac{\Omega_{BE}}{V} = -\frac{k_BT}{V}\ln(1-z) + \frac{k_BT}{\lambda_T^3}g_{5/2}(z)$$

在极限 $V\to\infty$ 下，可以认为 $z = 1 - 1/(n_0V)$，则

$$\lim_{V\to\infty}\left(-\frac{1}{V}\ln(1-z(V))\right) = 0, \quad \lim_{V\to\infty}\left(\frac{1}{V}\frac{z(V)}{1-z(V)}\right) = n_0$$

压强可以忽略第一项的贡献

$$P = \begin{cases} \frac{k_BT}{\lambda_T^3}g_{5/2}(z), & z<1 \\ \frac{k_BT}{\lambda_T^3}g_{5/2}(1), & z=1 \end{cases}$$

粒子密度

$$\langle n\rangle = \begin{cases} \frac{1}{\lambda_T^3}g_{3/2}(z), & z<1 \\ n_0 + \frac{1}{\lambda_T^3}g_{3/2}(1), & z=1 \end{cases}$$

玻色-爱因斯坦凝聚

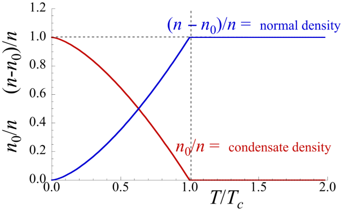
- 当 $T > T_c$：$\mu < 0$，$z < 1$
- 当 $T > T_c$：占据基态的粒子数 N_0 和总粒子数相比可以忽略
- $T < T_c$ 时：$\mu \approx 0$, $z \approx 1$, N_0 达到 N 同一量级，不可忽略

相变点

$$\langle n \rangle = \frac{1}{\lambda_T^3} g_{3/2}(1) = \frac{1}{\lambda_T^3} \mathrm{Zeta}(3/2)$$

序参量

$$\begin{aligned}\eta = \frac{n_0}{\langle n \rangle} &= \frac{\langle n \rangle - \frac{1}{\lambda_T^3} g_{3/2}(1)}{\langle n \rangle} \\ &= 1 - \frac{g_{3/2}(1)}{\langle n \rangle \lambda_T^3} = 1 - \frac{\lambda_{T_c}^3}{\lambda_T^3} \\ &= 1 - \left(\frac{T}{T_c}\right)^{3/2}\end{aligned}$$



玻色-爱因斯坦凝聚 热容

平均能量

$$E = -\frac{\partial \ln \Xi}{\partial \beta} = -\frac{3}{2}\Omega = \frac{3}{2}\frac{k_B T}{\lambda_T^3} V g_{5/2}(z)$$

$$c_V = \frac{1}{N}\left(\frac{\partial E}{\partial T}\right)_{V,N} = \frac{3}{2} k_B v \left[\frac{\partial}{\partial T}\frac{T}{\lambda_T^3} g_{5/2}(z) + \frac{T}{\lambda_T^3}\frac{\partial g_{5/2}(z)}{\partial z}\frac{\partial z}{\partial T}\right]$$

- 当 $T < T_c$ 时，$z = 1$，第二项为 0:

$$c_V = \frac{3}{2} k_B v \frac{5}{2\lambda_T^3} g_{5/2}(1)$$

- 在 $T = T_c$ 时，可以令 $\lambda_T^3 = g_{3/2}(1)/n$，同时 $v = V/N = 1/n$

$$c_V(T_c^-)/k_B = \frac{15}{4}\frac{g_{5/2}(1)}{g_{3/2}(1)} = 1.925$$

即

$$\frac{c_V}{k_B} = 1.925\left(\frac{T}{T_c}\right)^{3/2} \quad \text{for} \quad T < T_c$$

平均能量

$$E = -\frac{\partial \ln \Xi}{\partial \beta} = -\frac{3}{2}\Omega = \frac{3}{2}\frac{k_B T}{\lambda_T^3} V g_{5/2}(z)$$

$$c_V = \frac{1}{N}\left(\frac{\partial E}{\partial T}\right)_{V,N} = \frac{3}{2}k_B v\left[\frac{\partial}{\partial T}\frac{T}{\lambda_T^3} g_{5/2}(z) + \frac{T}{\lambda_T^3}\frac{\partial g_{5/2}(z)}{\partial z}\frac{\partial z}{\partial T}\right]$$

- 当 $T > T_c$ 时:
  由 $n = g_{3/2}(z)/\lambda_T^3$ 和 $\frac{\mathrm{d}n}{\mathrm{d}T} = 0$ 可得

$$0 = \frac{\mathrm{d}n}{\mathrm{d}T} = \frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{1}{\lambda_T^3}\right) g_{3/2}(z) + \frac{1}{\lambda_T^3}\frac{g_{3/2}(z)}{z}\frac{\mathrm{d}z}{\mathrm{d}T} = \frac{3g_{3/2}}{2\lambda_T^3 T} + \frac{g_{1/2}}{z\lambda_T^3}\frac{\mathrm{d}z}{\mathrm{d}T}$$

因此 $$\frac{1}{z}\frac{\mathrm{d}z}{\mathrm{d}T} = -\frac{3}{2}\frac{g_{3/2}}{g_{1/2}}\frac{1}{T}$$

利用 $z g_n'(z) = g_{n-1}(z)$，得到热容第二项

$$\frac{3}{2}k_B v\frac{T}{\lambda_T^3}\frac{g_{3/2}}{z}\frac{-3z g_{3/2}}{2T g_{1/2}} = -\frac{9}{4}k_B\frac{1}{n}\frac{g_{3/2}^2}{g_{1/2}} = -k_B\frac{9g_{3/2}}{4g_{1/2}}$$

玻色-爱因斯坦凝聚 热容

平均能量

$$E = -\frac{\partial \ln \Xi}{\partial \beta} = -\frac{3}{2}\Omega = \frac{3}{2}\frac{k_B T}{\lambda_T^3} V g_{5/2}(z)$$

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- 当 $T > T_c$ 时: c_V 的第一项为

$$\frac{3}{2} k_B v \frac{5}{2}\frac{1}{\lambda_T^3} g_{5/2}(z) = \frac{15}{4} k_B \frac{1}{n}\frac{1}{\lambda_T^3} g_{5/2}(z) = \frac{15 g_{5/2}(z)}{4 g_{3/2}(z)}$$

所以，总的热容为

$$c_V / k_B = \frac{15}{4}\frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4}\frac{g_{3/2}(z)}{g_{1/2}(z)}$$

玻色-爱因斯坦凝聚 热容

平均能量

$$E = -\frac{\partial \ln \Xi}{\partial \beta} = -\frac{3}{2}\Omega = \frac{3}{2}\frac{k_B T}{\lambda_T^3} V g_{5/2}(z)$$

$$c_V = \frac{1}{N}\left(\frac{\partial E}{\partial T}\right)_{V,N} = \frac{3}{2} k_B v \left[\frac{\partial}{\partial T}\frac{T}{\lambda_T^3} g_{5/2}(z) + \frac{T}{\lambda_T^3}\frac{\partial g_{5/2}(z)}{\partial z}\frac{\partial z}{\partial T}\right]$$

- 当 $T > T_c$ 时：
  若 $z \to 1^+$，$g_{1/2}(1)$ 发散，得到

$$c_V/k_B \to \frac{15}{4}\frac{1.341}{2.612} - \frac{9}{4}\frac{g_{3/2}(1)}{\infty} = 1.925$$

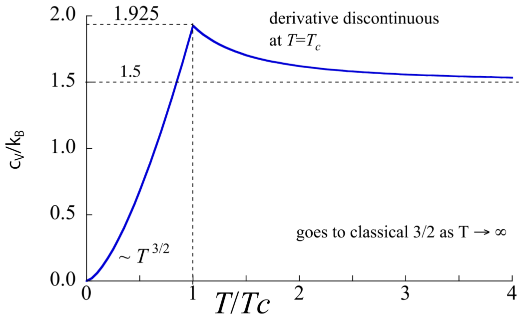
因此满足

$$c_V(T^-) = c_V(T^+)$$

但是

$$\frac{\mathrm{d}}{\mathrm{d}T} c_V(T^-) \neq \frac{\mathrm{d}}{\mathrm{d}T} c_V(T^+)$$

玻色-爱因斯坦凝聚 热容



- c_V 连续，对 T 的一阶导不连续
- $T \to \infty$，$c_V \to 3k_B/2$

玻色-爱因斯坦凝聚 实验

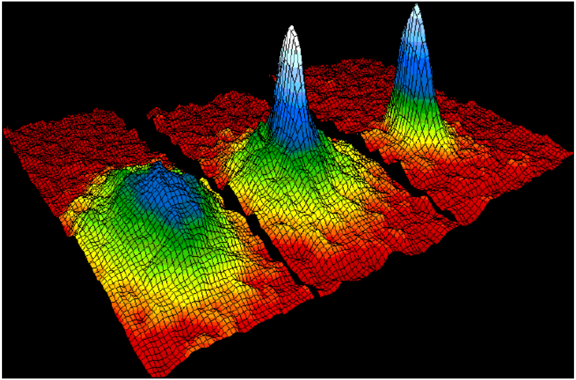
$$n\lambda_T^3 \geq g_{3/2}(1), \quad n\left(\frac{h}{\sqrt{2\pi m k_B T}}\right)^3 \geq 2.612$$

- 1924 年，Bose 和 Einstein 提出
- 极低温，如何保持原子的气体状态 $\rightarrow$ 气体处在极低的密度
- 当密度比标准状态的气体密度低 5 个数量级，使蒸汽液化或者固化的时间很长，而气体的热平衡时间很短
- 然而 n 越小，T_c 越低，就需要效率很高的冷却技术

$$n \approx 10^{14} \sim 10^{15}\text{cm}^{-3},\ T_c \text{ 约为 } \mu\text{K 的量级}$$

- 1995 年，Colorado 大学在碱金属 ^{87}Rb (Z=37) 气体中观测到了 BEC
  其中 $T = 172\,\text{nK}$, $n = 2.6 \times 10^{12}\,\text{cm}^{-3}$, 凝聚在基态的原子数约为 1000 个
- 1995 年，Rice 大学在碱金属 ^7Li 气体中观测到了 BEC
  其中 $T = 400\,\text{nK}$, $n = 10^{12}\,\text{cm}^{-3}$, 凝聚在基态的原子数约为 1000 个

玻色-爱因斯坦凝聚



大湾区大学

玻色-爱因斯坦凝聚

问：二维系统是否存在玻色凝聚？

玻色-爱因斯坦凝聚

问：二维系统是否存在玻色凝聚？

变量代换 $x^2 = \beta p^2/2m$,

$$\begin{aligned}\bar{N} &= \frac{z}{1-z} + \frac{2V}{\lambda_T^2}\int_{\lambda_T\sqrt{\pi}/L}^{\infty} \mathrm{d}x\, \frac{xz}{e^{x^2}-z} \\ &= \frac{z}{1-z} + \frac{2V}{\lambda_T^2}\int_{\lambda_T\sqrt{\pi}/L}^{\infty} \mathrm{d}x \sum_{n=1}^{\infty} xe^{-nx^2} z^n \\ &= \frac{z}{1-z} + \frac{2V}{\lambda_T^2}\sum_{n=1}^{\infty}\frac{z^n}{2n} \\ &= \frac{z}{1-z} + \frac{V}{\lambda_T^2} g_1(z)\end{aligned}$$

- $\sum_n \frac{z^n}{n}$ 要求 z 必须小于 1，否则它自身发散

  $z < 1 \rightarrow$ 不能形成 BEC

Outline

声子

固体中原子形成周期性排列结构，相邻原子之间形成耦合作用，每个原子在平衡位置做微振动 $\mathbf{q} = \mathbf{q}_0 + \mathbf{u}$

$$\Phi = \Phi_0 + \sum_{\alpha} \left(\frac{\partial \Phi}{\partial q_{r,\alpha}} \right) u_\alpha(r) + \frac{1}{2} \sum_{r,r',\alpha,\beta} \left(\frac{\partial^2 \Phi}{\partial q_{r,\alpha} \partial q_{r',\beta}} \right) u_\alpha(\mathbf{r}) u_\beta(\mathbf{r}') + \dots$$

- 原子平衡位置 $\frac{\partial \Phi}{\partial q} = 0$

$$E = \sum_{r,\alpha} \frac{1}{2} m \dot{u}_\alpha(\mathbf{r}) + \frac{1}{2} \sum_{r,r',\alpha,\beta} K_{\alpha\beta}(\mathbf{r} - \mathbf{r}') u_\alpha(\mathbf{r}) u_\beta(\mathbf{r}') + \Phi_0$$

- 傅里叶变换

$$u_\alpha(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tilde{u}(\mathbf{k})$$

声子

$$
\begin{aligned}
&\frac{1}{2N}\sum_{r,r',\alpha,\beta} K_{\alpha\beta}(\mathbf{r}-\mathbf{r}')\left(\sum_k e^{i\mathbf{k}\cdot\mathbf{r}}\tilde{u}_\alpha(\mathbf{k})\right)\left(\sum_{k'} e^{i\mathbf{k}'\cdot\mathbf{r}}\tilde{u}_\beta(\mathbf{k}')\right)\\
=&\frac{1}{2N}\sum_{r,r',\alpha,\beta}\sum_{k,k'} K_{\alpha\beta}(\boldsymbol{\rho})e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\rho}/2)}\tilde{u}_\alpha(\mathbf{k})e^{i\mathbf{k}'\cdot(\mathbf{R}-\boldsymbol{\rho}/2)}\tilde{u}_\beta(\mathbf{k}')\\
=&\frac{1}{2N}\sum_{k,k',\alpha,\beta}\sum_{\mathbf{R},\boldsymbol{\rho}} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{R}}\left(K_{\alpha\beta}(\boldsymbol{\rho})e^{i(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\rho}/2}\right)\tilde{u}_\alpha(\mathbf{k})\tilde{u}_\beta(\mathbf{k}')\\
=&\frac{1}{2}\sum_{k,k',\alpha,\beta}\delta(\mathbf{k}+\mathbf{k}')\left(\sum_\rho K_{\alpha\beta}(\boldsymbol{\rho})e^{i(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\rho}/2}\right)\tilde{u}_\alpha(\mathbf{k})\tilde{u}_\beta(\mathbf{k}')\\
=&\frac{1}{2}\sum_{k,\alpha,\beta}\left(\sum_\rho K_{\alpha\beta}(\boldsymbol{\rho})e^{i\mathbf{k}\cdot\boldsymbol{\rho}}\right)\tilde{u}_\alpha(\mathbf{k})\tilde{u}_\beta(-\mathbf{k})\\
=&\frac{1}{2}\sum_{k,\alpha,\beta}\tilde{K}_{\alpha\beta}(\mathbf{k})\tilde{u}_\alpha(\mathbf{k})\tilde{u}_\beta(-\mathbf{k})\\
=&\frac{1}{2}\sum_{k,\alpha,\beta}\tilde{K}_{\alpha\beta}(\mathbf{k})\tilde{u}_\alpha(\mathbf{k})\tilde{u}^*_\beta(\mathbf{k})
\end{aligned}
$$

声子

$$
\begin{aligned}
\sum_{\mathbf{r},\alpha}\frac{1}{2}m\dot{u}_\alpha(\mathbf{r})^2 &= \sum_{\mathbf{r},\alpha}\frac{1}{2}m\left(\frac{\mathrm{d}}{\mathrm{d}t}\sum_{\mathbf{k}}\frac{1}{\sqrt{N}}e^{i\mathbf{k}\cdot\mathbf{r}}\tilde{u}_\alpha(\mathbf{k})\right)\left(\frac{\mathrm{d}}{\mathrm{d}t}\sum_{\mathbf{k}'}\frac{1}{\sqrt{N}}e^{i\mathbf{k}'\cdot\mathbf{r}}\tilde{u}_\alpha(\mathbf{k}')\right)\\
&= \frac{1}{2N}m\sum_{\mathbf{k},\mathbf{k}',\mathbf{r},\alpha}e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}}\dot{\tilde{u}}_\alpha(\mathbf{k})\dot{\tilde{u}}_\alpha(\mathbf{k}')\\
&= \frac{1}{2}m\sum_{\mathbf{k},\mathbf{k}',\alpha}\delta(\mathbf{k}+\mathbf{k}')\dot{\tilde{u}}_\alpha(\mathbf{k})\dot{\tilde{u}}_\alpha(\mathbf{k}')\\
&= \frac{1}{2}m\sum_{\mathbf{k},\alpha}\dot{\tilde{u}}_\alpha(\mathbf{k})\dot{\tilde{u}}_\alpha(-\mathbf{k})\\
&= \sum_{\mathbf{k},\alpha}\frac{\tilde{p}_\alpha(\mathbf{k})\tilde{p}_\alpha(-\mathbf{k})}{2m}\\
&= \sum_{\mathbf{k},\alpha}\frac{\tilde{p}_\alpha(\mathbf{k})\tilde{p}^*_\alpha(\mathbf{k})}{2m}
\end{aligned}
$$

$$H = \sum_{\mathbf{k},\alpha} \frac{1}{2m} |\tilde{p}_\alpha(\mathbf{k})|^2 + \sum_{\mathbf{k},\alpha,\beta} \frac{\tilde{K}_{\alpha\beta}(\mathbf{k})}{2} \tilde{u}_\alpha(\mathbf{k}) u^*_\beta(\mathbf{k})$$

声子

$$H = \sum_{\mathbf{k},\alpha} \left[\frac{1}{2m} |\tilde{p}_\alpha(\mathbf{k})|^2 + \frac{\tilde{K}(\mathbf{k})}{2} |\tilde{u}_\alpha(\mathbf{k})|^2 \right]$$

- 对角化
- $3N$ 个独立的振子
- $\omega_\alpha(\mathbf{k}) = \sqrt{\frac{\tilde{K}(\mathbf{k})}{m}}$

声子

$$E = \sum_{i=1}^{3N} \hbar\omega_i \left(n_i + \frac{1}{2}\right) + \Phi_0, \quad n_i = 0, 1, 2, \ldots$$

声子

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配分函数

$$Z = \sum e^{-\beta H} = e^{-\beta E_0} \prod_i \sum_{n_i=0}^{\infty} e^{-\beta\hbar\omega_i n_i} = e^{-\beta E_0} \prod_i \frac{1}{1 - e^{-\beta\hbar\omega_i}}$$

固体内能

$$\bar{E} = -\frac{\partial \ln Z}{\partial \beta} = E_0 + \sum_i \frac{\hbar\omega_i}{e^{\beta\hbar\omega_i} - 1}$$

声子气体 爱因斯坦模型

- 爱因斯坦模型：所有模式的频率相同，都为 ω_E

$$E = E_0 + 3N \frac{\hbar\omega_E}{e^{\beta\hbar\omega_E} - 1}$$

$$C = \frac{\mathrm{d}E}{\mathrm{d}T} = 3Nk_B \left(\frac{T_E}{T}\right)^2 \frac{e^{-T_E/T}}{(1 - e^{-T_E/T})^2}$$

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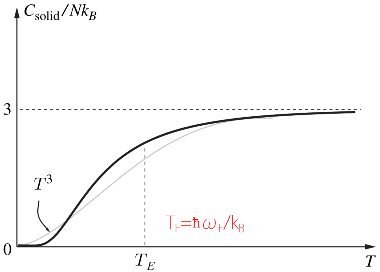

- $T \gg T_E$, $C \to 3Nk_B$
- $T \ll T_E$, $C \to 0$
- C 随温度指数衰减

声子气体 德拜模型

- 德拜 (Debye) 认为在低温时低频的声子容易被激发
- $\mathbf{k} = 0$ 对应的是晶胞的平移，即系统没有变化，因此 $\tilde{K}(k = 0) = 0$，由连续性

$$\lim_{\mathbf{k}\to 0} \tilde{K}(\mathbf{k}) = 0$$

- 在 $\mathbf{k}$ 很小时展开

$$\tilde{K}(\mathbf{k}) = Ak + Bk^2 + Ck^3 + \mathcal{O}(k^4)$$

$K(\rho) = K(-\rho)$ 保证 $\tilde{K}(\mathbf{k}) = \tilde{K}(-\mathbf{k})$，所以不存在奇数阶

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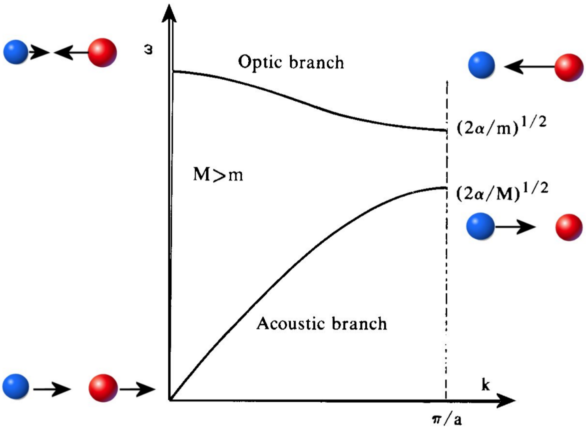
- 振动模式频率

$$\omega = \sqrt{\frac{Bk^2}{m}} = vk$$

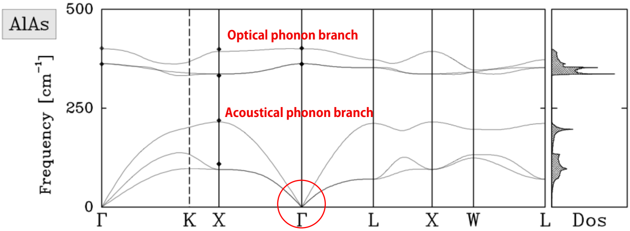
其中 $v = \sqrt{B/m}$ 为晶体中声子速度

声子 德拜模型



ε
Optic branch
$(2\alpha/m)^{1/2}$
M>m
$(2\alpha/M)^{1/2}$
Acoustic branch
k
π/a

声子 德拜模型


AlAs
500
250
0
Frequency [cm^{-1}]
Optical phonon branch
Acoustical phonon branch
Γ
K
X
Γ
L
X
W
L
Dos

声子 德拜模型

$$E = E_0 + \sum_{\mathbf{k},\alpha} \frac{\hbar v k}{e^{\beta\hbar v k} - 1} = E_0 + \frac{3V}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k} \frac{\hbar v k}{e^{\beta\hbar v k} - 1}$$

- **相空间积分**

$$\frac{\mathrm{d}q\mathrm{d}p}{h} = \frac{\mathrm{d}q\,\mathrm{d}\hbar k}{h} = \frac{\mathrm{d}q\mathrm{d}k}{2\pi}$$

- **德拜温度：存在一个最大的 k 对应的即是**

$$T_D = \frac{\hbar v k_{\mathrm{max}}}{k_B} \approx \frac{\hbar v}{k_B}\frac{\pi}{a}$$

a **为晶格常数**

声子 德拜模型

$$E = E_0 + \sum_{\mathbf{k},\alpha} \frac{\hbar v k}{e^{\beta\hbar v k} - 1} = E_0 + \frac{3V}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k} \frac{\hbar v k}{e^{\beta\hbar v k} - 1}$$

$T \gg T_D$: The classical limit

$$\begin{aligned} E(T) &= E_0 + \frac{3V}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k} \frac{\hbar v k}{(1 + \beta\hbar v k) - 1} \\ &= E_0 + 3V \frac{1}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}\, k_B T \end{aligned}$$

得到

$$E(T) = E_0 + 3Nk_B T, \quad C = 3Nk_B$$

声子 德拜模型

$$E = E_0 + \sum_{\mathbf{k},\alpha} \frac{\hbar v k}{e^{\beta\hbar v k} - 1} = E_0 + \frac{3V}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k} \frac{\hbar v k}{e^{\beta\hbar v k} - 1}$$

$T \ll T_D$: set $x = \beta\hbar v k$, thus one can have $\mathrm{d}^3 k = 4\pi x^2 \mathrm{d}x/(\beta\hbar v)^3$

$$\begin{aligned}\lim_{T\ll T_D} E(T) \approx & E_0 + \frac{3V}{8\pi^2}\left(\frac{k_B T}{\hbar v}\right)^3 4\pi k_B T \int_0^\infty \mathrm{d}x \, \frac{x^3}{e^x - 1} \\ = & E_0 + \frac{3V}{8\pi^2}\left(\frac{k_B T}{\hbar v}\right)^3 4\pi k_B T \frac{\pi^4}{15} \\ = & E_0 + \frac{\pi^2}{10} V \left(\frac{k_B T}{\hbar v}\right)^3 k_B T\end{aligned}$$

The heat capacity

$$C = \frac{\mathrm{d}E}{\mathrm{d}T} = k_B V \frac{2\pi^2}{5}\left(\frac{k_B T}{\hbar v}\right)^3 \propto T^3$$

Outline

费米系统

$$Z_{FD}(T,V,\mu)=\prod\left(1+e^{-\beta(\varepsilon-\mu)}\right)^2$$

平方代表的是自旋自由度

费米系统

$$Z_{FD}(T,V,\mu)=\prod\left(1+e^{-\beta(\varepsilon-\mu)}\right)^2$$

平方代表的是自旋自由度
系统巨势

$$\Omega_{FD}(T,V,\mu)=-k_BT\ln Z_{FD(T,V,\mu)}=-2k_BT\sum_l\ln\left(1+e^{-\beta(\varepsilon_l-\mu)}\right)$$

得到粒子数

$$\langle N\rangle=-\left(\frac{\partial\Omega_{FD}}{\partial\mu}\right)_{T,V}=\sum_l\frac{g}{e^{\beta(\varepsilon-\mu)}+1}=\sum_l\langle n_l\rangle$$

量子态 l 上的占据数

$$\langle n_l\rangle=\frac{g}{e^{\beta(\varepsilon_l-\mu)}+1}=\frac{gz}{e^{\beta\varepsilon_l}+z}$$

不同于玻色子，费米子的分布函数不会有发散的问题，所有逸度 $z=e^{\beta\mu}$ 可以是 $0\leq z\leq\infty$，也就是说 $0\leq\langle n_l\rangle\leq g$，每个量子态 l 上最多可以占据 g 个粒子，g 为量子态的简并度

费米气体 零温

When $T \to 0$, $\beta \to \infty$

$$n_l = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} = \begin{cases} 0, & \varepsilon > \mu \\ 1, & \varepsilon < \mu \end{cases}$$

- $T = 0\,\mathrm{K}$ 时，只有 $\varepsilon < \mu$ 的态被占据

费米气体 零温

$$
\begin{aligned}
n = \frac{N}{V} = \frac{g}{V} \sum_{\frac{\hbar^2 k^2}{2m} \le \varepsilon_F} 1 = \frac{g}{V} \frac{V}{(2\pi)^3} \int_{k^2 \le 2m\varepsilon_F/\hbar^2} \mathrm{d}\mathbf{k} \\
= \frac{g}{8\pi^3} \frac{4}{3} \pi \left(\frac{2m\varepsilon_F}{\hbar^2} \right)^{3/2}
\end{aligned}
$$

费米气体 零温

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$$= \frac{g}{8\pi^3} \frac{4}{3}\pi \left(\frac{2m\varepsilon_F}{\hbar^2} \right)^{3/2}$$

- 得到费米能量 (Fermi energy)

$$\varepsilon_F = \frac{\hbar^2}{2m} \left(\frac{6\pi^2 n}{g} \right)^{2/3}$$

  和费米波矢 (Fermi wavenumber): $k_F = \left(\frac{6\pi^2 n}{g} \right)^{1/3}$

- 态密度 (DOS)

$$g(\varepsilon) = \frac{\mathrm{d}n(\varepsilon)}{\mathrm{d}\varepsilon} = \frac{g}{4\pi^2} \left(\frac{2m}{\hbar} \right)^{3/2} \varepsilon^{1/2}$$

费米气体 零温

$$n = \frac{N}{V} = \frac{g}{V} \sum_{\frac{\hbar^2 k^2}{2m} \le \varepsilon_F} 1 = \frac{g}{V} \frac{V}{(2\pi)^3} \int_{k^2 \le 2m\varepsilon_F/\hbar^2} \mathrm{d}\mathbf{k}$$

$$= \frac{g}{8\pi^3} \frac{4}{3}\pi \left(\frac{2m\varepsilon_F}{\hbar^2} \right)^{3/2}$$

- 可以得到以下关系

$$\varepsilon_F \sim n^{2/3}, \quad k_F \sim n^{1/3}$$

  又由 $n \sim l^{-3}$, 得到 $k_F \sim 1/l$。(l 为粒子间的平均距离)
- DOS 可以写成 $g(\varepsilon) = C\sqrt{\varepsilon}$, C 为常数

$$n = \int_0^{\varepsilon_F} \mathrm{d}\varepsilon \, g(\varepsilon) = \frac{2}{3} C \varepsilon_F^{3/2} \Longrightarrow C = \frac{3}{2} \frac{n}{\varepsilon_F^{3/2}}$$

  得到 $g(\varepsilon_F) = \frac{3}{2} \frac{n}{\varepsilon_F}$

$$g(\varepsilon) = g(\varepsilon_F) \frac{g(\varepsilon)}{g(\varepsilon_F)} = g(\varepsilon_F) \frac{C\sqrt{\varepsilon}}{C\sqrt{\varepsilon_F}} = \frac{3}{2} \frac{n}{\varepsilon_F} \sqrt{\frac{\varepsilon}{\varepsilon_F}}$$

费米气体 零温

$$n = \frac{N}{V} = \frac{g}{V} \sum_{\frac{\hbar^2 k^2}{2m} \leq \varepsilon_F} 1 = \frac{g}{V} \frac{V}{(2\pi)^3} \int_{k^2 \leq 2m\varepsilon_F/\hbar^2} \mathrm{d}\mathbf{k}$$

$$= \frac{g}{8\pi^3} \frac{4}{3}\pi \left(\frac{2m\varepsilon_F}{\hbar^2} \right)^{3/2}$$

- **能量**

$$\frac{E}{V} = \int_0^{\varepsilon_F} \mathrm{d}\varepsilon\, g(\varepsilon)\varepsilon = \frac{3}{2} \frac{n}{\varepsilon_F^{3/2}} \frac{2}{5} \varepsilon_F^{5/2} = \frac{3}{5} n\varepsilon_F$$

每个粒子平均能量

$$\frac{E}{N} = \frac{E}{V} \frac{V}{N} = \frac{3}{5} \varepsilon_F$$

- **压强**

$$P = -\left(\frac{\partial E}{\partial V} \right)_{T,N} = -\frac{3}{5} N \left(\frac{\partial \varepsilon_F}{\partial V} \right)_{T,N}$$

由 $\varepsilon_F \sim n^{2/3} = \left(\frac{N}{V}\right)^{2/3}$ **得到**

$$n = \frac{N}{V} = \frac{g}{V} \sum_{\frac{\hbar^2 k^2}{2m} \leq \varepsilon_F} 1 = \frac{g}{V} \frac{V}{(2\pi)^3} \int_{k^2 \leq 2m\varepsilon_F/\hbar^2} \mathrm{d}\mathbf{k}$$

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每个粒子平均能量

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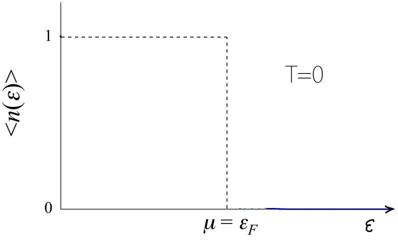
- **压强**

$$P = -\left(\frac{\partial E}{\partial V} \right)_{T,N} = -\frac{3}{5} N \left(-\frac{2}{3} \frac{\varepsilon_F}{V} \right) = \frac{2}{5} n\varepsilon_F$$

温度为零时，压强有限值

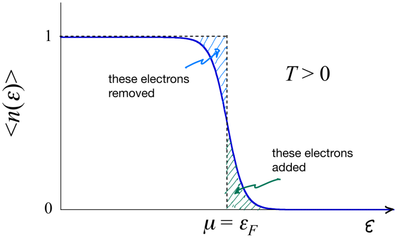
$T > 0$?

费米气体 有限温



- 零温时，只有费米面以下的态被填充

费米气体 有限温



- 升温：费米面以下的粒子可能被激发到费米面以上
- $\rightarrow$ 正则系综
- 费米面以下 (以上) 被激发的粒子数

$$g(\varepsilon_F - \Delta\varepsilon)\Delta\varepsilon < g(\varepsilon_F + \Delta\varepsilon)\Delta\varepsilon$$

由于 $g(\varepsilon) \propto \sqrt{\varepsilon}$. 为保证粒子数守恒，费米面也会随温度移动

$$
\begin{aligned}
I = \int A(E) f(E) \mathrm{d}E &= -\int K(E) f'(E) \mathrm{d}E \\
&= -\int \left[K(\mu) + K'(\mu)(E-\mu) + \frac{1}{2} K''(\mu)(E-\mu)^2 + \dots \right] f'(E) \mathrm{d}E \\
&= -\int \left[K(\mu) + \frac{1}{2} A'(\mu) (E-\mu)^2 + \dots \right] f'(E) \mathrm{d}E \\
&= \int_{-\infty}^{\mu} A(E) \mathrm{d}E + \frac{\pi^2}{6} (k_B T)^2 \left. \frac{\mathrm{d}A}{\mathrm{d}E} \right|_{E=\mu}
\end{aligned}
$$

- 索末菲尔德展开 (Sommerfeld expansion)
- 第一个等号用分部积分，并令 $K'(E) = A(E)$
- 第二行到第三行用到了函数在 $E = \mu$ 的奇偶性

费米气体 有限温

$$
\begin{aligned}
n &= \int_0^{\infty} \frac{g(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1} \\
&= \int_0^{\mu} g(\varepsilon)\mathrm{d}\varepsilon + \frac{\pi^2}{6}(k_B T)^2 g'(\varepsilon=\mu) \\
&= \int_0^{\varepsilon_F} g(\varepsilon)\mathrm{d}\varepsilon + \int_{\varepsilon_F}^{\mu} g(\varepsilon)\mathrm{d}\varepsilon + \frac{\pi^2}{6}(k_B T)^2 g'(\mu)
\end{aligned}
$$

由于 n 不随温度变化，上式红色部分为零

$$
(\mu - \varepsilon_F) g(\varepsilon_F) \approx -\frac{\pi^2}{6}(k_B T)^2 g'(\mu)
$$

因此得到

$$
\mu(T) = \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)}
$$

由于 $g(\varepsilon) = C\sqrt{\varepsilon}$

费米气体 有限温

$$
\begin{aligned}
n &= \int_0^\infty \frac{g(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1} \\
&= \int_0^\mu g(\varepsilon)\mathrm{d}\varepsilon + \frac{\pi^2}{6}(k_BT)^2 g'(\varepsilon=\mu) \\
&= \int_0^{\varepsilon_F} g(\varepsilon)\mathrm{d}\varepsilon + \int_{\varepsilon_F}^{\mu} g(\varepsilon)\mathrm{d}\varepsilon + \frac{\pi^2}{6}(k_BT)^2 g'(\mu)
\end{aligned}
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$$
(\mu-\varepsilon_F)g(\varepsilon_F) \approx -\frac{\pi^2}{6}(k_BT)^2 g'(\mu)
$$

因此得到

$$
\mu(T) = \varepsilon_F - \frac{\pi^2}{6}(k_BT)^2\frac{1}{2\varepsilon_F} = \varepsilon_F\left[1-\frac{\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2\right]
$$

- 单位体积内能量变化

$$\Delta U \approx [g(\varepsilon_F)k_B T]\,(k_B T) = g(\varepsilon)\,(k_B T)^2$$

- 比热容

$$c_V = 2g(\varepsilon_F)k_B^2 T = \frac{3n}{\varepsilon_F}k_B^2 T = 2nk_B\frac{T}{T_F}$$

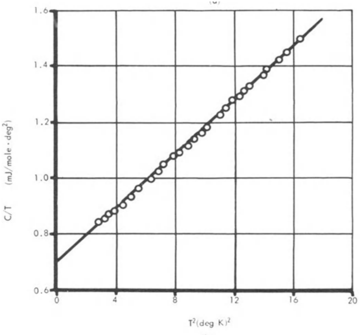
费米温度的量级 $T_F \sim 10^4\,\mathrm{K}$

- 晶体比热容 $c_V = c_V^{\mathrm{ions}} + c_V^{\mathrm{elec}}$

$$c_V^{\mathrm{ions}} = \frac{12\pi^4}{5}nk_B\left(\frac{T}{T_D}\right)^3, \quad c_V^{\mathrm{elec}} = \frac{\pi^2}{2}nk_B T\left(\frac{T}{T_F}\right)$$

一般有 $T_D \sim 100\,\mathrm{K}$

费米气体 有限温



Heat capacity of Cu

$$C^{\text{total}} = AT + BT^3$$

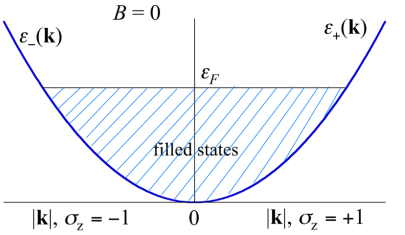
- Plot C/T versue T^2
- T^3 项在常温下占主导
- 足够低温下 T^1 项占主导

$$T < 0.1T_D \sim \mathcal{O}(1)\,\mathrm{K}$$

泡利顺磁性 (Pauli paramagnetism)

- **电子内禀自旋角动量** $\boldsymbol{\mu} = -\mu_B \boldsymbol{\sigma}$
- **塞曼劈裂** $-\boldsymbol{\mu} \cdot \mathbf{B} = \mu_B \sigma_z B$

$$\varepsilon_{\pm}(\mathbf{k}) = \varepsilon_0(\mathbf{k}) \pm \mu_B B$$



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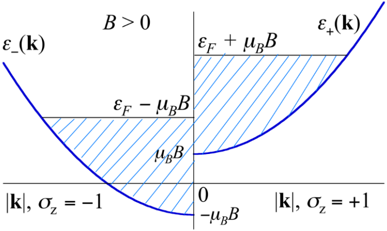

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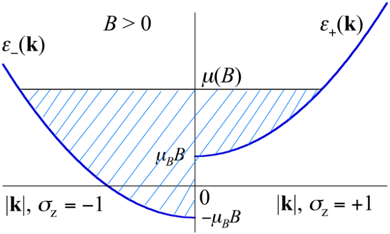

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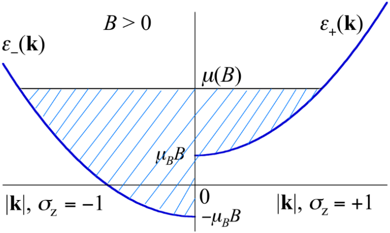


$$\frac{M}{V} = -\mu_B (n_+ - n_-) > 0 \rightarrow \quad \text{paramagnetic effect}$$

自旋正电子态密度

$$g_+(\varepsilon + \mu_B B) = \frac{1}{2} g(\varepsilon) \Longrightarrow g_+(\varepsilon) = \frac{1}{2} g(\varepsilon - \mu_B B)$$

粒子密度

$$n_+ = \int_{\varepsilon_{+\min}}^{\infty} \mathrm{d}\varepsilon \, g_+(\varepsilon) f(\varepsilon, \mu(B))$$

where

$$f(\varepsilon, \mu(B)) = \frac{1}{e^{(\varepsilon - \mu(B))/k_B T} + 1}$$

泡利顺磁性

自旋负电子态密度

$$g_-(\varepsilon + \mu_B B) = \frac{1}{2}g(\varepsilon) \Longrightarrow g_-(\varepsilon) = \frac{1}{2}g(\varepsilon + \mu_B B)$$

粒子密度

$$n_- = \int_{\varepsilon_{-\min}}^{\infty} \mathrm{d}\varepsilon\, g_-(\varepsilon) f(\varepsilon, \mu(B))$$

where

$$f(\varepsilon, \mu(B)) = \frac{1}{e^{(\varepsilon - \mu(B))/k_B T} + 1}$$

泡利顺磁性

$$
\begin{aligned}
\frac{M}{V} &= -\mu_B\left[n_+ - n_-\right] = \mu_B \int \mathrm{d}\varepsilon\, f(\varepsilon,\mu)\left[g_-(\varepsilon) - g_+(\varepsilon)\right] \\
&= \mu_B \int \mathrm{d}\varepsilon f(\varepsilon,\mu)\left[\frac{1}{2}g(\varepsilon+\mu_B B) - \frac{1}{2}g(\varepsilon-\mu_B B)\right] \\
&= \frac{1}{2}\mu_B \int \mathrm{d}\varepsilon\, g(\varepsilon)\left[f(\varepsilon,\mu+\mu_B B) - f(\varepsilon,\mu-\mu_B B)\right] \\
&= \frac{1}{2}\mu_B \int \mathrm{d}\varepsilon\, g(\varepsilon)\left[f(\varepsilon,\mu) + \frac{\partial f}{\partial \mu}(\mu_B B) - f(\varepsilon,\mu) + \frac{\partial f}{\partial \mu}(\mu_B B)\right] \\
&= \int \mathrm{d}\varepsilon\, g(\varepsilon)\mu_B^2 B\left(\frac{\partial f}{\partial \mu}\right)
\end{aligned}
$$

In $T \to 0$ limit

$$
\frac{M}{V} \to \mu_B^2 B g(\varepsilon_F)
$$

经典泡利顺磁性

根据玻尔兹曼分布，$\sigma_z = \pm 1$ 的占据概率：

$$P(\sigma_z) = \frac{e^{-\beta\mu_B B\sigma_z}}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}}$$

磁性密度

$$\begin{aligned}\frac{M}{V} &= \frac{N}{V}\frac{M}{N} = -n\mu_B\left[P(1) + (-1)P(-1)\right] = -n\mu_B \frac{e^{-\beta\mu_B B} - e^{\beta\mu_B B}}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} \\ &= n\mu_B \tanh(\beta\mu_B B)\end{aligned}$$

也可以定义磁化率

$$\chi_B = \frac{\mathrm{d}(M/V)}{\mathrm{d}B}$$

经典泡利顺磁性

$$\text{Quantum}: \frac{M}{V} = \int \mathrm{d}\varepsilon\, g(\varepsilon) \left(\frac{\partial f}{\partial \mu}\right) \mu_B^2 B, \quad \text{Classical}: \frac{M}{V} = n\mu_B \tanh(\beta\mu_B B)$$

- $T \to 0$, 有 $M/V \to \mu_B n$，即所有自旋都朝向一个方向；

$$\frac{M_Q}{M_C} \to \frac{3\mu_B B}{2\varepsilon_F} \ll 1$$

- (室温) 高温，有 $\tanh(\beta\mu_B B) \to \beta\mu_B B$,

$$\text{classical}: \frac{M_C}{V} = \frac{\mu_B^2 B n}{k_B T} \propto \frac{1}{T}$$

室温时仍然满足 $T \ll T_F$,

$$\text{quantum}: \frac{M_Q}{V} = \frac{3\mu_B^2 n B}{2\varepsilon_F}$$

磁化率比值

$$\frac{\chi_Q}{\chi_C} = \frac{M_Q}{M_C} = \frac{3}{2}\left(\frac{k_B T}{\varepsilon_F}\right) = \frac{3}{2}\frac{T}{T_F} \ll 1$$

费米系统

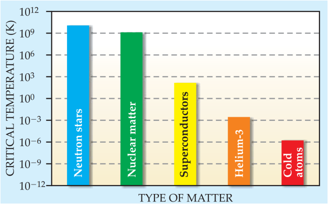
对于费米系统，它表现出的物理量，如 $\mu(T)$, c_V，χ，都与费米面处的态密度密切相关，$g(\varepsilon_F)$ 或者 $g'(\varepsilon_F)$，为什么?

费米系统

对于费米系统，它表现出的物理量，如 $\mu(T)$, c_V，χ，都与费米面处的态密度密切相关，$g(\varepsilon_F)$ 或者 $g'(\varepsilon_F)$，为什么?

- 对于 $k_BT \ll \varepsilon_F$ 的简并气体，只有费米面附近能量 k_BT 会被激发
- $\varepsilon_F - k_BT$ 以下的能量被全部填充
- 一个电子吸收大于 k_BT 的能量跑到费米面以上的态是不太可能发生的事件
- 可以被激发的电子有多少呢？$\approx g(\varepsilon_F)k_BT$

超导、超流、BEC、BCS



- 凝聚的粒子带电 $\rightarrow$ 超导

  定域规范对称性破缺: $U(1) \rightarrow \mathbb{Z}_2$

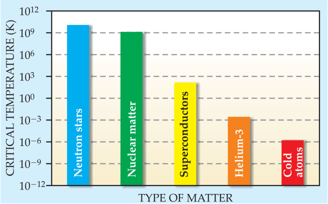
- 凝聚的粒子不带电 $\rightarrow$ 超流

  整体连续对称性破缺

- Bardeen-Cooper-Schrieffer (BCS)

  两个电子形成束缚对 (Cooper pairing)$\rightarrow$ 带电玻色子

超导、超流、BEC、BCS



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推荐阅读: Carlos A. R. Sá de Melo, When fermions become bosons: Pairing in ultracold gases

小结

- 玻色和费米气体的热力学函数
- 量子气体的统计效应
- 玻色-爱因斯坦凝聚
- 费米在零温和有限温的效应，泡利顺磁性