引入 $\boxed{\text{配分函数}}$

定义 $Z \equiv \sum_\lambda g_\lambda \cdot e^{-\beta\varepsilon_\lambda}$ 记下

总粒子数 $N = \sum_\lambda \bar{a}_\lambda = \sum_\lambda g_\lambda \cdot e^{-\alpha-\beta\varepsilon_\lambda}$

$= e^{-\alpha} \cdot \sum_\lambda g_\lambda \cdot e^{-\beta\varepsilon_\lambda}$

$= e^{-\alpha} \cdot Z$

得 $\alpha = -\ln \frac{N}{Z}$

能量 $\bar{E} = \sum_\lambda \varepsilon_\lambda \bar{a}_\lambda$

$$= \sum_\lambda \varepsilon_\lambda \cdot g_\lambda \cdot e^{-\alpha-\beta\varepsilon_\lambda}$$

$$= \sum_\lambda -\frac{d}{d\beta}\left[g_\lambda \cdot e^{-\alpha-\beta\varepsilon_\lambda}\right]$$

$$= -e^{-\alpha} \frac{d}{d\beta} \sum_\lambda g_\lambda e^{-\beta\varepsilon_\lambda}$$

$$= -e^{-\alpha} \frac{d}{d\beta} Z$$

$$= -\frac{N}{Z} \cdot \frac{d}{d\beta} Z$$

$$= -N \cdot \frac{d}{d\beta} \ln Z$$

$\beta = \frac{1}{kT}$

Boltzman 常数

MB分布的例子：二能级系统

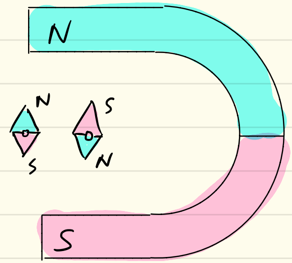
e.g. 稀磁系统

微观特性：

① 仅有两个能级 $\lambda = 1, 2$

② 每个能级简并度为 $g_\lambda = 1$

③ 能级能量 $\varepsilon_1 = -\varepsilon$; $\varepsilon_2 = \varepsilon$



$\lambda = 1, 2$

二能级系统配分函数

$$Z = g_1 \cdot e^{-\beta\varepsilon_1} + g_2 \cdot e^{-\beta\varepsilon_2}$$

$$= e^{\beta\varepsilon} + e^{-\beta\varepsilon}$$

通过 $N = e^{-\alpha} \cdot Z$ 得 $e^{-\alpha} = \dfrac{N}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}}$

MB分布 $\bar{a}_1 = g_1 \cdot e^{-\alpha-\beta\varepsilon_1} = \dfrac{N\ e^{+\beta\varepsilon}}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}}$.

$\bar{a}_2 = g_2 \cdot e^{-\alpha-\beta\varepsilon_2} = \dfrac{N\ e^{-\beta\varepsilon}}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}}$

验证 $\bar{a}_1 + \bar{a}_2 = N$

二能级系统在温度极限条件下粒子分布

$$\bar{a}_1 = \frac{N e^{+\beta\varepsilon}}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}}. \qquad \bar{a}_2 = \frac{N e^{-\beta\varepsilon}}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}} \qquad \beta = \frac{1}{kT}$$

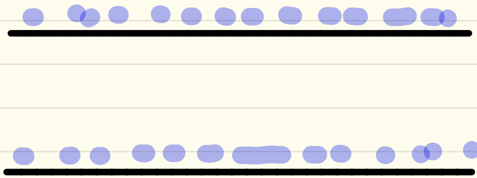
① $T \to +\infty$

$\hookrightarrow \beta \to 0$

得

$$\bar{a}_1 = \frac{N}{2}$$

$$\bar{a}_2 = \frac{N}{2}$$



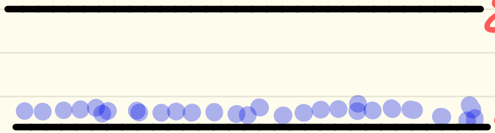
② $T \to 0$

$\hookrightarrow \beta \to +\infty$

得

$$\bar{a}_1 = N$$

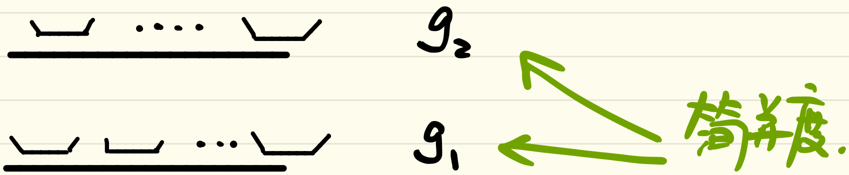
$$\bar{a}_2 = 0$$



课堂练习

某定域子系系统为三能级系统有能级 $\varepsilon_1=\varepsilon$ $\varepsilon_2=2\varepsilon$ $\varepsilon_3=4\varepsilon$，简并度 $g_1=1$，$g_2=2$，$g_3=4$。求在三个能级上的平均分布 $\overline{a_1}$，$\overline{a_2}$，$\overline{a_3}$ 并分析温度 $T\to+\infty$ 和 $T\to0$ 时的分布情况。总粒子数 N 已知

单个粒子出现在每个量子态的概率



在能级λ上出现的概率. $\dfrac{\bar{a}_\lambda}{N}$

.. 每个量子态 . . . . $\dfrac{\bar{a}_\lambda}{g_\lambda N}$

能量的计算

$$\beta = \frac{1}{kT}$$

对二能级系统

$$\bar{a}_\lambda = g_\lambda \cdot e^{-\alpha-\beta\varepsilon_\lambda}$$

$g_\lambda = 1$; $\varepsilon_1 = -\varepsilon$; $\varepsilon_2 = \varepsilon$

$$\bar{a}_1 = \frac{N\, e^{+\beta\varepsilon}}{e^{\beta\varepsilon}+e^{-\beta\varepsilon}} . \qquad \bar{a}_2 = \frac{N\, e^{-\beta\varepsilon}}{e^{\beta\varepsilon}+e^{-\beta\varepsilon}}$$

$$\bar{E} = \sum_\lambda \varepsilon_\lambda \cdot \bar{a}_\lambda$$

$$= -\varepsilon \frac{e^{\beta\varepsilon}}{e^{\beta\varepsilon}+e^{-\beta\varepsilon}} N + \varepsilon \frac{e^{-\beta\varepsilon}}{e^{\beta\varepsilon}+e^{-\beta\varepsilon}} N$$

双曲正切函数

$$= \varepsilon N \frac{e^{-\beta\varepsilon}-e^{\beta\varepsilon}}{e^{-\beta\varepsilon}+e^{\beta\varepsilon}}$$

$$= \varepsilon N \tanh(-\beta\varepsilon)$$