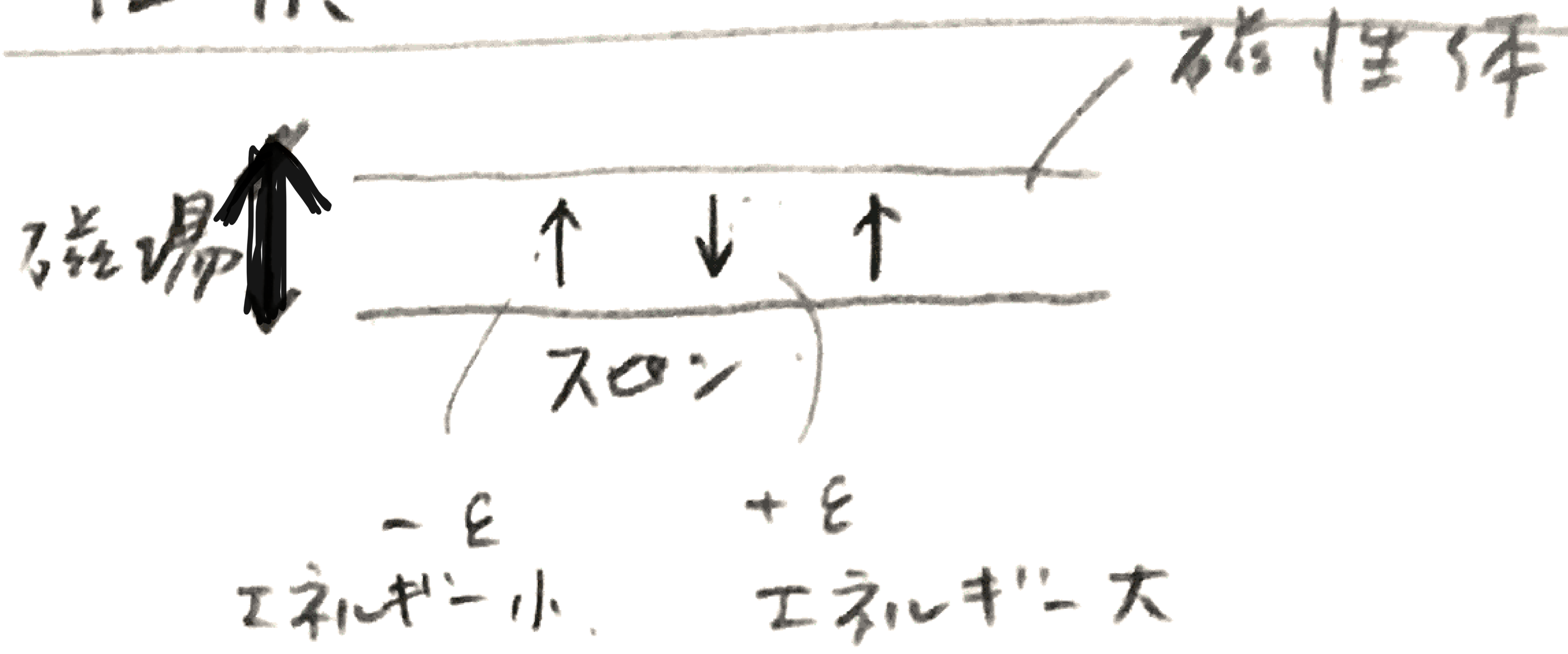
§3.4 2準位系



粒子数	N
上向きの数	$N_\uparrow$
下 〃	$N_\downarrow$

場合の数 $W(E, N) = \dfrac{N!}{N_\uparrow!\, N_\downarrow!}$

ただし $E = \varepsilon (N_\downarrow - N_\uparrow)$

$N = N_\downarrow + N_\uparrow$

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① エントロピー S

$$S = k_B \ln W$$

$$= k_B \left(N \ln N - N_\uparrow \ln N_\uparrow - N_\downarrow \ln N_\downarrow \right)$$

$$N_\uparrow = \frac{1}{2}\left(N - \frac{E}{\varepsilon}\right)$$

$$N_\downarrow = \frac{1}{2}\left(N + \frac{E}{\varepsilon}\right)$$

$$= k_B \left(N \ln N - \frac{1}{2}\left(N - \frac{E}{\varepsilon}\right) \ln \frac{1}{2}\left(N - \frac{E}{\varepsilon}\right) - \frac{1}{2}\left(N + \frac{E}{\varepsilon}\right) \ln \frac{1}{2}\left(N + \frac{E}{\varepsilon}\right) \right)$$

$$= k_B N \left(\ln N - \frac{1}{2}\left(1 - \frac{E}{\varepsilon N}\right)\left(\ln N + \ln\frac{1}{2}\left(1 - \frac{E}{\varepsilon N}\right)\right) - \frac{1}{2}\left(1 + \frac{E}{\varepsilon N}\right)\left(\ln N + \ln\frac{1}{2}\left(1 + \frac{E}{\varepsilon N}\right)\right)\right)$$

$$= -\frac{1}{2} k_B N \left(\left(1 - \frac{E}{\varepsilon N}\right) \ln\frac{1}{2}\left(1 - \frac{E}{\varepsilon N}\right) + \left(1 + \frac{E}{\varepsilon N}\right) \ln\frac{1}{2}\left(1 + \frac{E}{\varepsilon N}\right)\right)$$

//

② 温度 T

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N,V}$$

$$= -\frac{1}{2} k_B N \left(-\frac{1}{\varepsilon N} \ln\frac{1}{2}\left(1 - \frac{E}{\varepsilon N}\right) + \left(1 - \frac{E}{\varepsilon N}\right) \cdot \frac{2}{1 - \frac{E}{\varepsilon N}} \cdot \left(-\frac{1}{2\varepsilon N}\right) + \frac{1}{\varepsilon N} \ln\frac{1}{2}\left(1 + \frac{E}{\varepsilon N}\right) + \left(1 + \frac{E}{\varepsilon N}\right) \frac{2}{1 + \frac{E}{\varepsilon N}} \cdot \frac{1}{2\varepsilon N}\right)$$

$$= -\frac{k_B}{2\varepsilon}\left(\ln\frac{1}{2}\left(1 + \frac{E}{\varepsilon N}\right) - \ln\frac{1}{2}\left(1 - \frac{E}{\varepsilon N}\right)\right)$$

$$= -\frac{k_B}{2\varepsilon}\left(\ln\left(1 + \frac{E}{\varepsilon N}\right) - \ln\left(1 - \frac{E}{\varepsilon N}\right)\right)$$

$$\therefore T = -\frac{2\varepsilon}{k_B} \frac{1}{\ln \frac{1 + \frac{E}{\varepsilon N}}{1 - \frac{E}{\varepsilon N}}}$$

//

$$\ln \frac{1 + \frac{E}{\varepsilon N}}{1 - \frac{E}{\varepsilon N}} = -\frac{2\varepsilon}{k_B T}$$

$$\therefore \frac{1 + \frac{E}{\varepsilon N}}{1 - \frac{E}{\varepsilon N}} = e^{-\frac{2\varepsilon}{k_B T}}$$

$$\therefore \frac{E}{\varepsilon N} = \frac{e^{-\frac{2\varepsilon}{k_B T}} - 1}{e^{-\frac{2\varepsilon}{k_B T}} + 1} = \frac{e^{-\frac{\varepsilon}{k_B T}} - e^{\frac{\varepsilon}{k_B T}}}{e^{-\frac{\varepsilon}{k_B T}} + e^{\frac{\varepsilon}{k_B T}}}$$

$$\therefore E = -\varepsilon N \tanh \frac{\varepsilon}{k_B T}$$

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③ 比熱 $\frac{\partial E}{\partial T} = -\varepsilon N \left(\mathrm{sech}^2 \frac{\varepsilon}{k_B T}\right) \times \left(-\frac{\varepsilon}{k_B}\frac{1}{T^2}\right)$

$= N k_B \left(\frac{\varepsilon}{k_B T}\right)^2 \mathrm{sech}^2 \frac{\varepsilon}{k_B T}$

"ショットキー" 型 比熱
Schottky

☆ これらを図にしてみよう。

Maximaで

```
plot2d (- sinh(1/x)/cosh(1/x),[x,0,4]);
plot2d ( 1/x/x * sech(1/x)^2,[x,0,4]);
```

ついでに

```
taylor(log(1+x), x, 0, 10);
```