HW#5

6.22 6.26 6.31 6.37 6.52 (6.30 or Additional Problem)

6.22. a) Assume $n=0$

14/14

2 $$1 = \frac{1-x^{0+1}}{1-x}$$

When $n=1$ $$1+x = \frac{1-x^{1+1}}{1-x} = \frac{1-x^2}{1-x}$$ , it works.

Now, assuming that the formula works for $n-1$,

$$(1+x+\cdots+x^{n-1})+x^n = \frac{1-x^n}{1-x}+x^n$$

$$= \boxed{\frac{1-x^{n+1}}{1-x}}$$

We find the formula also works for $n$.

b) Allowed energy

2 $E = j\delta\mu B,\ (j-1)\delta\mu B,\ \cdots,\ -j\delta\mu B$

So the partition function:

$$Z = e^{-j\beta\delta\mu B} + e^{-(j-1)\beta\delta\mu B} + \cdots + e^{+j\beta\delta\mu B}$$

$$= e^{-j\beta\delta\mu B}\left(1 + e^{j\beta\delta\mu B} + \cdots e^{2j\beta\delta\mu B}\right)$$

$$= e^{-j\beta\delta\mu B}\,\frac{1-e^{(2j+1)\beta\delta\mu B}}{1-e^{\beta\delta\mu B}}$$

$$= e^{-bj}\,\frac{1-e^{(2j+1)b}}{1-e^{b}} = e^{-bj}\,\frac{e^{-b/2}(1-e^{(2j+1)b})}{e^{-b/2}-e^{b/2}}$$

$$= \frac{e^{-b(j+\frac{1}{2})}-e^{b(j+\frac{1}{2})}}{e^{-b/2}-e^{b/2}} = \boxed{\frac{\sinh[b(j+\frac{1}{2})]}{\sinh\frac{b}{2}}}$$

c) the average energy of one magnetic particle is

$$\bar{E} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{1}{Z}\frac{db}{d\beta}\frac{dZ}{db}$$

2

$$= -\delta_\mu B\left[(j+\tfrac{1}{2})\coth[b(j+\tfrac{1}{2})] - \tfrac{1}{2}\coth\tfrac{b}{2}\right]$$

The magnetization of N-particle system is:

$$M = -N\frac{\bar{E}}{B} = \boxed{N\delta_\mu\left[(j+\tfrac{1}{2})\coth[b(j+\tfrac{1}{2})] - \tfrac{1}{2}\coth\tfrac{b}{2}\right]}$$

d) $T\to 0$ $\quad b\to\infty$ $\quad \coth[b(j+\frac{1}{2})]\to 1$ $\quad \cot[\frac{b}{2}]\to 1$

2 $M = N\delta_\mu[(j+\frac{1}{2}) - \frac{1}{2}] = \boxed{N\delta_\mu j}$

All N particles are in lowest-energy state as expected.

e) $x \ll 1$

3

$$\coth x = \frac{\cosh x}{\sinh x} = \frac{e^x + e^{-x}}{e^x - e^{-x}} = \frac{(1+x+\frac{1}{2}x^2+\frac{1}{6}x^3)+(1-x+\frac{1}{2}x^3-\frac{1}{6}x^3)}{(1+x+\frac{1}{2}x^2+\frac{1}{6}x^3)-(1-x+\frac{1}{2}x^3-\frac{1}{6}x^3)}$$

$$= \frac{2+x^2}{2x+\frac{1}{3}x^3} = \frac{1}{x}(1+\frac{x^2}{2})(1+\frac{x^2}{6})^{-1} \approx \frac{1}{x}(1+\frac{x^2}{2})(1-\frac{x^2}{6})$$

$$\approx \frac{1}{x}(1+\frac{x^2}{2}-\frac{x^2}{6}) = \frac{1}{x}+\frac{x}{3}$$

When $T\to\infty$ $(j+\frac{1}{2})\coth[b(j+\frac{1}{2})] = \frac{1}{b}[1+\frac{b^2}{3}(j+\frac{1}{2})^2]$

$$\frac{1}{2}\coth[\tfrac{b}{2}] = \frac{1}{b}[1+\frac{b^2}{3}\cdot\frac{1}{4}]$$

$$M \approx N\delta_\mu\left[\frac{1}{b}+\frac{b}{3}(j+\tfrac{1}{2})^2 - \frac{1}{b} - \frac{b}{3}\cdot\frac{1}{4}\right]$$

$$= \frac{N\delta_\mu b}{3}j(j+1) = \boxed{\frac{N\delta_\mu^2 B j(j+1)}{3KT}}$$

f) $j=\frac{1}{2}$ $\quad M = N\delta_\mu[\coth b - \frac{1}{2}\coth(b/2)]$

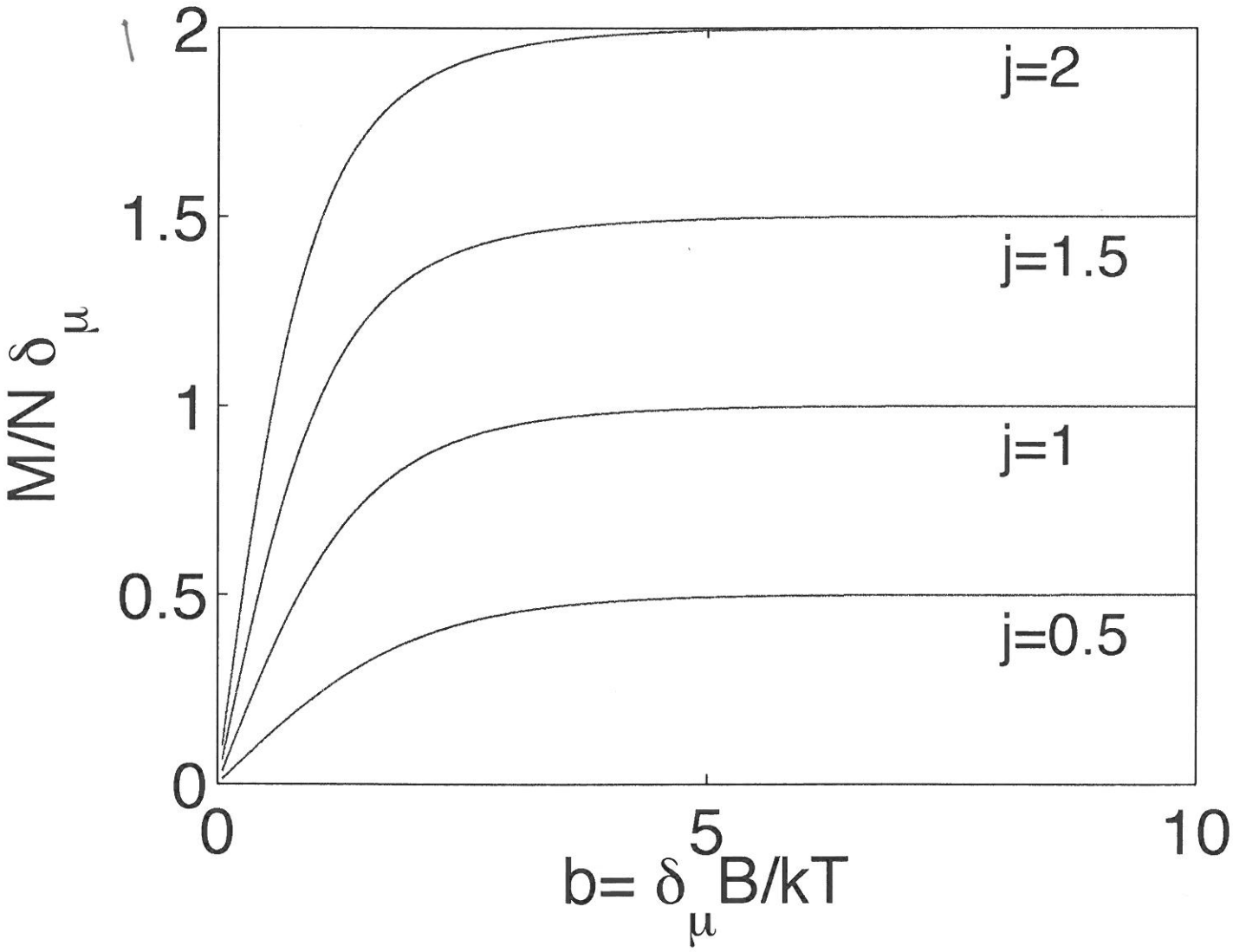
2

$$\frac{M}{N\delta_\mu} = \frac{e^b+e^{-b}}{e^b-e^{-b}} - \frac{1}{2}\frac{e^{b/2}+e^{-b/2}}{e^{b/2}-e^{-b/2}} = \frac{e^b+e^{-b}-\frac{1}{2}(e^{b/2}+e^{-b/2})^2}{e^b-e^{-b}}$$

$$\frac{M}{N\delta_\mu} = \frac{1}{2}\frac{(e^{b/2}-e^{-b/2})^2}{e^b-e^{-b}} = \frac{1}{2}\frac{e^{b/2}-e^{-b/2}}{e^{b/2}+e^{-b/2}} = \frac{1}{2}\tanh\frac{b}{2} \Rightarrow$$

set $\delta_\mu = 2\mu$

$M = N\mu\tanh(\beta\mu B)$


2
1.5
1
0.5
0
0
5
10
M/N δ μ
b= δ μ B/kT
j=2
j=1.5
j=1
j=0.5

6.26. From eq (6.30)

$$Z_{rot} = \sum_{j=0}^{\infty} (2j+1)\, e^{-j(j+1)\epsilon/kT}$$

At $T \to 0$

$$\bar{E} = \sum_{j=0}^{\infty} E(j)\,(2j+1)\,\frac{e^{-\beta\epsilon j(j+1)}}{Z}$$

Only keep the first two terms in $Z$.

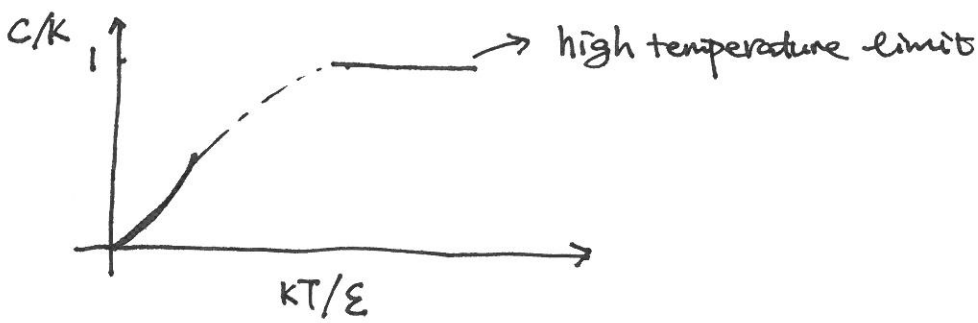
$Z = 1 + 3e^{-2\beta\epsilon}$, then

$$\bar{E} = \sum_{j=0}^{1} E(j)\cdot(2j+1)\,\frac{e^{-\beta\epsilon j(j+1)}}{Z} = \frac{0 + 3\cdot 2\varepsilon\, e^{-2\beta\epsilon}}{1+3e^{-2\beta\epsilon}} \simeq 6\varepsilon e^{-2\beta\varepsilon}$$

$$C = \frac{\partial \bar{E}}{\partial T} = 6\varepsilon\,\frac{\partial(e^{-2\beta\varepsilon})}{\partial\beta}\cdot\frac{\partial\beta}{\partial T}$$

$$= 6\varepsilon\cdot(-2\varepsilon)\,e^{-2\beta\varepsilon}\left(-\frac{1}{kT^2}\right)$$

$$= 3k\left(\frac{2\varepsilon}{kT}\right)^2 e^{-2\varepsilon/kT}$$



6.31 $Z = \sum_q e^{-\beta c|q|} = \frac{1}{\Delta q} \sum_q e^{-\beta c|q|} \Delta q$

8

In the limit $\Delta q \to 0$

$$Z = \frac{1}{\Delta q} \int_{-\infty}^{+\infty} e^{-\beta c|q|} dq = 2 \frac{1}{\Delta q} \int_0^{+\infty} e^{-\beta c q} dq$$

$$= \frac{2}{\beta c \Delta q}$$

$$\bar{E} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\beta c \Delta q}{2}\left(-\frac{2}{\beta^2 c \Delta q}\right) = \frac{1}{\beta} = \boxed{kT}$$

6.37 $\overline{v^2} = \int_0^\infty v^2 D(v)\, dv = \frac{4}{\sqrt{\pi}}\left(\frac{m}{2kT}\right)^{3/2} \int_0^\infty v^4 e^{-mv^2/2kT} dv$

$$= \frac{4}{\sqrt{\pi}}\left(\frac{m}{2kT}\right)^{3/2}\left(\frac{2kT}{m}\right)^{5/2} \int_0^\infty x^4 e^{-x^2} dx = \frac{8kT}{\sqrt{\pi}\, m} \cdot \frac{3\sqrt{\pi}}{8} = \frac{3kT}{m}$$

6.52. The allowed wavelength are

$\lambda_n = \frac{2L}{n}$ $\quad p_n = h/\lambda_n = hn/2L$

$E_n = p_n c = \frac{hcn}{2L}$

$$Z = \sum_n e^{-E_n/kT} = \sum_n e^{-hcn/2LkT}$$

$$= \int_0^\infty e^{-hcn/2LkT} dn = \frac{2LkT}{hc}$$

# Problem 6.30

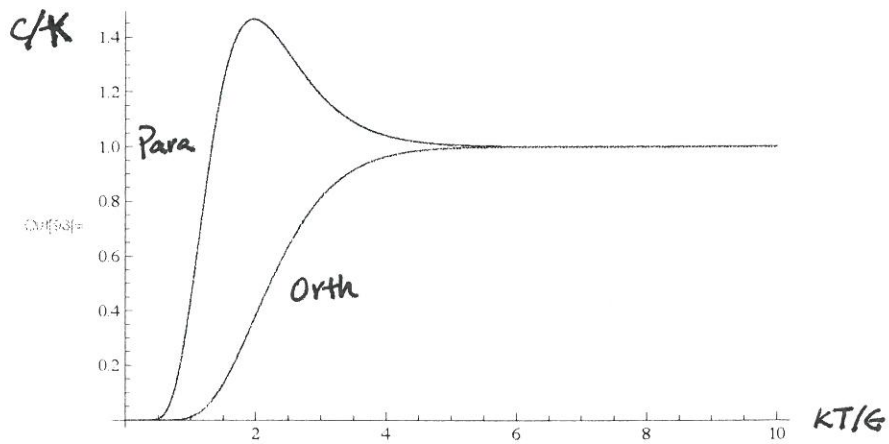
8/8

a)&b) For parahydrogen, only even j are allowed in the partition function. For orthohydrogen, only odd j are allowed.

```
In[87]:= Zpara = Sum[(2 j + 1) Exp[-j (j + 1) * b * epslon], {j, 0, 20, 2}];
         Epara = -(1 / Zpara) * D[Zpara, b] /. b → 1 / (k * T);
         Cpara = Simplify[D[Epara, T] /. T → t * epslon / k];
         Zorth = Sum[(2 j + 1) Exp[-j (j + 1) * b * epslon], {j, 1, 21, 2}];
         Eorth = -(1 / Zorth) * D[Zorth, b] /. b → 1 / (k * T);
         Corth = Simplify[D[Eorth, T] /. T → t * epslon / k];
         Plot[{Cpara / k, Corth / k}, {t, .001, 10}, PlotRange → Full]
```

2

Out[93]=

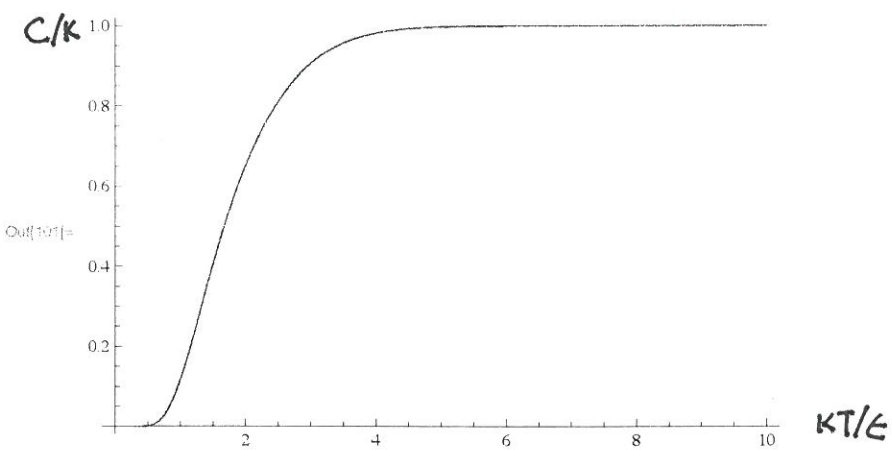



c) Normal gas is a mixture of 1/4 parahydrogen and 3/4 orthohydrogen.

```
In[100]:= Cnormal = .25 Cpara + .75 Corth;
          Plot[Cnormal / k, {t, .001, 10}, PlotRange → Full]
          FindRoot[Cnormal / k = .5, {t, 1.5, 2}]
```

2

Out[101]=



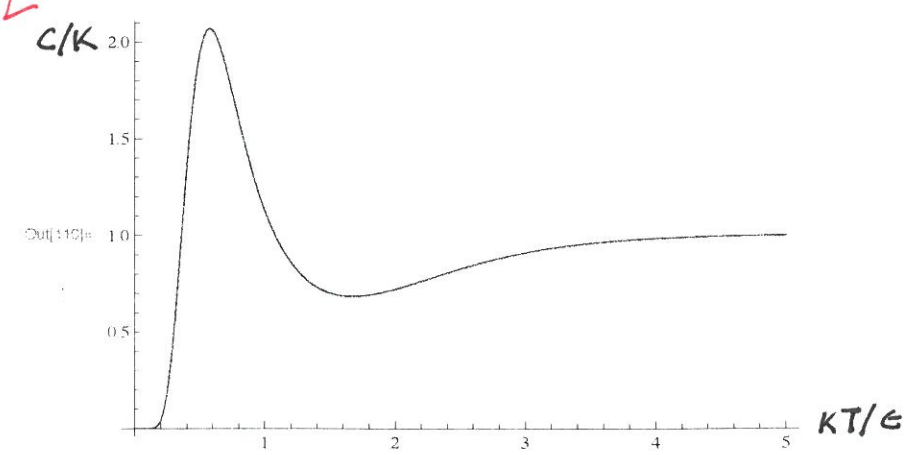

Out[102]= {t → 1.66924}

At t = kT/$\epsilon$=1.66924, $\epsilon$=0.0076eV, T = 150K, the heat capacity reaches half its asymptotic value.

d) Redefine the partition function under equilibrium:

```
In[102]:= Zequil = Zpara + 3 * Zorth;
          Eequil = -(1 / Zequil) * D[Zequil, b] /. b → 1 / (k * T);
          Cequil = Simplify[D[Eequil, T] /. T → t * epslon / k];
          Plot[Cequil / k, {t, .001, 5}, PlotRange → Full]
```

2




e) The deuterium we can calculate the heat capacity as a mixure of 2/3 ortho and 1/3 para

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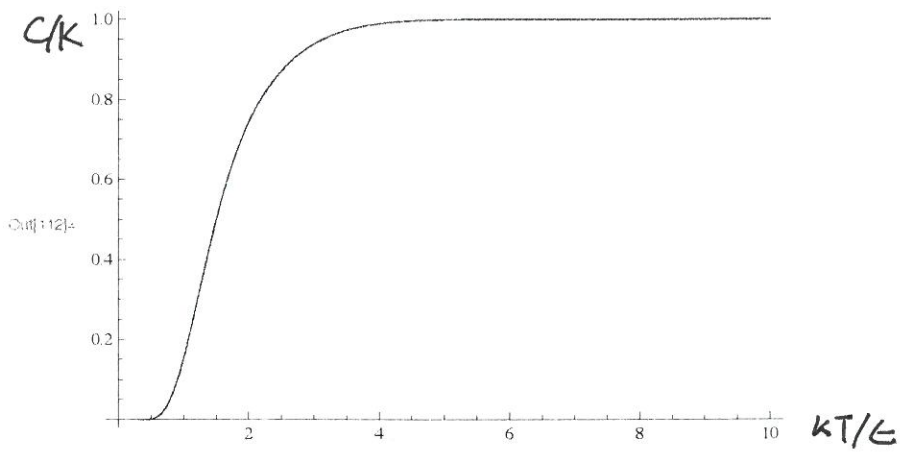
```
In[113]:= Cdeut = 2 / 3 * Corth + 1 / 3 * Cpara;
          Plot[Cdeut / k, {t, .001, 10}, PlotRange → Full]
```

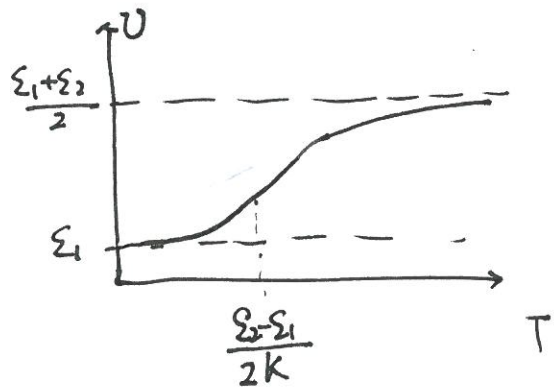


Additional Problem 2.

~~6-30~~ 8/8

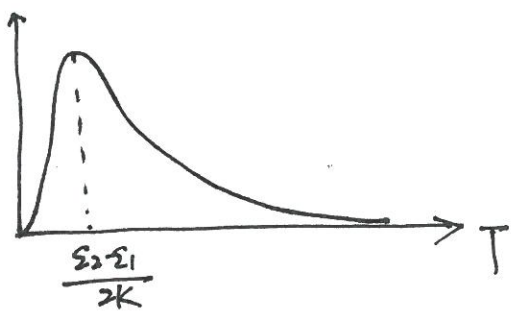
a) At low temperature, all particles are in lower energy state.

3 At high temperature, the difference between two states become insignificant. The particles are evenly distributed on two states.




b) C

2




c) $Z = e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2}$

3 $$\bar{E} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{\varepsilon_1 e^{-\beta\varepsilon_1} + \varepsilon_2 e^{-\beta\varepsilon_2}}{e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2}}$$

$$= \varepsilon_1 \cdot \frac{1}{1+e^{-\beta\Delta\varepsilon}} + \varepsilon_2 \frac{1}{1+e^{\beta\Delta\varepsilon}} \qquad \Delta\varepsilon = \varepsilon_2 - \varepsilon_1$$

$$C = \frac{\partial \bar{E}}{\partial T} = \frac{\partial \beta}{\partial T}\cdot\frac{\partial \bar{E}}{\partial \beta} = -\frac{1}{KT^2}\left[\frac{\varepsilon_1 \Delta\varepsilon e^{-\beta\Delta\varepsilon}}{(1+e^{-\beta\Delta\varepsilon})^2} - \frac{\varepsilon_2 \Delta\varepsilon e^{+\beta\Delta\varepsilon}}{(1+e^{\beta\Delta\varepsilon})^2}\right]$$

$$= \frac{\Delta\varepsilon^2}{4\cosh\left(\frac{\beta\Delta\varepsilon}{2}\right)^2 KT^2}$$