Assignment 3

2018113003

Q1)

→ Given: temp = T

$\varepsilon_0 = -\mu H,\ \varepsilon_1 = \mu H$

No of particles : N

Magnetic field : $\bar{H}$

To find: U, C_v

$$\Rightarrow U = \left(\frac{-\partial \ln Q}{\partial \beta}\right) = -\frac{1}{Q}\frac{\partial Q}{\partial \beta}$$ → for a single particle

∴ For N particles

$$U = -\frac{N}{Q}\frac{\partial Q}{\partial \beta}$$

For a particle

$$Q = \sum d_i e^{-\beta \varepsilon_i}$$

$$\Rightarrow Q = e^{-\beta\varepsilon_0} + e^{-\beta\varepsilon_1}$$

$$\therefore \frac{\partial Q}{\partial \beta} = -\varepsilon_0 e^{-\beta\varepsilon_0} - \varepsilon_1 e^{-\beta\varepsilon_1}$$

$$U = \frac{-N}{Q}\left(-(-\mu H)e^{+\beta\mu H} - (\mu H)e^{-\beta\mu H}\right)$$

$$= N\mu H\left(\frac{e^{-\beta\mu H} - e^{+\beta\mu H}}{e^{-\beta\mu H} + e^{\beta\mu H}}\right)$$

$$= -N\mu H \tanh(+\beta\mu H) \qquad \left(\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}\right)$$

$$\therefore\ U = -N\mu H \left(\tanh\left(\frac{\mu H}{k_B T} \right) \right)$$

$$C_V = -k_B \beta^2 \frac{\partial U}{\partial \beta}$$

$$\frac{\partial U}{\partial \beta} = \frac{\partial}{\partial \beta} \left(-N\mu H \tanh\left(\frac{\mu H \beta}{\cancel{k}} \right) \right)$$

$$= -N\mu H \left(\frac{\partial}{\partial \beta} \left(\frac{e^{2\beta\mu H} - 1}{e^{2\beta\mu H} + 1} \right) \right)$$

$$= -N\mu H \left(\frac{2\mu H (e^{2\beta\mu H} + 1) - 2\beta\mu H (e^{2\beta\mu H} - 1)}{(e^{2\beta\mu H} + 1)^2} \right)$$

$$= -N\mu H \left(\frac{2\mu H (2)}{(e^{2\beta\mu H} + 1)^2} \right)$$

$$= \frac{-4N\mu^2 H^2}{(e^{2\beta\mu H} + 1)^2}$$

$$\frac{\partial U}{\partial \beta} = -N\mu H \frac{\partial}{\partial \beta} \tanh(\beta\mu H)$$

$$= -N\mu H \left[\operatorname{sech}^2 \beta\mu H \right] \mu H$$

$$= -N(\mu H)^2 \operatorname{sech}^2 (\beta\mu H)$$

$$= -N(\mu H \operatorname{sech} \beta\mu H)^2$$

$$= -N\left(\mu H \operatorname{sech} \mu H / k_B T \right)^2$$

DELUXE
PAGE NO.:
DATE:

$$C_V = -k_B\left(\frac{1}{k_BT}\right)^2\left(-N\left(\mu H\,\mathrm{sech}\left(\mu H/k_BT\right)\right)^2\right)$$

$$= \frac{Nk_B}{k_B^2}\left(\frac{\mu H}{T}\,\mathrm{sech}\left(\mu H/k_BT\right)\right)^2$$

$$C_V = N/k_B\left(\frac{\mu H}{T}\,\mathrm{sech}\left(\frac{\mu H}{k_BT}\right)\right)^2$$

Q2)

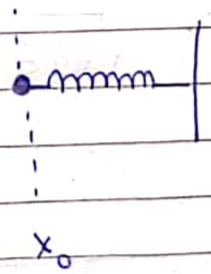
→ ~~Given: Single particle oscillator, Fregence v: Frequency : v=~~

Q2)

→ Given: Single particle oscillator, Frequency : ν
To find: $\Gamma_0(\mathcal{E})$, No of quantum states $\Omega_0(\mathcal{E})$ with Energy $\leq \mathcal{E}$

⇒ Let us take a 1D oscillator

$$q = A\sin(\omega t)$$
$$p/m = A\omega\cos(\omega t)$$



$$\therefore \frac{q^2}{A^2} + \frac{p^2}{A^2\omega^2 m^2} = 1$$

$$q^2 + \frac{p^2}{m^2\omega^2} = A^2$$

ω — used for frequency

$$\mathcal{E} = \frac{1}{2} kA^2$$

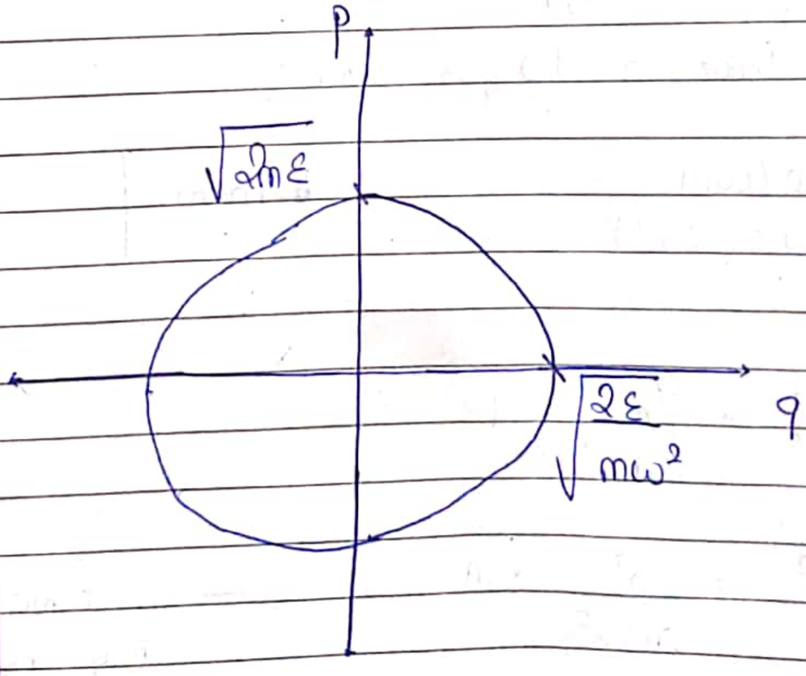
$$\therefore A^2 = \frac{2\mathcal{E}}{k}$$

$$\therefore q^2 + \frac{p^2}{m^2\omega^2} = \frac{2\mathcal{E}}{k}$$

$$\omega^2 = \frac{k}{m} \qquad k = m\omega^2$$

$$\Rightarrow q^2 + \frac{p^2}{m^2\omega^2} = \frac{2\mathcal{E}}{m\omega^2}$$

$$\frac{q^2}{\left(\frac{2\mathcal{E}}{m\omega^2}\right)} + \frac{p^2}{\left(2m\mathcal{E}\right)} = 1$$



To find: $\Gamma_0(\mathcal{E})$: Volume in phase space with Energy $< \mathcal{E}$

For a 2-D curve, $\Gamma_0(\mathcal{E}) \equiv$ Area under phase space

$$\therefore \Gamma_0(\mathcal{E}) = 4\int_0^{x_p} p(q)\,dq$$

$$p(q) = \pm\left(2m\mathcal{E}\right)^{1/2}\left[1 - \frac{q^2}{\left(\frac{2\mathcal{E}}{m\omega^2}\right)}\right]^{1/2} ; \quad x_p = \sqrt{\frac{2\mathcal{E}}{m\omega^2}}$$

in the Quadrant I

p, q — $+, +$

$$\therefore p(q) = \left(2m\mathcal{E}\right)^{1/2}\left(1 - \frac{q^2}{\left(\frac{2\mathcal{E}}{m\omega^2}\right)}\right)^{1/2}$$

$$\therefore \Gamma_0(\mathcal{E}) = 4\int_0 p(q)\,dq$$

$$= 4\left(2m\mathcal{E}\right)^{1/2}\int\left(1 - \frac{q^2}{2\mathcal{E}/m\omega^2}\right)^{1/2} dq$$

q ~~x~~ $q = \sqrt{\frac{2\mathcal{E}}{m\omega^2}}\,\sin x$

$$\therefore dq = \sqrt{2\mathcal{E}/m\omega^2}\,\cos x\,dx$$

$$T_0(\mathcal{E}) = 4\left(2m\mathcal{E}\right)^{1/2}\int_0^{x_t} \cancel{\sin} \cos x \left(\sqrt{\frac{2\mathcal{E}}{m\omega^2}}\cos x\,dx\right)$$

$$= 4\left(2m\mathcal{E}\left(\frac{2\mathcal{E}}{\cancel{m}\omega^2}\right)\right)^{1/2}\int_0^{\pi/2}\cos^2 x\,dx$$

$$= 4\left(\frac{4\mathcal{E}^2}{\omega^2}\right)^{1/2}\int_0^{\pi/2}\cos^2 x\,dx$$

$$= 8\mathcal{E}/\omega \int_0^{\pi/2}\cos^2 x\,dx$$

$$= \frac{8\mathcal{E}}{\omega}\int_0^{\pi/2}\left(\frac{\cos 2x + 1}{2}\right)dx$$

$$= \frac{4\mathcal{E}}{\omega}\left(\frac{\sin 2x}{2} + x\right)\Bigg|_0^{\pi/2}$$

$$= \frac{4\mathcal{E}}{\omega}\left(\pi/2\right)$$

$$T_0(\mathcal{E}) = \frac{2\pi\mathcal{E}}{\omega}$$

To find $\Omega(\mathcal{E}) \rightarrow$ No of quantum states with Energy $< \mathcal{E}$

For QM Harmonic oscillator

$\mathcal{E} = \hbar\omega(n + 1/2)$; $\Omega(\mathcal{E}) = n \Rightarrow \Omega(\mathcal{E}) = \frac{2\pi\mathcal{E}}{h\omega} - 1/2$

$\therefore$ At large Energies

$$\Omega(\mathcal{E}) \sim \frac{I_0(\mathcal{E})}{h} \qquad \left[\lim_{\mathcal{E}\to\infty} \Omega(\mathcal{E}) = \frac{2\pi\mathcal{E}}{h\omega} = \frac{I_0(\mathcal{E})}{h} \right.$$

Q3) $\rightarrow$ To show : $\overline{(\mathcal{E}-U)^2} = k_B T^2 C_V$,

$$\overline{(\mathcal{E}-U)^3} = k_B^2 \left\{ T^4 \left(\frac{\partial C_V}{\partial T}\right)_V + 2T^3 C_V \right\}$$

i) Proof of $\overline{(\mathcal{E}-U)^2} = k_B T^2 C_V$

$$\mathcal{E} = \sum \mathcal{E}_j, \; U = \sum \mathcal{E}_j e^{-\beta\mathcal{E}_j} \equiv \bar{\mathcal{E}}, \; \&$$
$$P_j = e^{-\beta\mathcal{E}_j}/Q$$

$$\Rightarrow U = \sum \mathcal{E}_j P_j \equiv \bar{\mathcal{E}}$$

$$\therefore \overline{(\mathcal{E}-U)^2} = \overline{(\mathcal{E}-\bar{\mathcal{E}})^2} \equiv \sigma_{\mathcal{E}}^2$$

$$\mathrm{Var}(\mathcal{E}) = \bar{\mathcal{E}^2} - \bar{\mathcal{E}}^2$$
$$= \sum \mathcal{E}^2 P_j - U^2$$
$$= \sum \mathcal{E}_j^2 \frac{e^{-\beta\mathcal{E}_j}}{Q} - \left(\sum \mathcal{E}_j \frac{e^{-\beta\mathcal{E}_j}}{Q}\right)^2$$

$$\mathrm{Var}(\mathcal{E}) = \frac{\sum \mathcal{E}_j^2 e^{-\beta\mathcal{E}_j}}{Q} - U^2$$

$$= -\frac{1}{Q} \frac{\partial}{\partial\beta} \left(\sum \mathcal{E}_j e^{-\beta\mathcal{E}_j} \right) - U^2$$

PAGE NO. :
DATE:

$$= -\frac{1}{\phi}\left[\frac{\partial}{\partial\beta}\left(\varepsilon U \phi\right)\right] - U^2$$

$$= -\frac{1}{\phi}\left[\phi\frac{\partial U}{\partial\beta} + U\frac{\partial\phi}{\partial\beta}\right] - U^2$$

$$= -\frac{\partial U}{\partial\beta} - U\left(\frac{1}{\phi}\frac{\partial\phi}{\partial\beta}\right) - U^2$$

$$= -\frac{\partial U}{\partial\beta} + U^2 - U^2 \qquad \left(U = -\frac{1}{\phi}\frac{\partial\phi}{\partial\beta}\right)$$

$$= -\frac{\partial U}{\partial\beta}$$

$$C_V = -k_B\beta^2\frac{\partial U}{\partial\beta}$$

$$\therefore k_B T^2 C_V = -\frac{\partial U}{\partial\beta} \equiv Var(\varepsilon)$$

$$\Rightarrow \overline{(\varepsilon - U)^2} = k_B T^2 C_V$$

ii) $\overline{(\varepsilon - U)^3} = k_B^2\left\{T^4\left(\frac{\partial C_V}{\partial T}\right)_V + 2T^3 C_V\right\}$

$$LHS = \overline{(\varepsilon - U)^3}$$

$$= \overline{(\varepsilon^3 - U^3 - 3U\varepsilon^2 + 3U^2\varepsilon)}$$

$$= (\overline{\varepsilon^3}) - U^3 - 3U(\overline{\varepsilon^2}) + 3U^2\bar{\varepsilon}$$

$$= (\overline{\varepsilon^3}) - U^3 - 3U\left(k_B T^2 C_V + U^2\right) + 3U^2(U)$$

$$= (\overline{\varepsilon^3}) - U^3 - 3U k_B T^2 C_V - \cancel{3U^3} + \cancel{3U^3}$$

DELUXE PAGE NO.: DATE:

$$\therefore \overline{(\varepsilon - U)^3} = \overline{(\varepsilon^3)} - U^3 - 3U k_B T^2 C_V$$

$$= \overline{(\varepsilon^3)} - U^3 - 3k_B T^2 \left(UC_V\right)$$

$$\overline{(\varepsilon^3)} = \frac{\sum \varepsilon_j^3 e^{-\beta\varepsilon_j}}{\phi}$$

$$= -\frac{1}{\phi}\frac{\partial}{\partial\beta}\left(\sum \varepsilon_j^2 e^{-\beta\varepsilon_j}\right)$$

$$= -\frac{1}{\phi}\frac{\partial}{\partial\beta}\left(\frac{-\partial}{\partial\beta}\left(\sum \varepsilon_j e^{-\beta\varepsilon_j}\right)\right)$$

$$= +\frac{1}{\phi}\frac{\partial}{\partial\beta}\left(\frac{\partial}{\partial\beta}\left(U\phi\right)\right)$$

$$= \frac{1}{\phi}\frac{\partial}{\partial\beta}\left(U\frac{\partial\phi}{\partial\beta} + \phi\frac{\partial U}{\partial\beta}\right)$$

$$= \frac{1}{\phi}\left(\frac{\partial U}{\partial\beta}\frac{\partial\phi}{\partial\beta} + U\frac{\partial^2\phi}{\partial\beta^2} + \frac{\partial\phi}{\partial\beta}\frac{\partial U}{\partial\beta} + \phi\frac{\partial^2 U}{\partial\beta^2}\right)$$

$$= \frac{1}{\phi}\left[U\frac{\partial^2\phi}{\partial\beta^2} + 2\frac{\partial\phi}{\partial\beta}\frac{\partial U}{\partial\beta} + \phi\frac{\partial^2 U}{\partial\beta^2}\right]$$

$$= \frac{U}{\phi}\frac{\partial^2\phi}{\partial\beta^2} + 2\left(\phi\,{}^1\!/_{\phi}\frac{\partial\phi}{\partial\beta}\right)\frac{\partial U}{\partial\beta} + \phi\frac{\partial^2 U}{\partial\beta^2}$$

$$= U/\phi\left(\frac{\partial}{\partial\beta}\left(-U\phi\right)\right) \mp 2U\left(\frac{\partial U}{\partial\beta}\right) + \frac{\partial}{\partial\beta}\left(\frac{\partial U}{\partial\beta}\right)$$

$$(\overline{\varepsilon^3}) = \mp U^2/\phi\left(\frac{\partial\phi}{\partial\beta}\right) \mp U\frac{\partial U}{\partial\beta} \mp 2U\left(\frac{\partial U}{\partial\beta}\right) + \frac{\partial}{\partial\beta}\left(\frac{\partial U}{\partial\beta}\right)$$

$$C_V = -k_B\beta^2\frac{\partial U}{\partial\beta}$$

$$\frac{\partial U}{\partial\beta} = -\frac{C_V}{k_B\beta^2}$$

$$\Rightarrow (\overline{\varepsilon^3}) = \pm U^3 + \frac{3C_V U}{k_B\beta^2} + \frac{\partial}{\partial\beta}\left(\frac{\partial U}{\partial\beta}\right)$$

$$\therefore \overline{(\varepsilon-U)^3} = (\overline{\varepsilon^3}) - U^3 - 3k_BT^2(UC_V)$$

$$= \cancel{U^3} + \cancel{3(C_VU)\left(\frac{k_B^2T^2}{k_B}\right)} - \cancel{3k_BT^2(UC_V)} + \frac{\partial^2 U}{\partial\beta^2} - \cancel{U^3}$$

$$\overline{(\varepsilon-U)^3} = \frac{\partial^2 U}{\partial\beta^2} \qquad \left[\frac{\partial f}{\partial\beta} = \frac{\partial f}{\partial T}\frac{\partial T}{\partial\beta}\right]$$

$$= \frac{\partial}{\partial\beta}\left(\frac{-C_V}{k_B\beta^2}\right) \qquad \left[\frac{\partial T}{\partial\beta} = \frac{\partial}{\partial\beta}\left(\frac{1}{k_B\beta}\right) = -k_BT^2\right]$$

$$= +k_BT^2\frac{\partial}{\partial T}\left(+C_V k_BT^2\right)$$

$$= k_B T^2 \left[\frac{\partial}{\partial T}\left(k_B T^2 C_V\right)\right]$$

$$= k_B T^2 \left[k_B\left(2TC_V + \cancel{k_B}T^2\left(\frac{\partial C_V}{\partial T}\right)\right)\right]$$

$$= k_B^2\left[T^4\left(\frac{\partial C_V}{\partial T}\right)_V + 2T^3 C_V\right]$$

$$= \underline{\underline{RHS}}$$

$$\therefore \overline{(E-U)^3} = k_B^2\left\{T^4\left(\frac{\partial C_V}{\partial T}\right)_V + 2T^3 C_V\right\}$$

Q4) →

$$\mathcal{H} = -\mu_B \bar{\sigma}\cdot\bar{H};$$

$\bar{\sigma}$ → pauli spin operator

μ_B → Bohr magneton

i) Density matrix in the diagonalized representation of σ_z

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Results for ideal monoatomic gas:

Known : $U = \frac{3}{2} N k_B T$

$$C_V = -k_B \beta^2 \frac{\partial U}{\partial \beta}$$

$$= \frac{+\cancel{k_B}}{\cancel{k_B^2 T^2}} \cancel{k_B T^2} \frac{\partial U}{\partial T}$$

$$= \frac{3}{2} N k_B$$

$$\therefore \overline{(\mathcal{E}-U)^2} = k_B T^2 \left(\frac{3}{2} N k_B \right)$$

$$\Rightarrow \frac{\overline{(\mathcal{E}-U)^2}}{U^2} = \frac{\cancel{k_B T^2} \left(\cancel{\frac{3}{2}} \cancel{N k_B} \right)}{\left(\frac{3}{2} N k_B \right)^{\cancel{2}} \cancel{T^2}}$$

$$= \frac{2}{3N}$$

For a monoatomic gas

$$\left(\frac{\partial C_V}{\partial T} \right)_V = 0$$

$$\therefore \overline{(\mathcal{E}-U)^3} = 2 k_B^2 T^3 \left(\frac{3}{2} N k_B \right)$$

$$\Rightarrow \frac{\overline{(\mathcal{E}-U)^3}}{U^3} = \frac{2 \cancel{k_B^3} \cancel{T^3} \cancel{N} \left(\cancel{\frac{3}{2}} \right)}{\left(\cancel{\frac{3}{2}} \right) \left(\frac{3}{2} \right)^2 (N \cancel{k_B T})^{\cancel{3}\, 2}} = \frac{8}{9N^2}$$

$\overline{(\mathcal{E}-U)^n}$ quantifies fluctuation of Energy from the mean.

$\Rightarrow$ $\dfrac{\overline{(\mathcal{E}-U)^n}}{U^n}$ quantifies the relative spread of fluctuation with respect to U as:

$$\frac{\overline{(\mathcal{E}-U)^n}}{U^n} = \overline{\left(\frac{\mathcal{E}-U}{U}\right)^n},$$

which from the trend observed is:

$$\overline{\left(\frac{\mathcal{E}-U}{U}\right)^n} \propto 1/N^{n-1}$$

This means that any moment of relative fluctuation is inversely related to amount of particles

$\Rightarrow$ Less the amount of particles, higher the fluctuation of Energy, and vice versa.

Q4)

→ $H = -\mu_B \bar{\sigma} . \bar{H}$;

μ_B → Bohr magneton
σ → Pauli spin operator

Feild is taken along z axis

$\therefore \bar{H} = H_0 \hat{z} \hat{k}$
$\bar{\sigma} = \sigma_x \hat{i} + \sigma_y \hat{j} + \sigma_z \hat{k}$

$\therefore H = -\mu_B \left(\bar{\sigma} . \bar{H} \right)$

$= -\mu_B H_0 \sigma_z$

$\Rightarrow H = -\mu_B H_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$;

$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\therefore$ For the basis $|\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ & $|\psi_1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$H|\psi_0\rangle = +|\psi_0\rangle \mathcal{E}$ $\qquad \mathcal{E} = -\mu_B H_0$
$H|\psi_1\rangle = -|\psi_1\rangle \mathcal{E}$

$\therefore \mathcal{E}_0 = +1\mathcal{E}, \ \mathcal{E}_1 = -1\mathcal{E}$

$\therefore \mathcal{Z} = \sum e^{-\beta \mathcal{E}_j} = e^{-\beta\mathcal{E}} + e^{\beta\mathcal{E}}$

$$\rho = \frac{1}{Q}\begin{pmatrix} e^{-\beta\varepsilon} & 0 \\ 0 & e^{\beta\varepsilon} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{e^{-\beta\varepsilon}}{e^{-\beta\varepsilon}+e^{\beta\varepsilon}} & 0 \\ 0 & \dfrac{e^{\beta\varepsilon}}{e^{-\beta\varepsilon}+e^{\beta\varepsilon}} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{1}{1+e^{2\beta\varepsilon}} & 0 \\ 0 & \dfrac{1}{1+e^{-2\beta\varepsilon}} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{1}{1+e^{2\beta(\mu_0 H)}} & 0 \\ 0 & \dfrac{1}{1+e^{-2\beta(\mu_0 H)}} \end{pmatrix}$$

OR :

$$\rho = \frac{1}{2\cosh(\beta\mu_0 H)}\begin{pmatrix} e^{+\mu_0 H\beta} & 0 \\ 0 & e^{-\mu_0 H\beta} \end{pmatrix}$$

$$\bar{M} = Tr\left(\hat{M}^{*}\hat{\rho}\right)$$

$$\bar{\sigma}_z = Tr\left(\hat{\sigma}_z\hat{\rho}\right)$$

$$= Tr\left(\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}e^{\beta\mu_0 H} & 0\\ 0 & e^{-\beta\mu_0 H}\end{pmatrix}\right)\left(\frac{1}{\phi}\right)$$

$$= \frac{1}{\phi}\, Tr\begin{pmatrix}e^{\beta\mu_0 H} & 0\\ 0 & -e^{-\beta\mu_0 H}\end{pmatrix}$$

$$= \frac{1}{\phi}\left(e^{\beta\mu_0 H} - e^{-\beta\mu_0 H}\right)$$

$$= \frac{e^{\beta\mu_0 H} - e^{-\beta\mu_0 H}}{e^{\beta\mu_0 H} + e^{-\beta\mu_0 H}}$$

$$= \tanh\left(\beta\mu_0 H\right)$$