Theoretical Statistical Physics

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## Mathematics

Normalization condition:
$\int_{\mathbb{R}^3} f_{(\vec{x})} d\vec{x} = 1$

Spherical coordinates:
$(0 \le \phi \le 2\pi; 0 \le \theta \le \pi)$
$x = r\cos(\phi)\sin(\theta); y = r\sin(\phi)\sin(\theta);$
$z = r\cos(\theta); |J| = r^2\sin(\theta)$

Sphere volume in n dimensions:
$V_{B_{n(r)}} = \frac{(r\sqrt{\pi})^n}{\Gamma(\frac{n}{2}+1)}$

Ellipse:
$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1; x_{(t)} = a\cos(t) \wedge y_{(t)} = b\sin(t)$

Binomial coefficient:
$\binom{N}{k} = \frac{N!}{k!(N-k)!}$

Variance:
$\sigma_x = \langle (x-\langle x\rangle^2)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$

Gaussian integral:
$\int_{-\infty}^{\infty} e^{-a(x-b)^2}dx = \sqrt{\frac{\pi}{a}}$

Gamma-Function:
$N! = \Gamma_{(N+1)} = \int_0^\infty e^x x^N dx$

Logarithm inequality:
$x\ln(x) \ge x-1$ ($x\ln(x)$ convex, $x-1$ tangent)

Taylor approximations:
$\tanh(x) = x - \frac{x^3}{3} + \mathcal{O}_{(x^5)}$

Stirling-approximation:
$N! \approx N^N e^{-N}\sqrt{2\pi N}\forall i \neq j$
$\ln(N!) \approx N\ln(N) - N \approx N\ln(N)$

Laplace-method:
$\int_a^b f_{(x)} e^{-Ng_{(x)}}dx \approx e^{-Ng_{(x_0)}} f_{(x_0)} \sqrt{\frac{2\pi}{N g''_{(x_0)}}}$ for $N\to\infty$ if $g_{x_0}$ is the minimum value of the function in the interval $[a,b]$, i. e.
$g'_{(x_0)} = 0 \wedge g''_{(x_0)} > 0 \wedge g_{(x_0)} = \min_{x\in[a,b]}(g_{(x)})$

Legendre transform:
$f^*_{(u)} = \sup_x(ux - f_{(x)})$, convex functions yield convex transforms, analogously for concaves.

Taylor expansion around $a$:
$f_{(x)} \approx$
$f_{(a)} + f'_{(a)}(x-a) + \frac{f''_{(a)}}{2!}(x-a)^2 + \frac{f'''_{(a)}}{3!}(x-a)^3$

Jacobian matrix:
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots \\ \frac{\partial f_2}{\partial x_1} & \ddots & \\ \vdots & & \end{pmatrix}$$

ODE-Ansätze:
$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{n}{x}y \Rightarrow y = Cx^n$

Curvature:
$f_{(a,b,c,...)}$ convex in $a \Leftrightarrow \frac{\partial^2 f}{\partial a^2} > 0$,
concave $\Leftrightarrow \frac{\partial^2 f}{\partial a^2} < 0$

Absolute differential:
$df_{(a,b,c,...)} = \frac{\partial f}{\partial a}da + \frac{\partial f}{\partial b}db + \frac{\partial f}{\partial c}dc + ...$

Analytic function:
$f_{(x,y,...)}$ analytic function of $x \Leftrightarrow$ Can locally be approximated by power series.
Compositions of analytic functions are always analytic.

## Differential forms

Differential form:
$\mu = f_{2(x_1,...,x_n)}dx_2 + f_{2(x_1,...,x_n)}dx_2 + ...f_{n(x_1,...,x_n)}dx_n$

Exactness:
$\mu$ exact $\Leftrightarrow \frac{\partial f_i}{\partial x_j} = \frac{\partial f_j}{\partial x_i}$. Falsify by showing this doesn't hold.
$\mu$ exact
$\Leftrightarrow \exists\phi : \mu = d\phi = \frac{\partial\phi}{\partial x_1}dx_1 + ... + \frac{\partial \phi}{\partial x_n}dx_n$. Show exactness by finding $\phi$.

Integrating factor:
$g$ is integrating factor $\Leftrightarrow g\nu$ exact for $\nu$ inexact. Find by guessing, or system of linear equations demanding exact summand product $g\nu$.

Solve ODE with integrating factor:
$\nu = 0 \leftrightarrow g\nu = 0$, arithmetically reorder to solvable form by treating $dx, dy...$ as variables and use $\frac{dy}{dx} = y'$.

Differential theorems::
$\left(\frac{\partial x}{\partial y}\right)_w \left(\frac{\partial y}{\partial z}\right)_w = \left(\frac{\partial x}{\partial z}\right)_w$
$\left(\frac{\partial y}{\partial x}\right)_z = \frac{1}{\left(\frac{\partial x}{\partial y}\right)_z}$
$\left(\frac{\partial x}{\partial y}\right)_z\left(\frac{\partial y}{\partial z}\right)_x\left(\frac{\partial z}{\partial x}\right)_y = -1$

## Matrices

Pauli matrices:
$\sigma_0 = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}; \sigma_1 = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}; \sigma_2 = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix};$
$\sigma_1 = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$

Density operator:
$\rho^\dagger = (\rho^T)^* = \rho; \mathrm{tr}(\rho) = 1; \rho \ge 0 \Leftrightarrow$ Alle Eigenwerte $\ge 0$

Dens. op. for pure state:
$\rho = |\psi\rangle\langle\psi| \Rightarrow \rho^2 = \rho$

Dens. op. for mixed state:
$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

Other:
Trace is basis independent.
$\mathrm{tr}(AB) = \mathrm{tr}(BA);$
$\mathrm{tr}(ABC) = \mathrm{tr}(CAB) = \mathrm{tr}(BCA);$
$\det(\exp(A)) = \exp(\mathrm{tr}(A))$ (for $A\in\mathbb{C}^{n\times n}$)
$\ln(\det(M)) = \mathrm{tr}(\ln(M))$

## Thermodynamics

First law of thermodynamics:
$\Delta U = \Delta Q - \Delta W$
$dU = C_V dT + \left(\frac{\partial U}{\partial V}\right)_T dV$

Gibbs fundamental relation:
$dU = TdS - pdV$

Work of quasistatic adiabatic change:
$W_{12} = -\int_{V_1}^{V_2} P_{(V)}dV$

Closed loop in PV-diag.:
$\Delta U = 0$

Isochoric process:
$\Delta W = 0$

Isobaric process:
$\Delta P = 0; \Delta W = P\Delta V$

Adiabatic process:
$\Delta Q = 0$

Differential Form of heat:
$\Delta Q = \underbrace{T}\, dS$
$dQ = cdT$

Differential form of entropy:
$dS = \frac{\delta Q}{T} = C_V\frac{dP}{P} + C_P\frac{dV}{V}$
$dS = \frac{\omega}{T} = C_V\frac{dT}{T} + \nu R\frac{dV}{T}$. To get $\Delta S$ integrate, $\Delta S$s are additive.

Maxwell relations:
$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V; \left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p;$
$\left(\frac{\partial V}{\partial T}\right)_p = -\left(\frac{\partial S}{\partial p}\right)_T; \left(\frac{\partial p}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T$

Thermodynamic potentials with [Natural Variables]:
Int. en.:
$U = \int\left(TdS - pdV + \sum_i \mu_i dN_i\right) \quad [S, V]$
Free energy: $F = U - TS \quad [T,V]$
Enthalpy: $H = U + pV \quad [S,p]$
Gibbs energy: $G = U + pV - TS \quad [T,p]$
Grand pot.:
$\Omega = \Phi_G = U - TS - \sum_i\mu_i N_i \quad [T,V]$

To show that $Y$ is a therm. pot. with nat. vars. $\alpha$ and $\beta$ show that $dY = ad\alpha + bd\beta$

Specific heat:
$C_V = \left(\frac{\partial U}{\partial T}\right)_V$

Volume dependence of $U$:
$\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial p}{\partial T}\right)_V - p$

Quasistatic adiabatic process of ideal gas:
$pV^{\frac{C_P}{C_V}} \equiv pV^\kappa$ = const.

Ideal gas law:
$pV = \nu RT = Nk_BT = \frac{N}{\beta}$

Van-der-Waals gas:
$p = \frac{nRT}{V-nb} - \frac{n^2a}{V^2}$

Aproximation for liquids:
$C_V \approx C_P$ (because almost no thermal expansion)

Efficiency of an engine:
General: $\eta = \frac{W}{Q}$
Otto: $\eta = 1 - \left(\frac{V_{min}}{V_{max}}\right)^{\kappa-1} = 1 - \frac{T_1}{T_2}$
Carnot (Maximum): $\eta = 1 - \frac{T_C}{T_H}$

Waste heat of generator:
$P_Q = P_{tot} - P_{use} = P_{use}(\frac{1}{\eta}-1) = P_{tot}(1-\eta)$

Temperature baths connected by carnot engine:
$T_f = \sqrt{T_1^iT_2^i}$
$W = c\left(\sqrt{T_1^i} - \sqrt{T_2^i}\right)^2$

Temperature change from mass flux:
$\Delta T = \frac{P}{\dot{M}c_P}$

Maxwell-Distribution:
Dist. $w_{(E)} = \mathcal{N}e^{-\beta E} = \mathcal{N}e^{-\frac{E}{k_BT}}$; Mean vel.
$\bar v = \sqrt{\frac{8k_BT}{\pi m}} = \sqrt{\frac{8RT}{\pi M_{molar}}}$; Most probable vel.
$v_{prob} = \sqrt{\frac{2k_BT}{m}} = \sqrt{\frac{2RT}{M_{molar}}}$; Mean squared vel.
$\sqrt{\bar{v^2}} = \sqrt{\frac{3k_BT}{m}} = \sqrt{\frac{3RT}{M_{molar}}}$

Virial coefficients:
Taylor expansion of formular for $p$ in $\frac{1}{V}$ around $\frac{1}{V} = 0$, then $p \approx \frac{B_{1(T)}}{V} + \frac{B_{2(T)}}{V^2} + \frac{B_{3(T)}}{V^3} + ...$

## Kinetic theory

Phase space volume constant:
$d^3xd^3p = d^3x'd^3p'$ constant in the case of a force $F$ that is only dependent on $x$ and no temporal derivative

Boltzmann transport equation:
$\left(\frac{\partial}{\partial t} + \vec v\cdot\vec\nabla_{\vec x} + \frac{\vec F}{m}\cdot\vec\nabla_{\vec v}\right) f_{(\vec x,\vec v)} = \frac{\partial f}{\partial x}|_{Stoß}$

Stoßzahlansatz:
$\frac{\partial f}{\partial x}|_{Stoß} = \int W_{(\vec v_1,\vec v_2,\vec v_3,\vec v)}\{f_{(\vec x,\vec v_1,t)}f_{(\vec x,\vec v_2,t)} - f_{(\vec x,\vec v_3,t)}f_{(\vec x,\vec v,t)}\}d\vec v_1 d\vec v_2 d\vec v_3$

Number density:
$n_{(\vec x)} = \int f_{(\vec x,\vec p)}d^3p$
If locally ideal gas: $p_{(\vec x)} = n_{(\vec x)}RT$

Internal energy from prob. dens. func.:
$U = \int\int f_{(\vec x,\vec p)}E_{(\vec x,\vec p)}d^3xd^3p$

Expectation value from number density:
$|x|^3 = \int|\vec x|^3 n_{(\vec x)}d^3x$

## Classical statistical mechanics

Partition functions and derivable parameters:
Canonical: $Z_C = \int e^{-\beta H}d\mu_C =$
$\frac{1}{h^{3N}N!}\int e^{-\frac{H_{(\vec p,\vec q)}}{k_BT}}d^{3N}\vec p d^{3N}\vec q$ with free energy $F_{(T,V,N)} = -k_BT\ln(Z_C)$ and internal energy

$U = -\frac{\partial \ln(Z_C)}{\partial \beta} = -\frac{\partial \ln(Z_C)}{\partial\left(\frac{1}{k_BT}\right)}$ and entropy

$S = -\left(\frac{\partial F}{\partial T}\right)_V$ and pressure $p = -\left(\frac{\partial F}{\partial V}\right)_T$.

Grand canonical:

$Z_G = \sum_{N=0}^{\infty} \int e^{-\beta H_{p,q} + \beta\bar{\mu}N} \frac{d\vec{p}d\vec{q}}{h^{3N}N!}$;

$\Omega = -\frac{1}{\beta}\ln(Z_C); S = \partial_T\Omega; p = \partial_V\Omega; N = \partial_\mu\Omega$

**Energy shell at energy $E$:**

$\mathcal{E} = \{x = (p,q) \in \Gamma | H_{(p,q)} = E\}$ (All points of Energy $E$ in phase space that can be reached → What geometric form does $H_{(x,p)} = E$ describe?)

**Ergodicity:**

System is ergodic when its motion covers entire energy shell in the system's phase space.

**Liouville-continuity-equation:**

$\frac{dw_t}{dt} = 0$ (Phase-space probability density has incompressible flow)

**Gibbs entropy:**

$S = -k_B \sum_i p_i \ln(p_i)$ or continuosly

$S = -\int w_{(x)} \ln(w_{(x)}) d\mu_{m(x)}$ (With $d\mu_{m(x)}$ e. g. as the unnormalized microcanonical measure: $d\mu_{m(x)} = \delta_{(E-H_{(x)})} d^{6N}x$)

**Gibbs variational principle:**

All ensembles maximize entropy in certain conditions. Difference is what constraints to impose. Microc. ens. assigns non-zero probability to states of a volume $V$, particle number $N$ and energy $E$. Canon. ens. $V$ and $N$ as well, but replaces E with average energy $\langle E\rangle$, i.e. temperature $T$ to maximize entropy. Gibbs' statement that canon. distribution $w_C$ maximizes entropy $S_C$ at $\langle H\rangle = \langle H\rangle_C$.

**Expectation value in distribution $\omega$:**

$\langle X\rangle = \int \omega X d\mu_\omega$ (with measure $d\mu_\omega$)

## Ising Model

**Gibbs fundamental relation for magnetic system (Magnetization $M$, magnetic field $h$):**

$dS_{(E,h)} = \frac{1}{T}dE + \frac{M}{T}dh$

$\frac{1}{T} = \frac{\partial S}{\partial E}|_h$

$\frac{M}{T} = \frac{\partial S}{\partial h}|_E$

With Entropy $S = k_B \ln(Z_M)$

For magnet: Microcanonical: $Z_M = \binom{N}{N_\downarrow}$

**Ideal paramagnet (m single spin magnetization):**

$H_{\vec{s}} = -hm \sum_{j=1}^{N} s_j$

Canon. par. func.: Sum over all spin configs' boltzmann factors $Z_C = \sum_s e^{-\beta H_{\vec{s}}}$

$E = -\frac{\partial \ln(Z_C)}{\partial\beta} = -Nmh\tanh\left(\frac{mh}{k_BT}\right)$

$M_{(h,T)} = -\frac{\partial F}{\partial h} = Nm\tanh\left(\frac{mh}{k_BT}\right)$

**Curie's Law:**

$M \approx \frac{Nm^2h}{k_BT}$ for $mh \ll k_BT$

$M \approx Nm$ for $mh \gg k_BT$

**One dimensional Ising model:**

$s_x = (-1)^{n_x + \frac{1-s_0}{2}}$ ($n_x$ number of flips up to x)

$H_{(s)} = J\sum_{x=1}^{L}(1 - s_{x-1}s_x) = 2J\ell$

Number of configurations with $\ell$ flips: $n = 2\binom{N}{\ell}$

$Z_L = \sum_s e^{-\beta H_{(s)}} = 2(1 + e^{-\beta 2J})^L$

## Mean field Ising Model

**Mean-field equation for magnetization per spin of Ising ferromagnet:**

$m = \tanh(2d\beta Jm + \beta h)$

## Solutions

**Reversible heat pump:**

Electric heater efficiency: $\eta_{EH} = 1$, efficiency of reversible heat engine (only Carnot reversible): $\eta_C = 1 - \frac{T_C}{T_H} = \frac{T_H - T_C}{T_H}$, efficiency of heat reversible heat pump exactly reciprocal to that: $\eta_{HP} = \frac{1}{\eta_C} = \frac{T_H}{T_H - T_C} \Rightarrow \frac{\eta_{HP}}{\eta_{EH}} = \frac{\frac{T_H}{T_H-T_C}}{1} = \frac{T_H}{T_H - T_C}$.

**Black body radiation:**

To derive $u_{(T)} = \sigma T^4$ from $U = u_{(T)}V$ and $p = \frac{1}{3}u_{(T)}$ plug into $\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial p}{\partial T}\right)_V - p \Rightarrow u = \frac{T}{3}\frac{du}{dT} - \frac{1}{3}u \Rightarrow \frac{du}{u} = 4\frac{dT}{T} \Rightarrow \ln(u) = \ln(T^4) + C_1 \Rightarrow u = T^4C_2 = \sigma T^4$.

To calculate entropy from Gibbs fundamental equation:

$dU = TdS - pdV \Rightarrow dS = \frac{dU}{T} + \frac{p}{T}dV$ calculate $dU = d(\sigma T^4V) = 4\sigma T^3VdT + T^4dV$. Insert $dU$ and $\frac{p}{T} = \frac{\sigma T^3}{3}$. Now integrate the term for $dS$, while holding either $T$ or $V$ constant ($\Rightarrow dT = 0$ or $dV = 0$), this yields $S = \frac{4}{3}\sigma VT^3 + S_0$. Using $S_{(0)} = 0 \Rightarrow S_0 = 0$.

The equation for adiabatic change of state implies that: Adiabatic $\Rightarrow \delta Q = TdS = 0 \Rightarrow VT^3 =$ const.

**Maxwell distribution:**

The Maxwell-distribution $w_{(\vec{p})} = \mathcal{N}e^{-\beta E_{(\vec{p})}} = \mathcal{N}e^{-\beta c|\vec{p}|}$, normalization

$\frac{1}{\mathcal{N}} = \int_{\mathbb{R}} e^{-\beta E_{(\vec{p})}}d^3p = 4\pi\int_0^\infty p^2 e^{-\beta c|\vec{p}|}dp = 4\pi\partial^2_{\beta c}\int_0^\infty e^{-\beta c|\vec{p}|}dp = 4\pi\partial^2_{\beta c}\frac{1}{\beta c} = \frac{8\pi}{(\beta c)^3} \Rightarrow \mathcal{N} = \frac{(\beta c)^3}{8\pi}$.

Expected energy: $\langle E\rangle = \int_{\mathbb{R}} E_{(\vec{p})}w_{(\vec{p})}d^3p =$

$-4\pi c\mathcal{N}\partial^3_{\beta c}\int_0^\infty e^{-\beta cp}dp = -4\pi c\mathcal{N}\partial^3_{\beta c}\frac{1}{\beta c} = 24\pi c\mathcal{N}\frac{1}{(\beta c)^4} = \frac{3}{\beta} = 3k_BT$

Expected squared energy: $\langle E^2\rangle = \int_{\mathbb{R}} E^2_{(\vec{p})}w_{(\vec{p})}d^3p = -4\pi c^2\mathcal{N}\partial^4_{\beta c}\int_0^\infty e^{-\beta cp}dp = 4\pi c^2\mathcal{N}\partial^4_{\beta c}\frac{1}{\beta c} = 96\pi c^2\mathcal{N}\frac{1}{(\beta c)^5} = \frac{12}{\beta^2} = 12k_B^2T^2$

Variance:

$\sigma_E^2 = \langle(E - \langle E\rangle)^2\rangle = \langle E^2\rangle - \langle E\rangle^2 = 3k_B^2T^2$

**Ideal paramagnet:**

Hamiltonian: $H_{(\vec{s})} = -hm\sum_{j=1}^{N} s_j$

Canonical partition function in this case is the sum over all spin configurations' boltzmann factors $Z_C = \sum_s e^{-\beta H_{(\vec{s})}} =$

$$\sum_{s_1\in\{\pm1\}}\sum_{s_2\in\{\pm1\}}...\exp\left(\beta hm\sum_{j=1}^{N}s_j\right) = \sum_{s_1\in\{\pm1\}}e^{\beta hms_1}\sum_{s_2\in\{\pm1\}}e^{\beta hms_2}... = \prod_{j=1}^{N}\sum_{s_j\in\{\pm1\}}e^{\beta hms_j} = \prod_{j=1}^{N}(e^{\beta hm} + e^{-\beta hm}) = (2\cosh(\beta hm))^N$$

Free energy:

$F = -\frac{\ln(Z_C)}{\beta} = -\frac{N}{\beta}\ln(2\cosh(\beta hm))$

Magnetization: $M = -\frac{\partial F}{\partial h} = \frac{N}{\beta}\frac{\sinh(\beta hm)}{\cosh(\beta hm)}\beta m = Nm\tanh(\beta hm)$

Internal energy:

$U = -\frac{\partial\ln(Z_C)}{\partial\beta} = -Nhm\tanh(\beta hm)$

Specific heat capacity:

$c_h = \frac{C_h}{N} = \frac{1}{N}\frac{\partial U}{\partial T}|_h = \frac{1}{N}\frac{\partial U}{\partial\beta}\frac{\partial\beta}{\partial T} = -hm\left(hm - hm\frac{\sinh^2(\beta hm)}{\cosh^2(\beta hm)}\right)\left(-\frac{1}{k_BT^2}\right) = k_B\frac{\beta^2h^2m^2}{\cosh^2(\beta hm)}$

Magnetic susceptibility:

$\chi = \frac{\partial M}{\partial h} = k_B\frac{\beta^2Nm^2}{\cosh^2(\beta hm)}$

**3-level-system:**

Example for $H = \begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \eta\\ 0 & \eta & 0\end{pmatrix}$ and

$A = \begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}$

Canonical density operator: $\rho_C = e^{\beta(F-H)} =$

$\exp\left(\beta\frac{1}{(} - \beta\ln(Z_C))\right)\exp(-\beta H) =$

$\exp\left(\ln\left(\frac{1}{Z_C}\right)\right)\exp(-\beta H) = \frac{1}{Z_C}e^{-\beta H}$. Using

that $H = \begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \eta\\ 0 & \eta & 0\end{pmatrix} \Rightarrow H^N =$

$\begin{pmatrix}(-\epsilon)^n & 0 & 0\\ 0 & 0 & \eta^n\\ 0 & \eta^n & 0\end{pmatrix}$ for odd $n$, and

$\begin{pmatrix}(-\epsilon)^n & 0 & 0\\ 0 & \eta^n & 0\\ 0 & 0 & \eta^n\end{pmatrix}$ for even $n$, it follows that

$e^{-\beta H} = \sum_{n=1}^{\infty}\frac{1}{n!}(-\beta H)^n =$

$$\begin{pmatrix}\frac{\beta^1\epsilon^1}{1!} + \frac{\beta^2\epsilon^2}{2!}\dots & 0 & 0\\ 0 & \frac{\beta^2\eta^2}{2} + \frac{\beta^4\eta^4}{4!}\dots & -\beta\eta - \frac{\beta^3\eta^3}{3!}\dots\\ 0 & -\beta\eta - \frac{\beta^3\eta^3}{3!}\dots & \frac{\beta^2\eta^2}{2} + \frac{\beta^4\eta^4}{4!}\dots\end{pmatrix} =$$

$$\begin{pmatrix}e^{\beta\epsilon} & 0 & 0\\ 0 & \frac{e^{-\beta\eta}}{2} + \frac{e^{\beta\eta}}{2} & \frac{e^{-\beta\eta}}{2} - \frac{e^{\beta\eta}}{2}\\ 0 & \frac{e^{-\beta\eta}}{2} - \frac{e^{\beta\eta}}{2} & \frac{e^{-\beta\eta}}{2} + \frac{e^{\beta\eta}}{2}\end{pmatrix} =$$

$$\begin{pmatrix}e^{\beta\eta} & 0 & 0\\ 0 & \cosh(\beta\epsilon) & -\sinh(\beta\epsilon)\\ 0 & -\sinh(\beta\epsilon) & \cosh(\beta\epsilon)\end{pmatrix}.$$

Partition function must normalize density operator: $Z = \mathrm{tr}\left(e^{-\beta H}\right) = e^{\beta\epsilon} + e^{-\beta\eta} + e^{\beta\eta}$

Free energy:

$F = -\frac{1}{\beta}\ln(Z_C) = -\frac{1}{\beta}\ln\left(e^{\beta\epsilon} + e^{-\beta\eta} + e^{\beta\eta}\right)$

Energy expectation value: $\langle H\rangle = \mathrm{tr}(\rho_C H) =$

$$\mathrm{tr}\left(\frac{1}{Z_C}\begin{pmatrix}-\epsilon e^{\beta\eta} & 0 & 0\\ 0 & -\eta\sinh(\beta\epsilon) & \eta\cosh(\beta\epsilon)\\ 0 & \eta\cosh(\beta\epsilon) & -\eta\sinh(\beta\epsilon)\end{pmatrix}\right)$$

$-\frac{1}{Z_C}(\epsilon e^{\beta\epsilon} + 2\eta\sinh(\beta\epsilon))$

Expected value of observable:

$\langle A\rangle = \mathrm{tr}(\rho_C A) =$

$$\mathrm{tr}\left(\frac{1}{Z_C}\begin{pmatrix}0 & \cosh(\beta\eta) & -\sinh(\beta\eta)\\ e^{\beta\epsilon} & -\sinh(\beta\eta) & \cosh(\beta\eta)\\ 0 & \cosh(\beta\eta) & -\sinh(\beta\eta)\end{pmatrix}\right) =$$

$-\frac{2}{Z_C}\sinh(\beta\eta)$

Low temperature behavior:

$\langle H\rangle - \frac{\epsilon e^{\beta\epsilon} + \eta(e^{\beta\eta} - e^{-\beta\eta})}{e^{\beta\epsilon} + e^{-\beta\eta} + e^{\beta\eta}} \xrightarrow{\beta\to\infty} -\eta$ and

$\langle A\rangle - \frac{e^{-\beta\eta} - e^{\beta\eta}}{e^{\beta\epsilon} + e^{-\beta\eta} + e^{\beta\eta}} \xrightarrow{\beta\to\infty} -1$