

Critical Exponents

①

as critical point is approached $\Rightarrow$ system "signals" onset of phase transition by fluctuations on a macroscopic scale $\Rightarrow$ below critical point ~~magnetization~~ order parameter becomes non-zero

$$\varepsilon = \frac{T - T_c}{T_c}$$

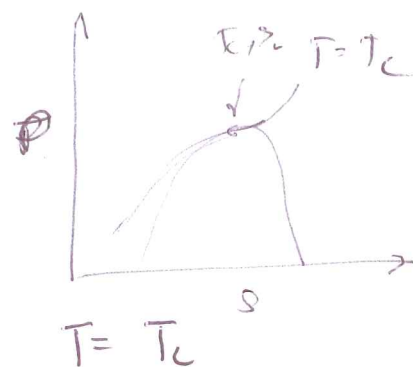
near T_c - thermodynamic functions have the form
 $f(\varepsilon) = A\varepsilon^\lambda (1 + B\varepsilon^\gamma + \dots)$ ($\gamma > 0$)

$$\lambda = \lim_{\varepsilon \rightarrow 0} \frac{\ln f(\varepsilon)}{\ln \varepsilon}$$

PVT System

- degree of critical isotherm

$$\frac{p - p_c}{p_c^0} = A_0 \left| \frac{s - s_c}{s_c} \right|^\delta \text{ sign}(s - s_c)$$



how pressure varies as a function of density around T_c, p_c, s_c along the critical isotherm

(p_c^0 - pressure of ideal gas at p_c, T_c) [value $6 > \delta \geq 4$]

- degree of the coexistence curve

$$\frac{s_l - s_g}{s_c} = A_\beta (-\varepsilon)^\beta$$

as we approach T_c from below, the difference in densities will have some temperature dependence

β [value $\beta \approx 0.34$]

Heat Capacity

(2)

as $T \rightarrow T_c$ from above such that $V = V_c$

$$C_v = A_+^* (+\epsilon)^{\alpha}$$

as $T \rightarrow T_c$ from below such that $V = V_c$

$$C_v = A_-^* (-\epsilon)^{\alpha'}$$

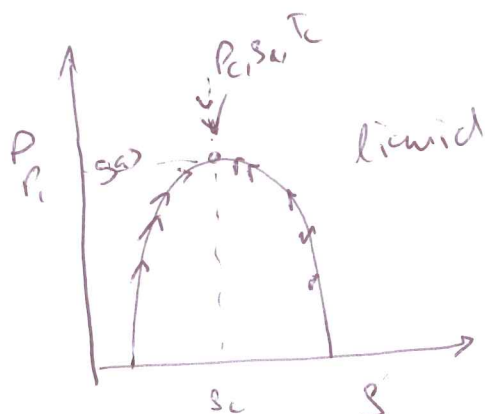
$$\alpha \sim 0.1 \quad \alpha' \sim 0.1$$

Isobaric Compressibility

$$\frac{\kappa_T}{\kappa_0} = \begin{cases} A_+^* (-\epsilon)^{-\delta'} & T < T_c \\ A_-^* (\epsilon)^{-\delta} & T > T_c \end{cases} \quad \begin{matrix} s = s_c(T) \text{ or } s = s_g(T) \\ s = s_0 \end{matrix}$$

for $T > T_c \Rightarrow$ approach T_c along critical isochore

for $T < T_c \Rightarrow$ approach T_c along coexistence curve



[value: $\delta' \sim 1.2 \quad \delta \sim 1.3$]

Magnetic System

specific heat

$$C_B \sim \begin{cases} \left(\frac{T - T_c}{T_c} \right)^\alpha \\ \left(\frac{T_c - T}{T_c} \right)^{\alpha'} \end{cases}$$

from above

$$[\text{value: } \alpha \approx -0.03 \quad \alpha' \approx -0.02]$$

from below

susceptibility

$$\chi_T = \left(\frac{\partial m}{\partial B} \right)_T \sim \left(\frac{T - T_c}{T_c} \right)^{-\gamma} \quad [\gamma \approx 1.3]$$

$T \rightarrow T_c$ from above

magnetization

$$m_0 \sim (T_c - T)^\beta$$

from below $[\beta \approx 0.35]$

at

[recall β for PVT = 0.34]

$$\text{at } T_c \quad m \sim B^{1/\delta}$$

analogous to $p - p_c = (\delta p - \delta_c)^\delta$

$\delta \approx 4.3$ for iron
(4.0 for water)

exponent inequalities

$$C_V = x_g C_{Vg} + x_e C_{Ve} + \frac{x_g T}{s_g^3 k_T^g} \left(\frac{\partial s_g}{\partial T} \right)_{\text{ex}}^2 + \frac{x_e T}{s_e^3 k_T^e} \left(\frac{\partial s_e}{\partial T} \right)_{\text{ex}}^2$$

(derived in homework)

||

$$C_V \geq \frac{x_g T}{s_g^3 k_T^g} \left(\frac{\partial s_g}{\partial T} \right)_{\text{ex}}^2 \quad (\text{all quantities} \geq 0)$$

critical point: $x_g \rightarrow 1/2$

$$s_g \rightarrow s_c$$

$$k_T \sim (T_c - T)^{-\gamma'}$$

$$\left(\frac{\partial s_g}{\partial T} \right)_{\text{ex}} \sim (T_c - T)^{\beta' - 1}$$

$$C_V \geq \frac{1}{2} \frac{T_c B (T_c - T)^{\gamma' + 2\beta' - 2}}{s_c^3}$$

B - constant

$$\ln C_V \geq (2 - \gamma' - 2\beta') \ln(-\epsilon)$$

$$\frac{\ln C_V}{\ln(-\epsilon)} \quad C_V \sim (-\epsilon)^{\alpha'}$$

$$\boxed{\alpha' + \gamma' + 2\beta' \geq 2} \Rightarrow \text{Rushbrooke inequality}$$

Correlation functions

- can be measured by X-ray or neutron scattering

$$G^{(1)}(i, j) \equiv \langle \vec{S}_i \cdot \vec{S}_j \rangle \quad (\text{for spin system})$$

- translational invariance $\Rightarrow$ depends only on $|\vec{r}_i - \vec{r}_j|$
- isotropic system: independent of direction of $|\vec{r}_i - \vec{r}_j|$
- general definition for systems other than spin systems

$$G^{(1)}(i, j) = \langle \phi(\vec{r}_i) \cdot \phi(\vec{r}_j) \rangle$$

$\phi(\vec{r})$ - can be a scalar, vector, tensor depending on system

- want to know at what distance do order parameters (local) $\phi(\vec{r})$, $\phi(\vec{r})$ become uncorrelated

$$G_c^{(1)}(i, j) = \langle \phi(\vec{r}_i) \cdot \phi(\vec{r}_j) \rangle - |\langle \phi(\vec{r}) \rangle|^2$$

- above T_c $\langle \phi \rangle = 0 \Rightarrow G_c^{(1)}(i, j) = G_\phi^{(1)}(i, j)$

- below T_c $G_c^{(1)}(i, j) \rightarrow$ sensitive to fluctuations only

- at $T_c \Rightarrow$ evidence suggests: $G_c^{(1)} \rightarrow$ power law behaviour

$$G_c^{(1)}(r) \sim \frac{1}{r^{d-2+\eta}} \quad \eta - \text{critical exponent}$$

$$0 \leq \eta \leq 1$$

- away from $T_c \Rightarrow$ usually

we have

$$G_c^{(1)}(r) \sim e^{-r/\xi}$$

ξ - correlation length

$$\xi \sim |T - T_c|^{-\nu} \quad (\nu \text{ typically } \frac{2}{3})$$

correlation length diverges at critical point

Correlation functions $\longleftrightarrow$ susceptibilities

example: Ising model

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i$$

$$Q = \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \beta B \sum_i \sigma_i}$$

magnetization: $\frac{1}{\beta} \left. \frac{\partial \ln Q}{\partial B} \right|_{B=0} = \frac{1}{\beta} \frac{1}{Q} \left. \frac{\partial Q}{\partial B} \right|_{B=0} = \frac{1}{\beta Q} \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \beta B \sum_i \sigma_i} \left(\sum_i \sigma_i \right)$

$$= M \quad (\text{extensive}) \quad (= N \langle \sigma \rangle)$$

taking one more derivative with respect to βB will give ~~can~~ the susceptibility

$$\chi = \frac{1}{N} \frac{\partial M}{\partial (\beta B)} = \frac{\sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta H} (\sum_i \sigma_i) (\sum_j \sigma_j)}{N Q} - \left[\frac{\sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta H} (\sum_i \sigma_i)^2}{N Q^2} \right]$$

$$= \frac{1}{N} \sum_{i,j} \langle \sigma_i \sigma_j \rangle - \frac{M^2}{N}$$

due to translational invariance

$$= \frac{1}{N} \sum_j \langle \sigma_0 \sigma_j \rangle - \frac{M^2}{N}$$

can replace $\frac{1}{N} \sum_j \langle \sigma_0 \sigma_j \rangle - \frac{M^2}{N}$ with correlation function

$$\chi = \sum_j [\langle \sigma_0 \sigma_j \rangle - \langle \sigma_0 \rangle \langle \sigma_j \rangle] = \sum_j G_c^{(2)}(j)$$

take continuous limit: becomes an integral

$$\Rightarrow \chi = 1 \nu \int_0^\infty r dr G_c^{(2)}(r)$$

Scaling: thermodynamic functions around T_c scale as fns of
Homogeneous Functions $\Downarrow$ exponents

function is homogeneous if

$$F(\lambda x) = g(\lambda) F(x) \quad \lambda=1 \Rightarrow g(1)=1$$

$$F(\lambda \mu x) = g(\lambda) F(\mu x) = g(\lambda) g(\mu) F(x) \\ = g(\lambda \mu) F(x)$$

$$\Downarrow \\ g(\lambda \mu) = g(\lambda) g(\mu)$$

$$\frac{d}{d\mu} g(\lambda \mu) = \lambda g'(\lambda \mu) = g(\lambda) g'(\mu) \quad \mu=1 \quad g'(1) = p$$

$$\lambda g'(\lambda) = g(\lambda) p$$

$\Downarrow$
integrate from 1 to λ

$$\Rightarrow \frac{g'(\lambda)}{g(\lambda)} = \frac{p}{\lambda}$$

$$\Downarrow \\ \ln g(\lambda) = p \ln \lambda \Rightarrow g(\lambda) = \lambda^p$$

$$F(\lambda x) = \lambda^p F(x) \quad \lambda = x^{-1}$$

$$F(1) = \lambda^p x^{-p} F(x)$$

$$\Rightarrow F(x) = x^p F(1)$$

write two-variable homogeneous fn. as

$$\Rightarrow f(\lambda^p x, \lambda^q y) = \lambda f(x, y)$$

$$\lambda = y^{-1/q}$$

$$\Downarrow \\ f\left(\frac{x}{y^{p/q}}, 1\right) = y^{-1/q} f(x, y)$$

$$\Rightarrow f(x, y) = y^{1/q} f\left(\frac{x}{y^{p/q}}, 1\right)$$

Widom Scaling

- consider free-energy of a magnetic system
- write it as a sum of a regular and a singular term: -

$$g(T, B) = g_r(T, B) + g_s(T, B)$$

$$g_s(T, B) \rightarrow g_s(\varepsilon, B) \quad \varepsilon = \frac{T - T_c}{T_c}$$

around phase transition: need to consider only $g_s(\varepsilon, B)$, since it contains all the singular behaviour of response functions

- assumption: g_s is a homogeneous function of its arguments

$$g_s(\lambda^p \varepsilon, \lambda^q B) = \lambda g_s(\varepsilon, B)$$

- definition of critical exponent β :

$$M(\varepsilon, B=0) \sim (-\varepsilon)^\beta$$

$$\Rightarrow \frac{\partial g_s(\lambda^p \varepsilon, \lambda^q B)}{\partial B} = \lambda \frac{\partial g_s(\varepsilon, B)}{\partial B}$$

$$\lambda^q M(\lambda^p \varepsilon, \lambda^q B) = \lambda M(\varepsilon, B)$$

$$\text{at } \lambda = (-\varepsilon)^{-1/p} \quad \text{at } B = 0$$

$$(-\varepsilon)^{-q/p} M((- \varepsilon)^{-1/p} \varepsilon, 0) = (-\varepsilon)^{-1/p} M(\varepsilon, 0)$$

$$M(\varepsilon, 0) = (-\varepsilon)^{\frac{1-q}{p}} M(1, 0)$$

$$\Rightarrow \beta = \frac{1-q}{p}$$

- determine δ in a similar way

$$n(0, B) = |B|^{1/\sigma} \text{sign}(B)$$

$$\text{set } \epsilon = 0, \lambda = B^{-1/q}$$

$$\lambda^q n(\lambda^p 0, \lambda^q B) = \lambda n(0, B)$$

$$B^{-1+1/q} n(0, 1) = n(0, B)$$

$$n(0, B) = B^{(1-q)/q} n(0, 1) = |B|^{1/\sigma} \text{sign}(B)$$

$$\Rightarrow \delta = \frac{q}{1-q}$$

magnetic susceptibility

$$\chi = - \left. \frac{\partial^2 g}{\partial B^2} \right|_T \sim \begin{cases} (-\epsilon)^{-\delta'} & T < T_c \\ (-\epsilon)^{-\delta} & T > T_c \end{cases}$$

~~to~~ to obtain χ differentiate n w.r to B

$$\lambda^q n(\lambda^p \epsilon, \lambda^q B) = \lambda n(\epsilon, B)$$

$$\lambda^{2q} \chi(\lambda^p \epsilon, \lambda^q B) = \lambda \chi(\epsilon, B)$$

$$\text{set } B=0 \quad \lambda = \epsilon^{-1/p}$$

$$\epsilon^{-2q/p} \chi(1, 0) = \epsilon^{-1/p} \chi(\epsilon, 0)$$

$$\chi(\epsilon, 0) = \epsilon^{\frac{1-2q}{p}} \chi(1, 0)$$

$$\frac{1-2q}{p} = -\delta \quad \Rightarrow \delta = \delta'$$

heat capacity

$$C_B \sim -T \left(\frac{\partial^2 G}{\partial T^2} \right)_B \sim (\epsilon)^{-\alpha}$$

$$\lambda^{1/p} C_B(\lambda^p \epsilon, \lambda^q B) = \lambda C_B(\epsilon, B)$$

$$B=0 \quad \lambda = \epsilon^{-1/p}$$

$$C_B(\epsilon, 0) = \epsilon^{(1-2p)/p} C_B(1, 0)$$

$$\alpha = \frac{(1-2p)}{p} \quad 2 - \frac{1}{p} \quad \alpha = 2^1$$

combine equations

$$\beta = \frac{1-q}{p}$$

$$\delta = \frac{q}{1-q}$$

$$\gamma = \frac{2q-1}{p}$$

↓

$$\delta(1-q) = q$$

$$\delta - \delta q = q$$

$$\delta = q/(1-\delta)$$

$$q = \frac{\delta}{1+\delta}$$

$$\beta = \frac{1-q}{p} = \frac{1}{(1+\delta)p}$$

$$\gamma = \frac{2\delta-1-\delta}{\delta(1+\delta)} = \frac{\delta-1}{\delta(\delta+1)} = \frac{1}{(\delta+1)\beta}$$

$$\frac{\delta-1}{\delta(\delta+1)} = \frac{1}{(\delta+1)\beta}$$

Relation between
critical exponents

$$\boxed{\beta(\delta-1) = \gamma}$$

combine

$$\beta = \frac{1-q}{p}$$

$$\delta = \frac{q}{1-q}$$

$$\alpha = 2 - \frac{1}{p}$$

$$\delta(1-q) = q$$

$$\delta - \delta q = q$$

$$\delta = \cancel{q} + \delta q(\delta+1)$$

$$q = \frac{\delta}{\delta+1}$$

$$\rightarrow 2 - 2 = -\frac{1}{p}$$

$$2 - 2 = \frac{1}{p}$$

$$p = \frac{1}{2-\alpha}$$

$$\frac{\beta}{2-\alpha} = \frac{1}{\delta+1} \Rightarrow \beta(\delta+1) = 2-\alpha$$

$$\boxed{\beta\delta + \beta + \alpha = 2}$$

relation between critical exponents

these relations are experimentally verifiable

$\Rightarrow$ they hold

$\Rightarrow$ the underlying assumption

$$\mathcal{G}_s(\varepsilon, B) = B^{1/\alpha} \mathcal{G}\left(\frac{\varepsilon}{B^{p/\alpha}}, 1\right)$$

in other words: the dependence of the singular part of the free energy can be reduced to a single-variable function times a scaling factor

Kadanoff Decimation

- consider d-dimensional Ising model

$$H(\{S_i\}) = -K \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i$$

- divide lattice into blocks of L^d (a -distance between lattice sites)

$$L^d \ll \xi \quad \xi - \text{correlation length}$$

- total number of blocks: $\frac{N}{L^d}$

- total spin of one block:

$$S_I' = \sum_{i \in I} S_i$$

- $L^d \ll \xi \Rightarrow$ block spins will be highly correlated

- define new spin variable

$$S_I' = \tau S_I \quad S_I = \pm 1 \quad \tau = L^d$$

block Hamiltonian:

$$H(\{S_I'\}) = -K_L \sum_{\langle I,J \rangle} S_I' S_J' - B_L \sum_I S_I'$$

K_L - effective interaction between blocks

B_L - effective B-field

for free energy per site $g(\epsilon, B) \Rightarrow$ write for block

$$g(\epsilon_L, B_L) = L^d g(\epsilon, B)$$

$$\text{correlation length: } \xi_L(\epsilon_L, B_L) = L^{-1} \xi(\epsilon, B)$$

- introduce scaling for ε, B

$$\varepsilon_L = L^x \varepsilon \quad B_L = L^y B$$

$$B \sum_{I=1}^N S_I = B \sum_{I=1}^{N/L^d} S'_I = \underbrace{B L^d}_{\omega} \sum_{I=1}^{N/L^d} S'_I$$

$$B_L = L^y B$$

- $g(\varepsilon_L, B_L) = g(L^x \varepsilon, L^y B) = L^d g(\varepsilon, B) \Rightarrow$ scaled free energy

- introduce: Block correlation function

$$C(r_L, \varepsilon_L) = \langle S_I S_J \rangle - \langle S_I \rangle \langle S_J \rangle$$

$$= \mathbb{E}^{-2} [\langle S'_I S'_J \rangle - \langle S'_I \rangle \langle S'_J \rangle]$$

$$= \mathbb{E}^{-2} \sum_{\substack{I \in I \\ J \in J}} [\langle S_I S_J \rangle - \langle S_I \rangle \langle S_J \rangle]$$

$$= \mathbb{E}^{-2} L^{2d} C(r, \varepsilon)$$

$$r_L = \frac{r}{L}$$

$$\Downarrow \quad \Downarrow \quad C\left(\frac{r}{L}, \varepsilon L^x\right) = L^{2(d-y)} C(r, \varepsilon)$$

choose $L = r/a$

$$C(r, \varepsilon) = \left(\frac{r}{a}\right)^{2(y-d)} C\left(1, \varepsilon \left(\frac{r}{a}\right)^x\right)$$

$$\nu: \xi \sim |T - T_c|^{-\nu} \Rightarrow r/\xi = r \varepsilon^\nu \quad \Downarrow \quad \boxed{x = -\nu}$$

$$\text{at } T_c \quad C(r, 0) \sim r^{2y-2d} = r^{2-\eta-d}$$

$$2y-2d = 2-\eta+d$$

$$\boxed{y = 1 - \frac{\eta}{2}}$$

$$\text{since } g(L^x \epsilon, L^y \beta) = L^d g(\epsilon, \beta)$$

$$\text{and } g_s(\lambda^p \epsilon, \lambda^q \beta) = \lambda g_s(\epsilon, \beta)$$

$$\Rightarrow y = dq \quad x = dp$$

$$\text{From Widom scaling } \delta = \frac{q}{1-q} \Rightarrow q = \frac{\delta}{1+\delta}$$

$\Downarrow$

$\Downarrow$

it is thus possible to relate critical exponents

$$\gamma = \frac{d\delta}{1+\delta} = 1 - \frac{u}{2}$$

$$\nu = \frac{2-\alpha}{d}$$

$$\eta = 2-d \left(\frac{\delta-1}{\delta+1} \right)$$

Ising correlation functions (1D)

- interested in calculating $\langle f(\sigma_i) f(\sigma_j) \rangle$

σ_i - spin at site i ;

σ_j - spin at site j ;

$$\langle f(\sigma_i) f(\sigma_j) \rangle = \frac{\sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta J \sum_i \sigma_i \sigma_{i+1}} f(\sigma_i) f(\sigma_j)}{\sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta J \sum_i \sigma_i \sigma_{i+1}}}$$

$$f(\sigma_i) = \begin{pmatrix} f(+1) & 0 \\ 0 & f(-1) \end{pmatrix} = f_{\mu\nu}$$

transfer matrix: $\langle \sigma_i | e^{-\beta J \sigma_i \sigma_{i+1}} | \sigma_{i+1} \rangle$

$$T_{\mu\nu} = \begin{pmatrix} e^{-\beta J} & e^{\beta J} \\ e^{\beta J} & e^{-\beta J} \end{pmatrix}$$

$$\begin{aligned} \langle f(\sigma_i) f(\sigma_j) \rangle &= \frac{\text{Tr } T^i f T^{j-i} f T^{N-j}}{\text{Tr } T^N} \\ &= \frac{\text{Tr } T^i f T^{j-i} f T^{N-j}}{\text{Tr } T^N} \\ &= \frac{\text{Tr } f T^{j-i} f T^{N-j+i}}{\text{Tr } T^N} \\ &= \frac{\text{Tr } f T^j f T^{N-j}}{\text{Tr } T^N} \end{aligned}$$

diagonalize T and use new basis

$$\begin{pmatrix} e^{-\beta J} & e^{\beta J} \\ e^{\beta J} & e^{-\beta J} \end{pmatrix} \Rightarrow (e^{-\beta J} - \lambda)^2 - e^{2\beta J} = 0$$

$$\lambda^2 - 2\lambda e^{-\beta J} + e^{-2\beta J} - e^{2\beta J} = 0$$

$$\lambda = \frac{2e^{-\beta J} \pm \sqrt{4e^{-2\beta J} - 4(e^{-2\beta J} - e^{2\beta J})}}{2}$$

$$\lambda = e^{-\beta J} \pm e^{\beta J} = 2 \cosh \beta J, 2 \sinh \beta J$$

λ_+ λ_-

in this new basis F will no longer be diagonal

~~$\langle \delta(\sigma_i) \delta(\sigma_j) \rangle =$~~

we can write $T^n = \lambda_m^n \delta_{mp}$

$$\begin{aligned} \langle \delta(\sigma_i) \delta(\sigma_j) \rangle &= \frac{1}{Z} \sum_m \lambda_m^n \delta_{mp} \\ &= \frac{\sum_m \sum_p \lambda_m^n \delta_{mp} F_{pq} \lambda_q^{N-n} F_{qm}}{\sum_m \lambda_m^N} \\ &= \frac{\sum_{mp} \lambda_m^n F_{mp} \lambda_p^{N-n} F_{pm}}{\sum_m \lambda_m^N} \\ &= \frac{\sum_{mp} \lambda_m^N F_{mp} \left(\frac{\lambda_p}{\lambda_m}\right)^{N-n} F_{pm}}{\sum_m \lambda_m^N} \\ &= \left\langle |F_{mp}|^2 \left(\frac{\lambda_p}{\lambda_m}\right)^{N-n} \right\rangle \end{aligned}$$

Since F is symmetric we have: contributing term $m=0$ ($m=1$) suppressed

$$\langle \delta(\sigma_i) \delta(\sigma_j) \rangle = F_{00}^2 + F_{01}^2 \left(\frac{\lambda_1}{\lambda_0}\right)^{N-n}$$

$$\Rightarrow G_c^{(2)}(n) = F_{01}^2 \left(\frac{\lambda_1}{\lambda_0}\right)^{N-n} \approx e^{-n/\xi} \Rightarrow \xi = \frac{1}{\ln(\lambda_0/\lambda_1)}$$