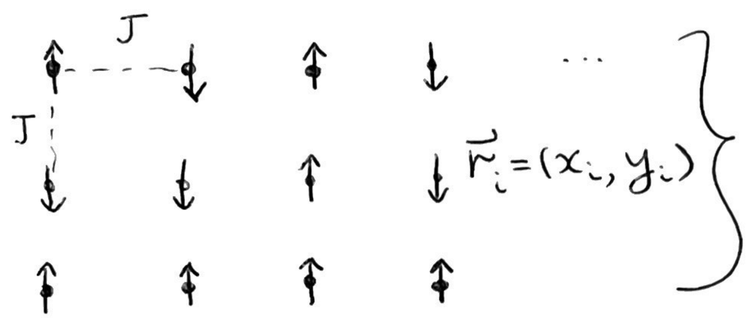
Lecture 14

2D Ising model on a square lattice

magnetic field

$$\mathcal{H} = -J \underbrace{\sum_{\langle ij \rangle}}_{\text{sums once over each coupling } J} S_i S_j - H \Big(\underbrace{\sum_{i=1}^{N} S_i}_{= M, \text{ total magnetization}} \Big)$$

$S_i = \pm 1$, $i = 1, \dots, N$



N spins

Consider ...

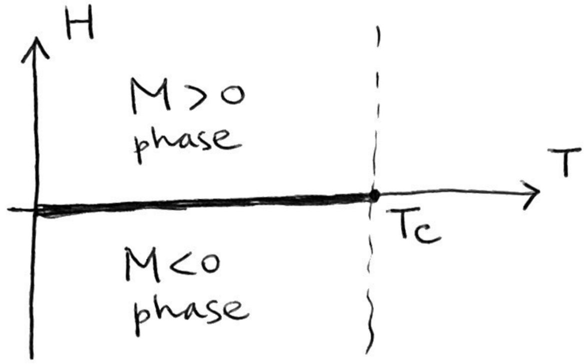
$H = 0$: critical T $\left[\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j \right]$

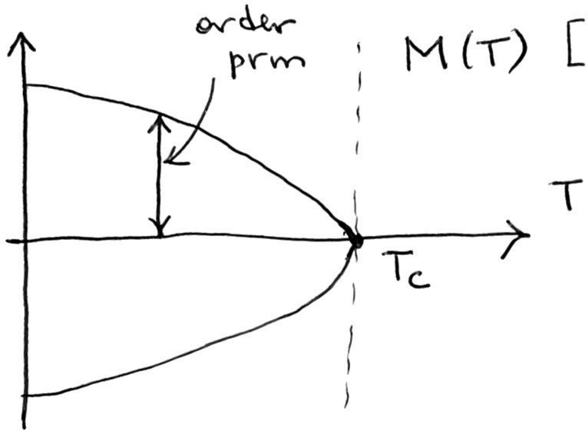
$T > T_c$: finite correlation length (~ cluster size), short-range order

$T = T_c$: ∞ correlation length, ordered structures on every length scale (self-similarity)

$T < T_c$: $M = \sum_i S_i \neq 0$ spontaneously, clusters of spins of the same sign (long-range order). As $T \to 0$, all spins are aligned up or down.

Magnetic phase transitions:





$M(T)$ [$\neq 0$ below T_c]

Spin-spin correlation functions:

$$\Gamma(\vec{r}_i, \vec{r}_j) = \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle$$

2D position of spin i

thermal average

Translational invariance:

$$\langle s_i \rangle = \langle s_j \rangle \equiv \langle s \rangle,$$

$$\Gamma(\vec{r}_i, \vec{r}_j) = \Gamma(\underbrace{|\vec{r}_i - \vec{r}_j|}_{= r}) = \langle s_i s_j \rangle - \langle s \rangle^2$$

Note that $\Gamma(0) = \underbrace{\langle s_i^2 \rangle}_{= \langle s^2 \rangle} - \langle s \rangle^2 = 1 - \langle s \rangle^2$.

$\underline{T > T_c}$: $\langle s \rangle = 0$

$$\Gamma(r) \sim \frac{1}{r^{\tau}} e^{-r/\xi}$$

corr'n length

$\underline{T < T_c}$: $\langle s \rangle \neq 0$

$\underline{T = T_c}$:

$$\Gamma(r) \sim \frac{1}{r^{d-2+\eta}}$$

\# dims — critical exp

Note that

$$\langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2 = \beta^{-2} \frac{\partial^2}{\partial H^2} \log Z ,$$

where $\underset{(T,H)}{Z} = \sum_r e^{-\beta \underbrace{E_r}_{\text{energy of state } r}}$

On the other hand,

$$\chi_T = \left(\frac{\partial \langle M \rangle}{\partial H} \right)_T = - \left(\frac{\partial^2 \overbrace{F}^{= -k_B T \log Z}}{\partial H^2} \right)_T = \beta^{-1} \left(\frac{\partial^2 \log Z}{\partial H^2} \right)_T .$$

χ_T: isothermal susceptibility

Thus, $\underline{\langle M^2 \rangle - \langle M \rangle^2 = \beta^{-1} \chi_T}$

Furthermore, $\langle (M - \langle M \rangle)^2 \rangle =$

$$= \left\langle \left(\sum_i (s_i - \langle s_i \rangle) \right) \left(\sum_j (s_j - \langle s_j \rangle) \right) \right\rangle =$$

$$= \sum_{i,j} \left[\langle s_i s_j \rangle - \langle s \rangle^2 \right] = \sum_{i,j} \Gamma(|\vec{r}_i - \vec{r}_j|) = N \sum_i \Gamma(r_i) \simeq$$

choose $|\vec{r}_i - \underbrace{\vec{r}_j}_{= \vec{r}_0 = \vec{0}}| = r_i$

$$\simeq N \int_0^\infty dr\, \underline{\underline{r^{d-1} \Gamma(r)}} .$$

Finally,

$$\chi_T \sim N \int_0^\infty dr\, r^{d-1} \underbrace{\Gamma(r)}_{\sim \frac{1}{r^{d-2+\eta}}}$$

$\rightarrow$ the $\int$ diverges at the upper limit if $\eta < 2$

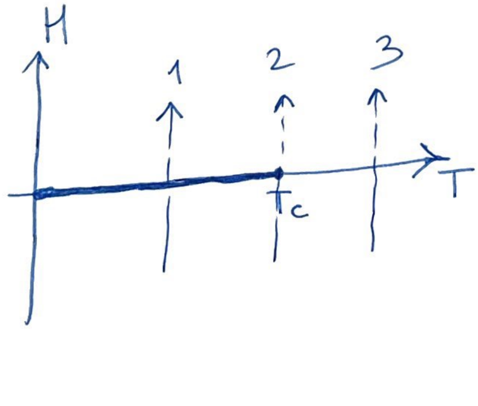
$\uparrow$ diverges at $T = T_c$ [implies divergent fluct's in M]

Ising model: consider $F = U - TS$

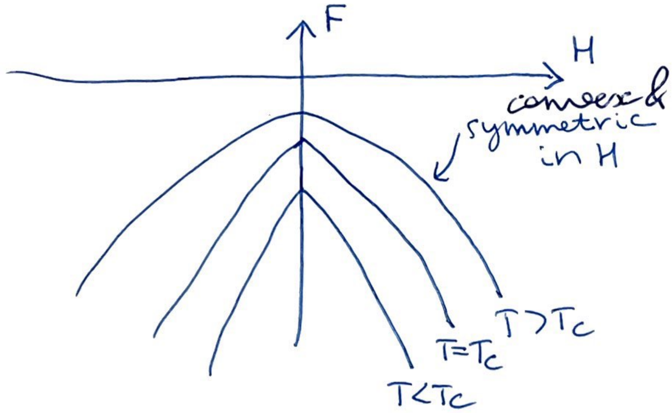
<u>1st order transition</u>: finite discontinuity in one or more of 1st derivative of F

<u>Continuous (2nd order) transition</u>: 1st derivatives continuous but 2nd derivatives discont. <u>or</u> infinite

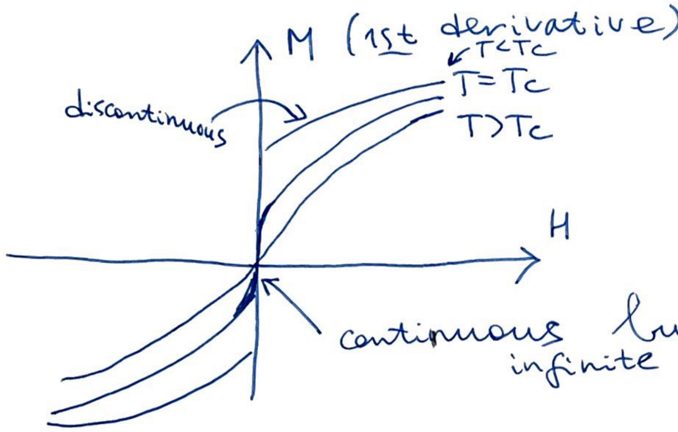
e.g. divergent susceptibility $\Rightarrow$
$\Rightarrow$ divergent fluct's of $M \Rightarrow$
$\Rightarrow$ infinite corr'n length (i.e., power-law decay of correlations)



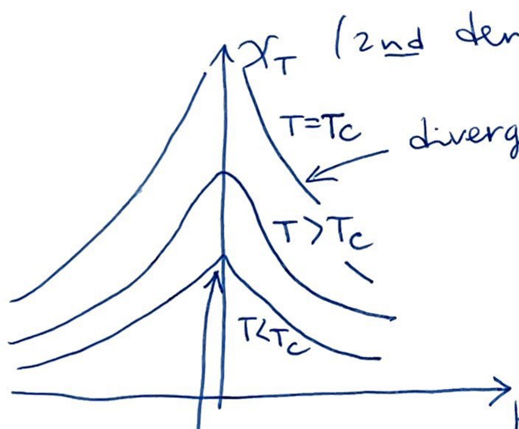
As a function of H:



Cusp develops at $T=T_c$ and stays at $T<T_c$



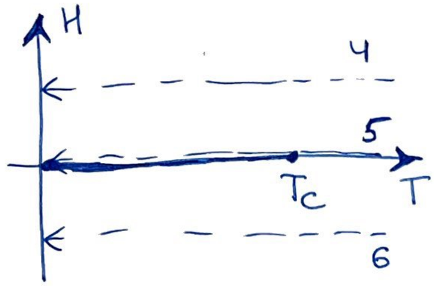
continuous but with infinite slope

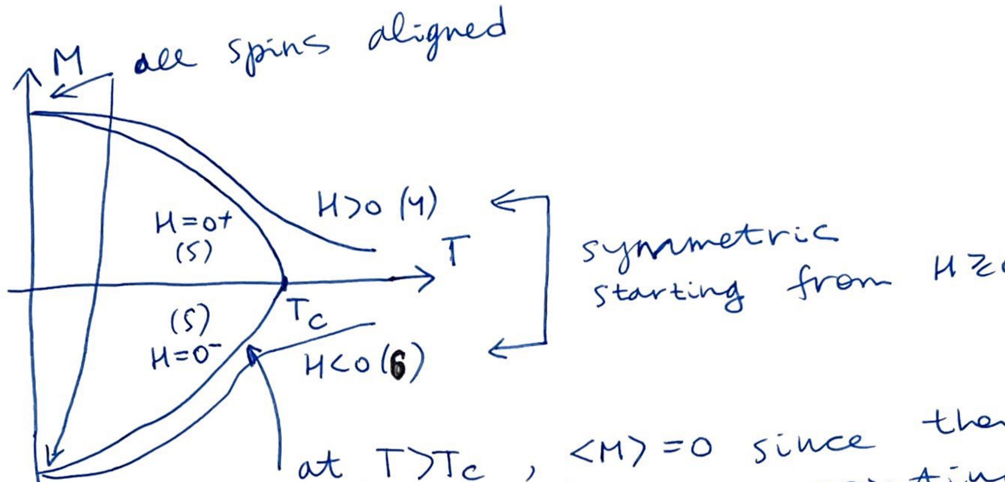


diverges (continuous phase transition)

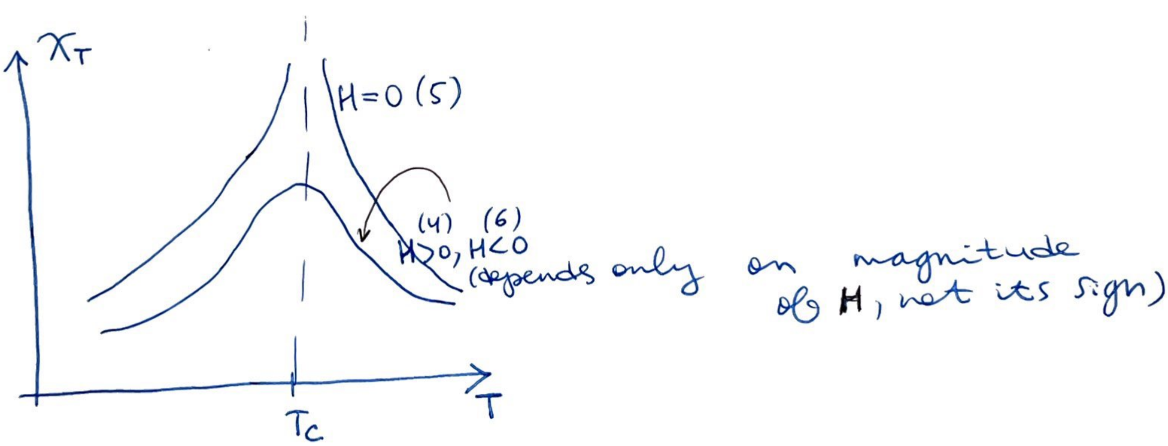
cusp at 1st order phase transition ($H=0$)

As a function of T:





at $T>T_c$, $\langle M\rangle=0$ since there're clusters of spins pointing up and down, & no preference between them. At $T=T_c$, one cluster "takes over" by chance, & then reaches saturation as $T\downarrow$



Critical exponents

Consider $t = \frac{T-T_c}{T_c}$

Critical exp. definition $\lambda = \lim_{t\to 0} \frac{\log|G(t)|}{\log|t|} \Rightarrow |G(t)| \sim |t|^\lambda$, or $G(t) \sim |t|^\lambda$.

For example,

$M \sim (-t)^\beta \quad [H=0] \quad \Rightarrow \beta \simeq \frac{1}{2}$ from the plot

$\chi_T \sim |t|^{-\gamma} \quad [H=0] \quad \Rightarrow \gamma > 0$ (χ_T diverges)

$$\Gamma(r) \sim \frac{1}{r^{d-2+\eta}}$$

Note that the same exponent works for χ_T above & below T_c (non-trivial!)

Corr'n length $\xi \sim |t|^{-\nu} \Rightarrow \nu > 0$

Universality

T_c depends on the system, but critical exponents are much more universal.

For example, in the 3D Ising model:

sc, bcc, fcc $\quad K_c = \frac{k_B T_c}{J} = 0.22, 0.16, 0.10$ respectively

But $\beta = 0.327$ is the same in all cases. So systems fall into universality classes $\Rightarrow$ can work with the simplest system of its class

Consider

$$C_H = T\left(\frac{\partial S}{\partial T}\right)_H = T\,\frac{\partial(S,H)}{\partial(T,H)} = T\,\frac{\dfrac{\partial(S,H)}{\partial(T,M)}}{\dfrac{\partial(T,H)}{\partial(T,M)}} \;\text{(=)}$$

$$\frac{\partial(S,H)}{\partial(T,H)} = \begin{vmatrix} \frac{\partial S}{\partial T} & \frac{\partial S}{\partial H} \\ \frac{\partial H}{\partial T} & \frac{\partial H}{\partial H} \end{vmatrix} = \left(\frac{\partial S}{\partial T}\right)_H \qquad \leftarrow (H,T) \text{ variables}$$

$$\frac{\partial(T,H)}{\partial(T,M)} = \begin{vmatrix} \frac{\partial T}{\partial T} & \frac{\partial T}{\partial M} \\ \frac{\partial H}{\partial T} & \frac{\partial H}{\partial M} \end{vmatrix} = \left(\frac{\partial H}{\partial M}\right)_T \qquad \leftarrow (M,T) \text{ variables}$$

$$\frac{\partial(S,H)}{\partial(T,M)} = \begin{vmatrix} \frac{\partial S}{\partial T} & \frac{\partial S}{\partial M} \\ \frac{\partial H}{\partial T} & \frac{\partial H}{\partial M} \end{vmatrix} = \qquad \leftarrow (M,T) \text{ variables}$$

$$= \left(\frac{\partial S}{\partial T}\right)_M \left(\frac{\partial H}{\partial M}\right)_T - \left(\frac{\partial S}{\partial M}\right)_T \left(\frac{\partial H}{\partial T}\right)_M$$

$$\text{(=)}\; T\,\frac{\left(\frac{\partial S}{\partial T}\right)_M \left(\frac{\partial H}{\partial M}\right)_T - \left(\frac{\partial S}{\partial M}\right)_T \left(\frac{\partial H}{\partial T}\right)_M}{\left(\frac{\partial H}{\partial M}\right)_T} =$$

$$= \underbrace{T\left(\frac{\partial S}{\partial T}\right)_M}_{C_M} - T\,\frac{\left(\frac{\partial S}{\partial M}\right)_T \left(\frac{\partial H}{\partial T}\right)_M}{\left(\frac{\partial H}{\partial M}\right)_T}$$

1^{st} law:

$dU = TdS - pdV$

Here, $V = \text{const}$ and

$dU = TdS - \underbrace{M}_{\text{no units}}\, d\underbrace{H}_{\text{units of energy}}$

Note that $\quad Z(H,T) = \sum_r e^{-\beta E_r}$

$$F_{(H,T)} = -k_B T \log Z(H,T) = U - TS$$

$$dF = \overbrace{dU} - TdS - SdT =$$

$$= \cancel{TdS} - MdH - \cancel{TdS} - SdT =$$

$$= -MdH - SdT$$

$\Leftarrow$

Entropy: $\quad S = -\left(\frac{\partial F}{\partial T}\right)_H$

Magnetization: $\quad M = -\left(\frac{\partial F}{\partial H}\right)_T$

$$\hookrightarrow \left(\frac{\partial S}{\partial H}\right)_T = \left(\frac{\partial M}{\partial T}\right)_H$$

OK, so $$(C_H - C_M)\left(\frac{\partial H}{\partial M}\right)_T = -T\left(\frac{\partial S}{\partial M}\right)_T \left(\frac{\partial H}{\partial T}\right)_M \qquad (*)$$

Likewise, $$d\tilde{u} = TdS + HdM = TdS - MdH + MdH + HdM = du + d(\underbrace{HM}_{\text{energy stored in magnetic field}})$$

$$d\tilde{F} = d\tilde{u} - TdS - SdT = HdM - SdT \Rightarrow \begin{cases} H = \left(\frac{\partial \tilde{F}}{\partial M}\right)_T, \\ S = -\left(\frac{\partial \tilde{F}}{\partial T}\right)_M \end{cases}$$

$$\Leftarrow \quad \left(\frac{\partial H}{\partial T}\right)_M = -\left(\frac{\partial S}{\partial M}\right)_T$$

$(*)$ gives $$(C_H - C_M)\left(\frac{\partial H}{\partial M}\right)_T = T\left(\frac{\partial H}{\partial T}\right)_M^2$$

$$\frac{\left(\frac{\partial H}{\partial T}\right)_M^2}{\left(\frac{\partial H}{\partial M}\right)_T} \overset{?}{=} \frac{\left(\frac{\partial M}{\partial T}\right)_H^2}{\left(\frac{\partial M}{\partial H}\right)_T}$$

$$\left(\frac{\partial M}{\partial H}\right)_T \left(\frac{\partial H}{\partial T}\right)_M \left(\frac{\partial H}{\partial T}\right)_M \overset{?}{=} \left(\frac{\partial H}{\partial M}\right)_T \left(\frac{\partial M}{\partial T}\right)_H \left(\frac{\partial M}{\partial T}\right)_H$$

$$\left(\frac{\partial M}{\partial H}\right)_T \left(\frac{\partial H}{\partial T}\right)_M \left(\frac{\partial T}{\partial M}\right)_H = -1$$

$$\left(\frac{\partial H}{\partial M}\right)_T \left(\frac{\partial M}{\partial T}\right)_H \left(\frac{\partial T}{\partial H}\right)_M = -1$$

$$\Rightarrow -\left(\frac{\partial M}{\partial T}\right)_H \left(\frac{\partial H}{\partial T}\right)_M = -\left(\frac{\partial H}{\partial T}\right)_M \left(\frac{\partial M}{\partial T}\right)_H \qquad 1 = 1$$

So, $$(C_H - C_M) = T\frac{\left(\frac{\partial M}{\partial T}\right)_H^2}{\underbrace{\left(\frac{\partial M}{\partial H}\right)_T}_{\chi_T}} \Rightarrow \chi_T (C_H - C_M) = T\left(\frac{\partial M}{\partial T}\right)_H^2$$

So, $\chi_T(C_H - C_M) = T\left(\frac{\partial M}{\partial T}\right)_H^2$.

Since $C_M \geq 0$ & $\chi_T \geq 0$, we have:

$$\boxed{C_H \geq \frac{T}{\chi_T}\left(\frac{\partial M}{\partial T}\right)_H^2}$$

as $t \to 0^-$ $(T \to T_c^-)$ in zero field $(H=0)$, we have: $t = \frac{T-T_c}{T_c}$

$$\begin{cases} C_H = a_1(\underbrace{-t}_{>0})^{-\alpha} & a_1 \geq 0 \text{ since } C_H \geq 0 \\ \chi_T = a_2(-t)^{-\gamma} & a_2 \geq 0 \text{ since } \chi_T \geq 0 \\ \left(\frac{\partial M}{\partial T}\right)_H = a_3(-t)^{\beta-1} & a_3 < 0 \text{ since } M \searrow \text{ as } T \nearrow \end{cases}$$

Then $a_1(-t)^{-\alpha} \geq \frac{T_c}{a_2}(-t)^{\gamma} a_3^2 (-t)^{2(\beta-1)}$, or

$$(-t)^{-\alpha-\gamma-2(\beta-1)} \geq \underbrace{\frac{T_c}{a_1 a_2} a_3^2}_{K>0},$$

$$\underbrace{-\log(-t)}_{>0}\,[\alpha+\gamma+2(\beta-1)] \geq \underbrace{\log K}_{\text{may be } <0 \text{ or } >0}$$

$$\alpha+\gamma+2(\beta-1) \geq \frac{\log K}{-\log(-t)} \to 0 \text{ as } t \to 0^-$$

Thus, $\boxed{\alpha+\gamma+2\beta \geq 2}$

However, we know from the exact solution of the 2D Ising model that

$\alpha = 0, \beta = \frac{1}{8}, \gamma = \frac{7}{4} \Rightarrow \alpha + \gamma + 2\beta = 2$, in fact

Need RG methods to see why the equality holds

Auxiliary relations:

1. $f(x,y)$ $\quad \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial y}\right)_f \left(\frac{\partial y}{\partial f}\right)_x \overset{?}{=} -1 \qquad [**]$
$x(f,y)$
$y(f,x)$

Indeed,

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy =$$

$$= \left(\frac{\partial f}{\partial x}\right)_y \left[\left(\frac{\partial x}{\partial f}\right)_y df + \left(\frac{\partial x}{\partial y}\right)_f dy \right] + \left(\frac{\partial f}{\partial y}\right)_x dy$$

$$= \underbrace{\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial f}\right)_y}_{=1} df + \underbrace{\left[\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial y}\right)_f + \left(\frac{\partial f}{\partial y}\right)_x \right]}_{=0} dy$$

$\Downarrow$

$[**]$ follows

2. $$\frac{\partial(u,v)}{\partial(x,y)} = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{vmatrix}$$

Note that $\quad \frac{\partial(u,v)}{\partial(x,y)} = -\frac{\partial(v,u)}{\partial(x,y)}$

$$\frac{\partial(u,y)}{\partial(x,y)} = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial y} \end{vmatrix} = \left(\frac{\partial u}{\partial x}\right)_y$$

Finally, $\quad \frac{\partial(u,v)}{\partial(x,y)} = \frac{\partial(u,v)}{\partial(t,s)} \frac{\partial(t,s)}{\partial(x,y)}$

$\uparrow$ can be checked by direct substitution