Mathematical Statistical Physics

29 July - 3 August 2013, YITP, Kyoto

Phase separation, interfaces and wetting in two dimensions. Exact results from field theory

Gesualdo Delfino

SISSA, Trieste

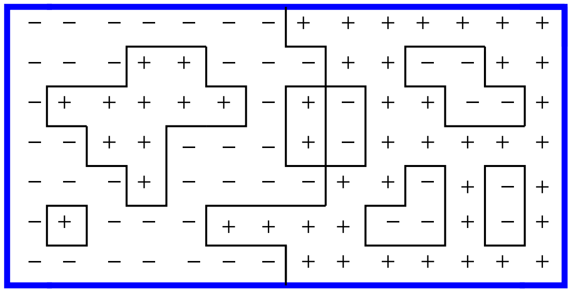
Based on :

GD, J. Viti, Phase separation and interface structure in two dimensions from field theory, J. Stat. Mech. (2012) P10009 [arXiv:1206.4959]

GD, A. Squarcini, Interfaces and wetting transition on the half plane. Exact results from field theory, J. Stat. Mech. (2013) P05010 [arXiv:1303.1938]

GD, A. Squarcini, Multiple interfaces, to appear

phase separation classical topic of statistical mechanics emphasizing role of boundary conditions and notion of interface



exact analytic results for bulk magnetization have been available for 2D Ising

issues in 2D:

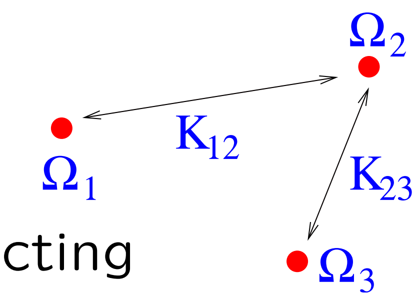
- general results
- role of integrability
- universality

answers provided by field theory

Pure phases and kinks

ferromagnet with spin σ taking discrete values, and 2nd order transition at T_c

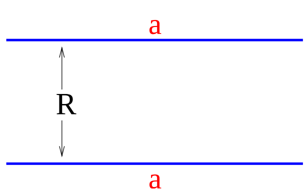
scaling limit $\leftrightarrow$ Euclidean field theory



below T_c : degenerate vacua $|\Omega_a\rangle$

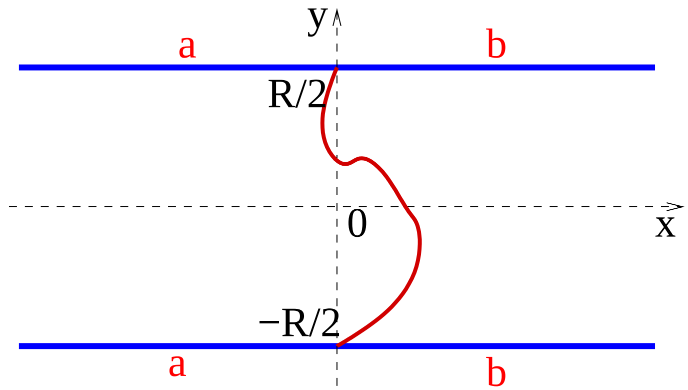
elementary excitations in 2D : kinks $|K_{ab}(\theta)\rangle$ connecting $|\Omega_a\rangle$ and $|\Omega_b\rangle$ $\quad (e,p) = (m_{ab}\cosh\theta, m_{ab}\sinh\theta)$

$|\Omega_a\rangle$, $|\Omega_b\rangle$ non-adjacent if connected by $|K_{ac_1}(\theta_1)K_{c_1c_2}(\theta_2)\dots K_{c_{j-1}b}(\theta_j)\rangle$ with $j > 1$ only

$\lim_{R\to\infty}$  : pure phase a $\quad \langle\sigma\rangle_a \equiv \langle\Omega_a|\sigma(x,y)|\Omega_a\rangle$

Phase separation (adjacent phases)

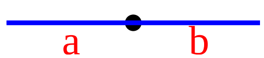
surface tension :



$$\Sigma_{ab} = -\lim_{R\to\infty} \frac{1}{R} \ln \frac{Z_{ab}(R)}{Z_a(R)}$$

boundary states :

$$|B_{ab}(\pm\tfrac{R}{2})\rangle =$$



$$= e^{\pm\frac{R}{2}H}\left[\int \frac{d\theta}{2\pi} f(\theta)|K_{ab}(\theta)\rangle + \sum_c \int |K_{ac}K_{cb}\rangle + \ldots\right]$$

$$|B_a(\pm\tfrac{R}{2})\rangle =$$

$$= e^{\pm\frac{R}{2}H}\left[|\Omega_a\rangle + \sum_c \int |K_{ac}K_{ca}\rangle + \ldots\right]$$

$$\begin{cases} Z_{ab}(R) = \langle B_{ab}(\frac{R}{2})|B_{ab}(-\frac{R}{2})\rangle \sim \dfrac{|f(0)|^2}{\sqrt{2\pi m_{ab}R}}\, e^{-m_{ab}R} \\ Z_a(R) = \langle B_a(\frac{R}{2})|B_a(-\frac{R}{2})\rangle \sim \langle\Omega_a|\Omega_a\rangle = 1 \end{cases} \Longrightarrow \quad \Sigma_{ab} = m_{ab}$$

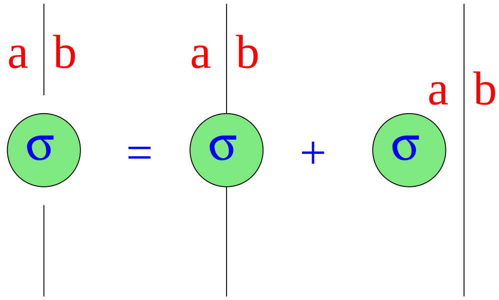
magnetization profile :

$$\langle\sigma(x,0)\rangle_{ab} = \frac{1}{Z_{ab}}\langle B_{ab}(\tfrac{R}{2})|\sigma(x,0)|B_{ab}(-\tfrac{R}{2})\rangle \qquad \theta_{12}\equiv\theta_1-\theta_2$$

$$\sim \frac{|f(0)|^2}{Z_{ab}}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\,F^{\sigma}_{ab}(\theta_1|\theta_2)\,e^{-m[(1+\frac{\theta_1^2}{4}+\frac{\theta_2^2}{4})R-i\theta_{12}x]} \qquad mR\gg 1$$

$$F^{\sigma}_{ab}(\theta_1|\theta_2)\equiv\langle K_{ab}(\theta_1)|\sigma(0,0)|K_{ab}(\theta_2)\rangle$$

$$= i\frac{\langle\sigma\rangle_a-\langle\sigma\rangle_b}{\theta_{12}-i\epsilon}+\sum_{n=0}^{\infty}c_n\,\theta_{12}^n+2\pi\,\delta(\theta_{12})\langle\sigma\rangle_a$$



[Berg, Karowski, Weisz, '78; Smirnov, 80's; GD, Cardy, '98] Does not require integrability

$$\Rightarrow \quad \langle\sigma(x,0)\rangle_{ab} = \tfrac{1}{2}[\langle\sigma\rangle_a+\langle\sigma\rangle_b]-\tfrac{1}{2}[\langle\sigma\rangle_a-\langle\sigma\rangle_b]\,\mathrm{erf}(\sqrt{\tfrac{2m}{R}}\,x)$$

$$+c_0\sqrt{\frac{2}{\pi mR}}\,e^{-2mx^2/R}+\ldots \qquad \mathrm{erf}(z)\equiv\frac{2}{\sqrt{\pi}}\int_0^z dt\,e^{-t^2}$$

$$\langle\sigma(x,0)\rangle_{ab} = \frac{1}{2}[\langle\sigma\rangle_a + \langle\sigma\rangle_b] - \frac{1}{2}[\langle\sigma\rangle_a - \langle\sigma\rangle_b]\,\mathrm{erf}\left(\sqrt{\frac{2m}{R}}\,x\right)$$

$$+c_0\sqrt{\frac{2}{\pi m R}}\,e^{-2mx^2/R} + \dots$$

Ising: $\langle\sigma\rangle_+ = -\langle\sigma\rangle_-$, $c_0 = 0$ (by parity); $\langle\sigma\rangle_{-+} \sim \langle\sigma\rangle_+ \mathrm{erf}(\sqrt{\frac{2m}{R}}x)$

matches lattice result [Abraham, '81]

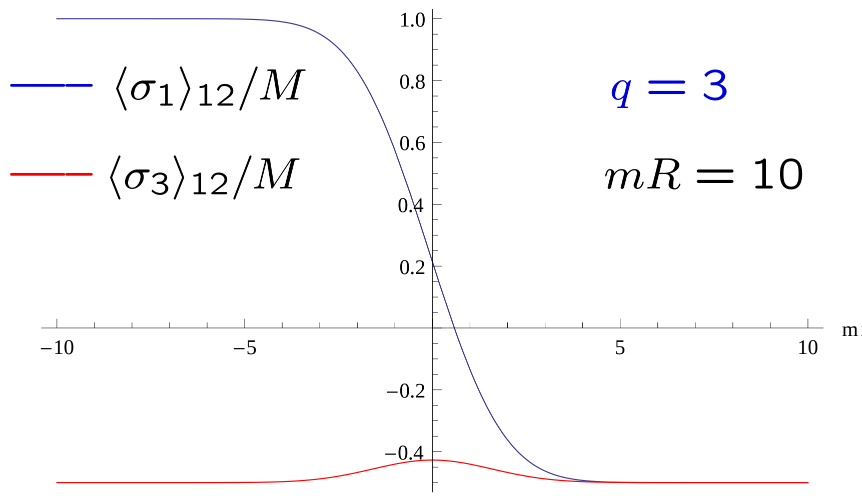
q-state Potts:

$\sigma_c(x) = \delta_{s(x),c} - 1/q\,, \quad c = 1,\dots,q$

$\langle\sigma_c\rangle_a = (q\delta_{ac} - 1)\frac{M}{q-1}$

$c_0^{ab,c} = [2 - q(\delta_{ac} + \delta_{bc})]B(q)$

$B(3) = \frac{M}{4\sqrt{3}}, \quad B(4) = \frac{M}{3\sqrt{3}}$



- non-local (erf) term amounts to sharp separation between pure phases
- local (gaussian) term sensitive to interface structure

percolation:

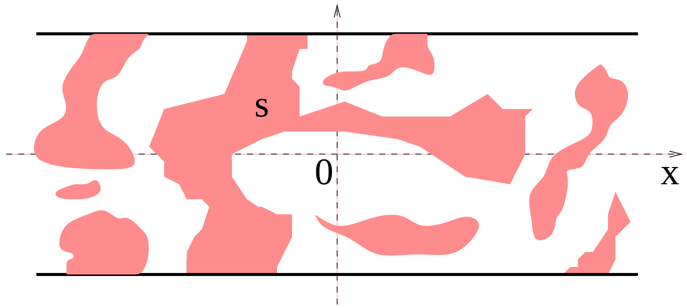
sites randomly occupied with probability p

on the plane: infinite cluster for $p > p_c$

P=prob. site $\in$ infinite cluster

maps on $q \to 1$ Potts

on the strip, take only configurations without clusters connecting left and right parts of the boundary

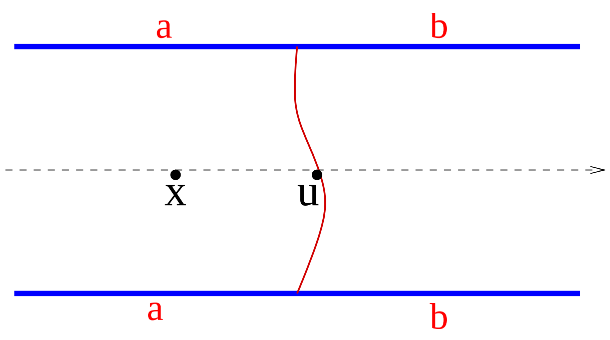


$P_s(x,0)$=prob. $(x,0) \in$ cluster spanning at $x<0$ $(p > p_c)$

$$= \frac{P}{2}\left[1 - \mathrm{erf}\left(\sqrt{\frac{2m}{R}}\,x\right) - \gamma\sqrt{\frac{2}{\pi m R}}e^{-2mx^2/R} + \cdots\right]$$

Passage probability and interface structure

$$\langle\sigma(x,0)\rangle_{ab} = \int_{-\infty}^{+\infty} du\, \sigma_{ab}(x|u)\, p(u)$$



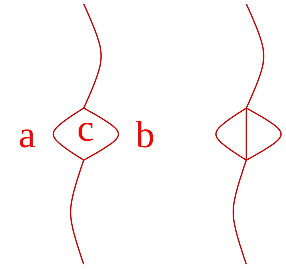
$p(u)du$ = passage probability in $(u, u+du)$

$$\sigma_{ab}(x|u) = \Theta(u-x)\langle\sigma\rangle_a + \Theta(x-u)\langle\sigma\rangle_b + A_0\delta(x-u) + A_1\delta'(x-u) + \ldots$$

$$\Theta(x) \equiv \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$

matches field theory for $p(u) = \sqrt{\frac{2m}{\pi R}}\, e^{-2mu^2/R}$, $\quad A_0 = \frac{c_0}{m}$

- local terms account for branching



for $y \neq 0$ field theory leads to

$$p(u;y) = \frac{1}{\rho(y)}\sqrt{\frac{2m}{\pi R}}\, e^{-2mu^2/R\rho^2(y)} \qquad \forall\, |y| < \frac{R}{2} \text{ as } R \to \infty$$

$$\rho(y) = \sqrt{1 - (\frac{y}{R/2})^2}$$

$\Longrightarrow$ the interface behaves as a brownian bridge

- brownian bridge property rigorously known for Ising and Potts [Greenberg, Joffe, '05; Campanino, Joffe, Velenik, '08]

- field theory says that it holds for any interface between adjacent phases

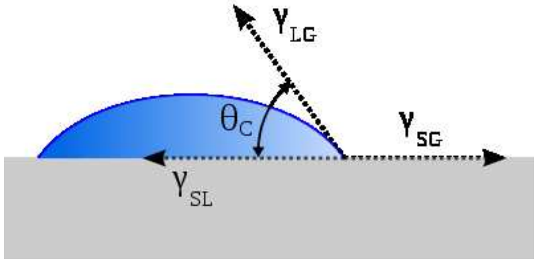
Wetting

is the ability of a phase to maintain contact with a surface

phenomenological description in terms of contact angle θ_c

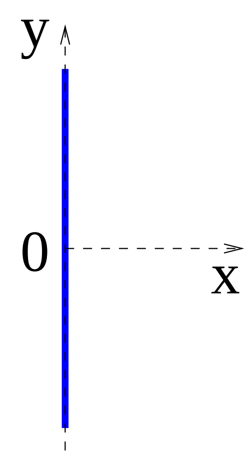
$0 < \theta_c < \pi$: partial wetting

$\theta_c = 0$: complete wetting



equilibrium condition at contact points known as Young's law

half plane :



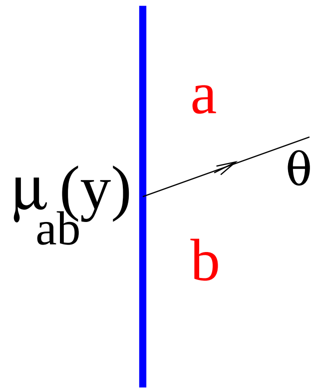
B_a = boundary condition at $x = 0$
breaking the symmetry in direction a

$$\langle\sigma(x,y)\rangle_{B_a} = {}_{B_a}\langle\Omega|\sigma(x,y)|\Omega\rangle_{B_a} \to \langle\sigma\rangle_a\,, \quad x\to\infty$$

$$H_{B_a}\,|\Omega\rangle_{B_a} = E_B\,|\Omega\rangle_{B_a} \qquad\qquad H_{B_a}\,|K_{ba}(\theta)\rangle_{B_a} = (E_B + m\cosh\theta)\,|K_{ba}(\theta)\rangle_{B_a}$$

boundary condition changing fields :

$\mu_{ab}(y)$ switches from B_a to B_b



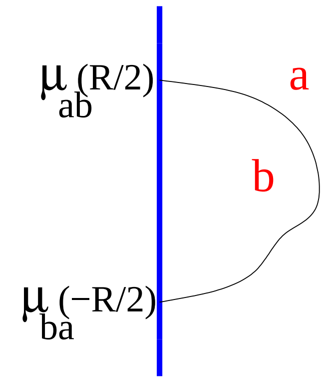
$$_{B_a}\langle\Omega|\mu_{ab}(y)|K_{ba}(\theta)\rangle_{B_a} = e^{-ym\cosh\theta}\mathcal{F}_\mu(\theta)$$

$$\mathcal{F}_\mu(\theta) = a\,\theta + O(\theta^2)$$

pinned interfaces :

$$Z_{B_{aba}} = {}_{B_a}\langle \Omega | \mu_{ab}(\tfrac{R}{2}) \mu_{ba}(-\tfrac{R}{2}) | \Omega \rangle_{B_a}$$

$$\sim \int \frac{d\theta}{2\pi} |\mathcal{F}_\mu(\theta)|^2 \, e^{-mR\cosh\theta} \sim \frac{|a|^2 \, e^{-mR}}{2\sqrt{2\pi}(mR)^{3/2}}$$



$$\langle \sigma(x,0) \rangle_{B_{aba}} = Z^{-1}_{B_{aba}} \, {}_{B_a}\langle \Omega | \mu_{ab}(\tfrac{R}{2}) \sigma(x,0) \mu_{ba}(-\tfrac{R}{2}) | \Omega \rangle_{B_a}$$

$$\sim \frac{1}{Z_{B_{aba}}} \int \frac{d\theta_1}{2\pi} \frac{d\theta_2}{2\pi} \, \mathcal{F}_\mu(\theta_1) \, F^\sigma_{ab}(\theta_1|\theta_2) \, \mathcal{F}^*_\mu(\theta_2) \, e^{-m[(1+\frac{\theta_1^2}{4}+\frac{\theta_2^2}{4})R - i\theta_{12}x]}$$

$$\sim \langle \sigma \rangle_b + (\langle \sigma \rangle_a - \langle \sigma \rangle_b) \left[\mathrm{erf}(\sqrt{\tfrac{2m}{R}}\, x) - \sqrt{\tfrac{8m}{\pi R}}\, x \, e^{-\frac{2m}{R}x^2} \right], \qquad mR,\, mx \gg 1$$

$$\langle \sigma(x,0) \rangle_{B_{aba}} \to \begin{cases} \langle \sigma \rangle_a \,, & x \to \infty \\ \langle \sigma \rangle_b \,, & R \to \infty \end{cases}$$ wall-interface distance $\sim \sqrt{R}$

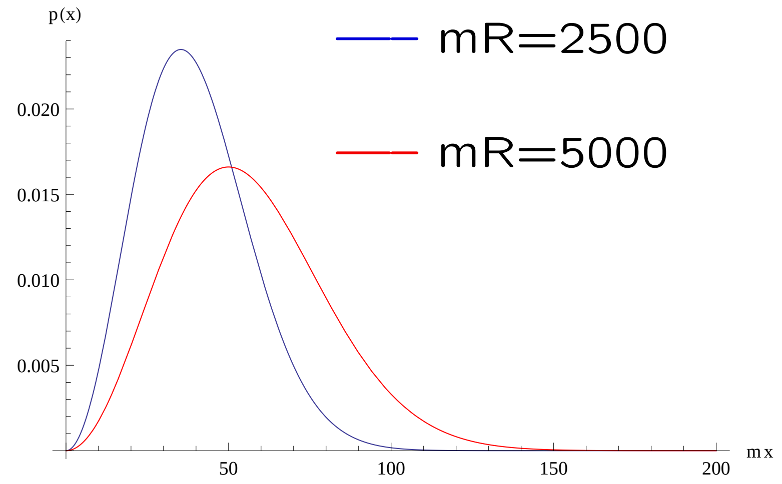
Ising: $\langle \sigma \rangle_+ = -\langle \sigma \rangle_-$; matches lattice result [Abraham, '80]

passage probability :

$$\langle \sigma(x,0) \rangle_{B_{aba}} \sim \langle \sigma \rangle_a \int_0^x du\, p(u) + \langle \sigma \rangle_b \int_x^\infty du\, p(u)\,, \qquad mx \gg 1$$

matches field theory for

$$p(x) = \frac{4}{\sqrt{\pi}} \left(\frac{2m}{R}\right)^{3/2} x^2\, e^{-2mx^2/R}$$



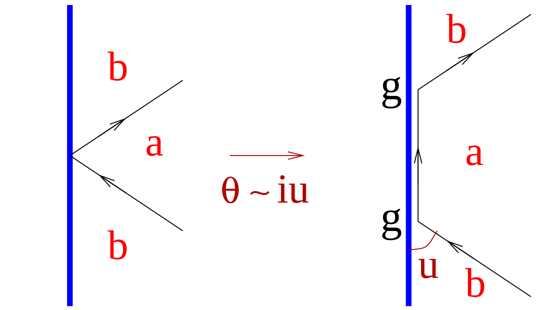
general result provided :

i) adjacent phases

ii) no boundary bound states

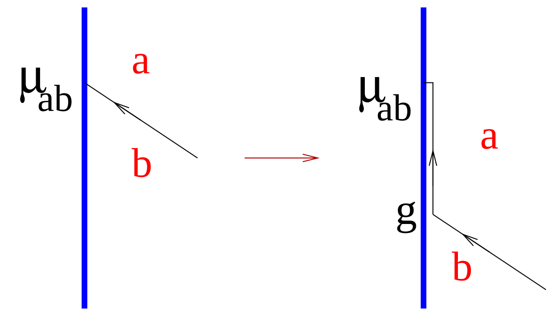
boundary bound states:

kink-boundary amplitude has pole at $\theta = iu$



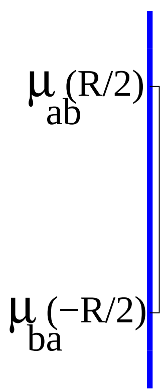
$$|K_{ba}(\theta \simeq iu)\rangle_{B_a} \sim |\Omega\rangle_{B'_a}$$

$$E_{B'} = E_B + m\cos u\,, \qquad 0 < u < \pi$$



$$\mathcal{F}_\mu(\theta \simeq iu) \simeq \frac{ig}{\theta - iu}\ {}_{B_a}\langle\Omega|\mu_{ab}(0)|\Omega\rangle_{B'_a}$$

$|\Omega\rangle_{B'_a}$ now leading as $R \to \infty$



$$Z_{B_{aba}} \sim \left|{}_{B_a}\langle\Omega|\mu_{ab}(0)|\Omega\rangle_{B'_a}\right|^2 e^{-mR\cos u}$$

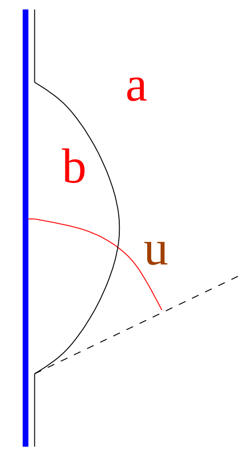
$$\langle\sigma(x,0)\rangle_{B_{aba}} = \langle\sigma(x,0)\rangle_{B'_a} + O(e^{-mR(1-\cos u)})$$

$$\langle\sigma(x \gg \tfrac{1}{m}, 0)\rangle_{B_{aba}} \to \langle\sigma\rangle_a \ \forall R \quad \Rightarrow \quad mR \text{ diverges faster than } 1/u^2$$

field theory $\longleftrightarrow$ wetting phenomenology dictionary :

splitting and recombination of B'_a $\longleftrightarrow$ partial wetting

u = contact angle



$E_{B'} = E_B + m \cos u$ $\longleftrightarrow$ Young's condition

$m(\cos u - 1)$ = spreading coefficient

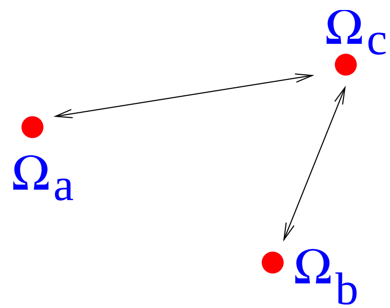
$u = 0$ $\longleftrightarrow$ complete wetting

$\lambda \int dy\, \phi(0, y)$ boundary interaction : $u = u(\frac{(T_c - T)^{(1-x_\phi)\nu}}{\lambda})$

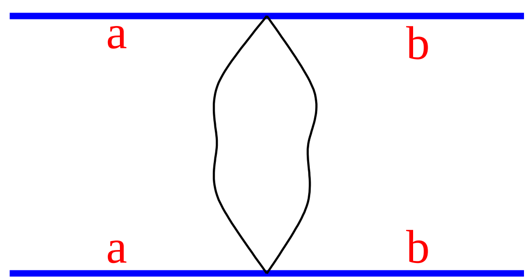
$u = 0$ determines wetting transition temperature $T_w(\lambda) < T_c$

Double interfaces

suppose going from $|\Omega_a\rangle$ to $|\Omega_b\rangle$ requires two kinks



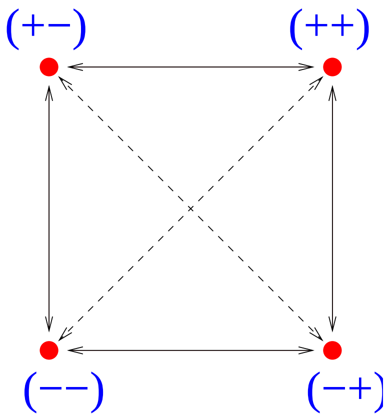
$$|B_{ab}(\pm\tfrac{R}{2})\rangle = e^{\pm\frac{R}{2}H}\left[\sum_c \int d\theta_1 d\theta_2\, f_{acb}(\theta_1,\theta_2)\, |K_{ac}(\theta_1)K_{cb}(\theta_2)\rangle + \ldots\right]$$



Ashkin-Teller

$\sigma_1, \sigma_2 = \pm 1$

$$H = -\sum_{\langle x_1 x_2 \rangle} \{J[\sigma_1(x_1)\sigma_1(x_2) + \sigma_2(x_1)\sigma_2(x_2)] + J_4\,\sigma_1(x_1)\sigma_1(x_2)\sigma_2(x_1)\sigma_2(x_2)\}$$



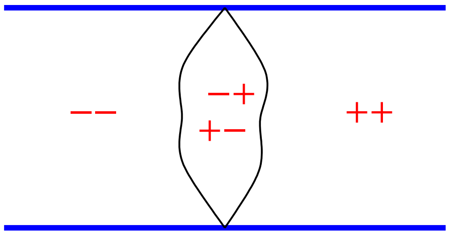
4 degenerate vacua below T_c

scaling limit $\rightarrow$ sine-Gordon

$$\Sigma_{(++)(+-)} = m$$

$$\Sigma_{(++)(--)} = \begin{cases} 2m \sin\frac{\pi\beta^2}{2(8\pi-\beta^2)}\,, & J_4 > 0 \\ 2m\,, & J_4 \leq 0 \end{cases}$$

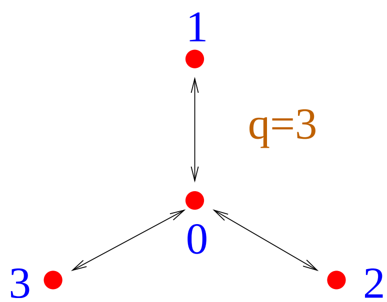
$$\frac{4\pi}{\beta^2} = 1 - \frac{2}{\pi}\arcsin\left(\frac{\tanh 2J_4}{\tanh 2J_4 - 1}\right) \text{ on square lattice}$$

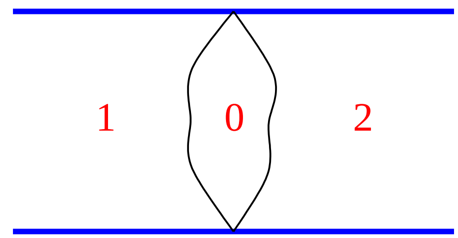


double interface between $(--)$ and $(++)$ for $J_4 \leq 0$

(dilute for $q \le 4$) Potts model at T_c

kinks relate ordered vacua to disordered one [GD, '99; GD, Cardy, '00]





field theory gives

$$\langle\sigma_1(x,0)\rangle_{12} \sim \frac{\langle\sigma_1\rangle_1}{2}\left[\frac{q-2}{2(q-1)}\left(1-\frac{2}{\pi}\,e^{-2z^2}-\frac{2z}{\sqrt{\pi}}\,\text{erf}(z)e^{-z^2}+\text{erf}^2(z)\right)\right.$$

$$\left.+\frac{q}{q-1}\left(\frac{z}{\sqrt{\pi}}\,e^{-z^2}-\text{erf}(z)\right)\right] \qquad\qquad z\equiv\sqrt{\frac{2m}{R}}\,x$$

(cf. asymptotics of Ising $\langle\sigma\sigma\sigma\rangle$ [McCoy, Wu, '78; Abraham, Upton, '93])

$\Rightarrow$ passage probability $\;p(x_1,x_2)=\frac{2m}{\pi R}\,(z_1-z_2)^2\,e^{-(z_1^2+z_2^2)}$

mutually avoiding interfaces

Conclusion

- field theory yields exact asymptotic results for phase separation in 2D

- reason is not integrability, but that interfaces are particle trajectories $\Rightarrow$ results are general

- notion of interface emerges directly in the continuum

- although $mR \gg 1$ projects to low energies, relativistic particles essential for kinematical poles ($\longrightarrow$ erf) and contact angle

- phase separation basic application of kinematical poles, massive boundary states and boundary changing operators, boundary bound states

- SLE describes fractal curves at criticality; connection with the off-critical case of this talk?