Lattice Models: Exact Methods and Combinatorics

18 – 22 May 2015, GGI Arcetri, Florence

Phase Separation, Interfaces and Wetting in Two Dimensions

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Based on :

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

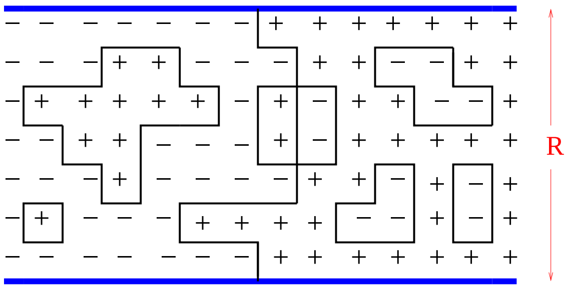
GD, A. Squarcini, Interfaces and wetting transition on the half plane. Exact results from field theory, J. Stat. Mech. (2013) P05010

GD, A. Squarcini, Exact theory of intermediate phases in two dimensions, Annals of Physics 342 (2014) 171

GD, A. Squarcini, Phase separation in a wedge. Exact results, PRL 113 (2014) 066101

GD, Order parameter profiles in presence of topological defect lines, J. Phys. A 47 (2014) 132001

Introduction



Ising ferromagnet: phase separation emerges when $T < T_c$, $R \gg \xi$

exact magnetization profile [Abraham, '81]

Issues :

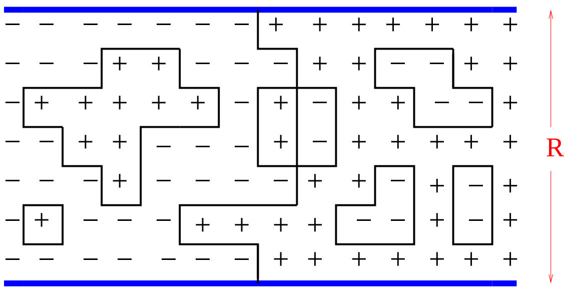
– role of integrability

– other universality classes

– structure of the interfacial region

– different geometries

Introduction



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– role of integrability

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– different geometries

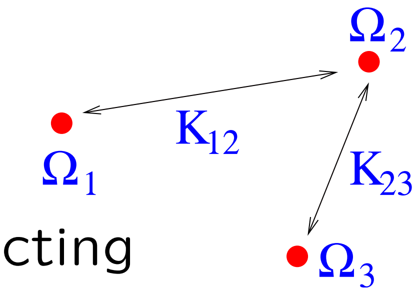
field theory yields exact answers and suggests applications in $D > 2$

Pure phases and kinks

bulk system at a spontaneous symmetry breaking point

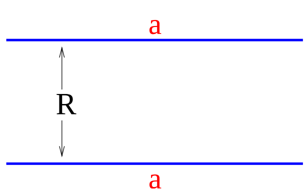
scaling limit $\leftrightarrow$ Euclidean field theory $\leftrightarrow$ QFT with imaginary time

coexisting phases $\leftrightarrow$ degenerate vacua $|\Omega_a\rangle$



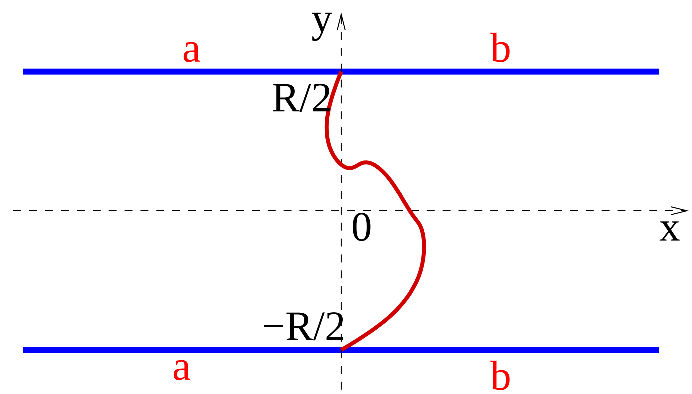
elementary excitations in 2D : kinks $|K_{ab}(\theta)\rangle$ connecting $|\Omega_a\rangle$ and $|\Omega_b\rangle$ $\quad (e,p) = (m_{ab} \cosh\theta, m_{ab} \sinh\theta)$

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

$\lim_{R\to\infty}$ 

: pure phase a $\qquad \langle\sigma\rangle_a \equiv \langle\Omega_a|\sigma(x,y)|\Omega_a\rangle$

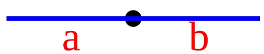
Phase separation (adjacent phases)



interfacial free energy :

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

boundary states :

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

$|B_a(\pm\frac{R}{2})\rangle =$  $= e^{\pm\frac{R}{2}H} [|\Omega_a\rangle + \sum_c \int |K_{ac}K_{ca}\rangle + \dots]$

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

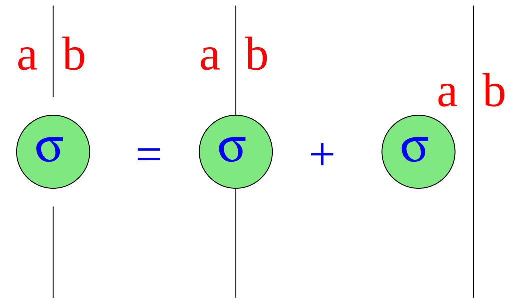
order parameter profile :

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

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

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

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



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

$\Rightarrow$

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

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

kinematical pole at $\theta_{12}=0$ accounts for phase separation in 2D

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

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

Ising: $\langle\sigma\rangle_+ = -\langle\sigma\rangle_-\,,\ c_0 = 0 \quad \Rightarrow \quad \langle\sigma\rangle_{-+} \sim \langle\sigma\rangle_+\,\mathrm{erf}(\sqrt{\tfrac{2m}{R}}x)$

matches lattice result [Abraham, '81]

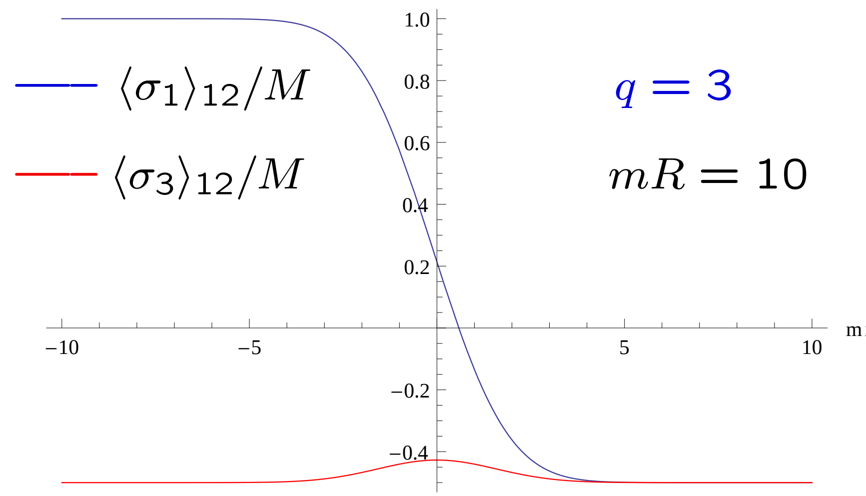
q-state Potts ($q \le 4$):

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

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

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

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

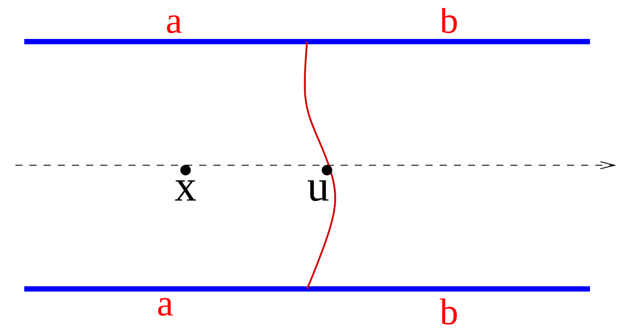


- non-local (erf) term amounts to sharp separation between pure phases
- local (gaussian) term sensitive to interface structure

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 $(u, u + du)$

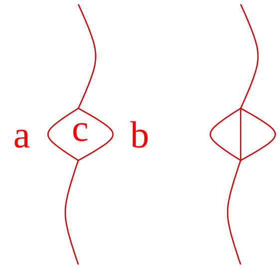


$$\sigma_{ab}(x|u) = \Theta(u-x)\langle\sigma\rangle_a + \Theta(x-u)\langle\sigma\rangle_b + A_0\delta(x-u) + A_1\delta'(x-u) + \dots$$

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

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

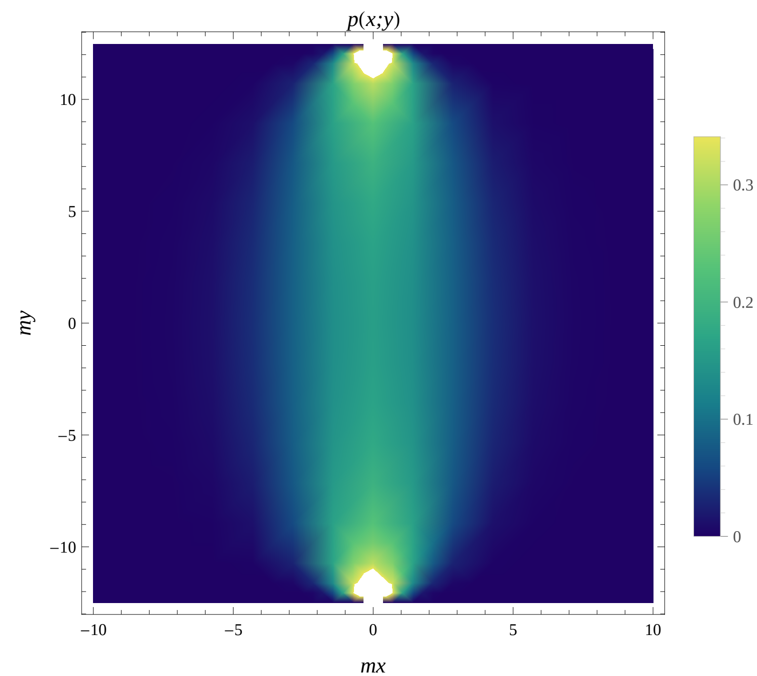
- local terms account for branching



for $y \neq 0$ the passage probability density becomes

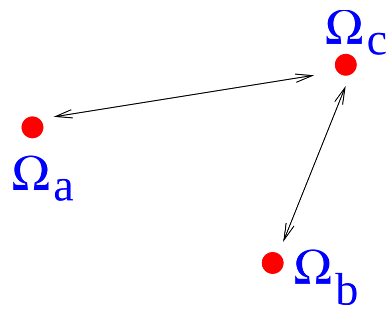
$$p(x;y) = \frac{1}{\kappa}\sqrt{\frac{2m}{\pi R}}\, e^{-\chi^2}$$

$$\kappa(y) \equiv \sqrt{1 - 4y^2/R^2} \qquad\qquad \chi \equiv \sqrt{\frac{2m}{R}}\,\frac{x}{\kappa}$$

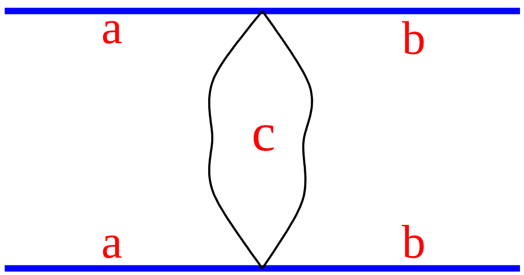


Double interfaces

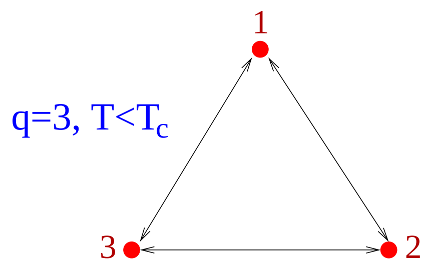
suppose going from $|\Omega_a\rangle$ to $|\Omega_b\rangle$ requires two kinks

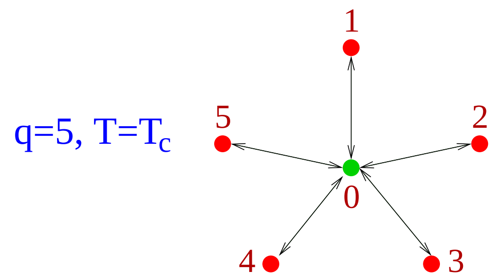


$$|B_{ab}(\pm\tfrac{R}{2})\rangle = e^{\pm\frac{R}{2}H}\,[\int d\theta_1 d\theta_2\, f_{acb}(\theta_1,\theta_2)\,|K_{ac}(\theta_1)K_{cb}(\theta_2)\rangle + \ldots]$$

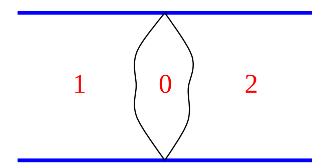


q-**state Potts:** the order of the transition changes at $q = 4$





$q \to 4^+$, $T = T_c$: field theory gives



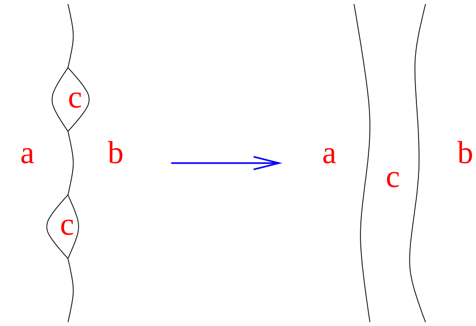
$$\langle \sigma_1(x,0) \rangle_{12} \sim \frac{\langle \sigma_1 \rangle_1}{2} \left[\frac{q-2}{2(q-1)} \left(1 - \frac{2}{\pi} e^{-2z^2} - \frac{2z}{\sqrt{\pi}} \mathrm{erf}(z) e^{-z^2} + \mathrm{erf}^2(z) \right) \right.$$

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

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

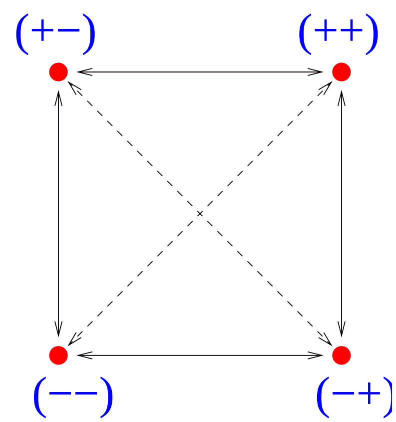
mutually avoiding interfaces

Wetting transition



Ashkin-Teller : $\sigma_1, \sigma_2 = \pm 1$

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

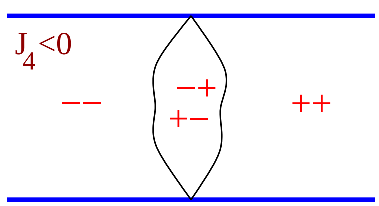


4 degenerate vacua below T_c

scaling limit $\rightarrow$ sine-Gordon

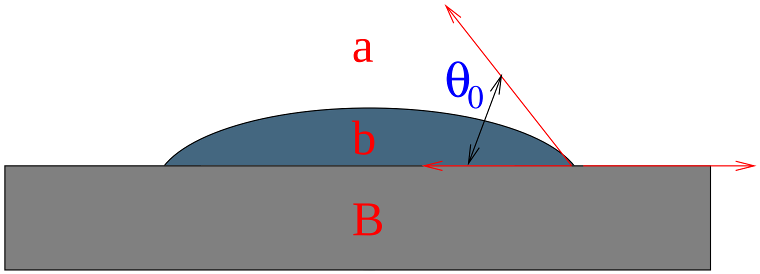
$$\Sigma_{(++)(+-)} = m \quad \forall J_4$$

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



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

Boundary wetting



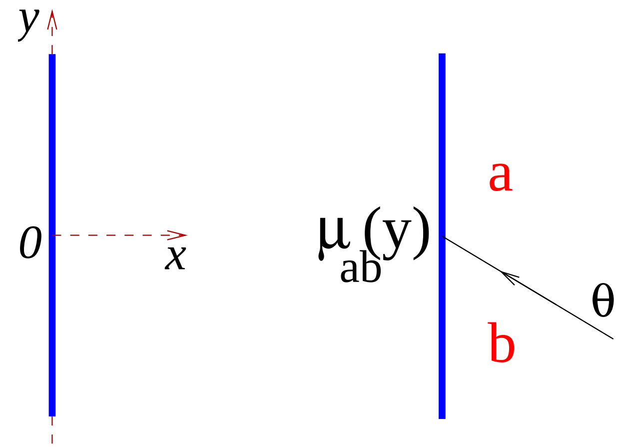
phenomenological description in terms of contact angle θ_0

wetting transition for $\theta_0 = 0$

equilibrium condition at contact points (Young's law, 1805):

$$\Sigma_{Ba} = \Sigma_{Bb} + \Sigma_{ab} \cos\theta_0$$

field theory :



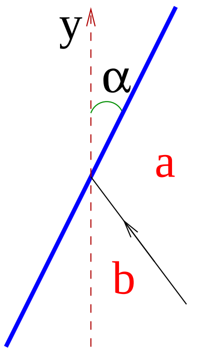
B_a boundary condition selecting the vacuum $|\Omega_a\rangle_0$ whit energy E_0

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

$$_0\langle\Omega_a|\mu_{ab}(y)|K_{ba}(\theta)\rangle_0 = e^{-ym\cosh\theta}\mathcal{F}_0^{\mu}(\theta)$$

forbid the particle to stay on the boundary $\Rightarrow$ $\mathcal{F}_0^{\mu}(\theta) = c\,\theta + O(\theta^2)$

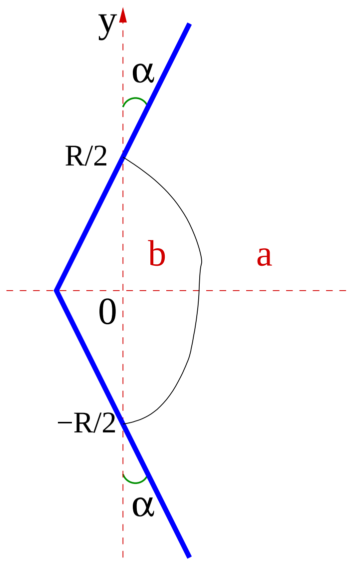
Lorentz boost $\mathcal{B}_\Lambda$ sends $\theta \to \theta + \Lambda$



$\mathcal{B}_{-i\alpha}$ rotates by an angle α: $\mathcal{F}_0^{\mu}(\theta) = \mathcal{F}_\alpha^{\mu}(\theta - i\alpha)$

$\mathcal{F}_\alpha^{\mu}(\theta) \simeq c(\theta + i\alpha)$ for θ, α small

interface in a wedge :

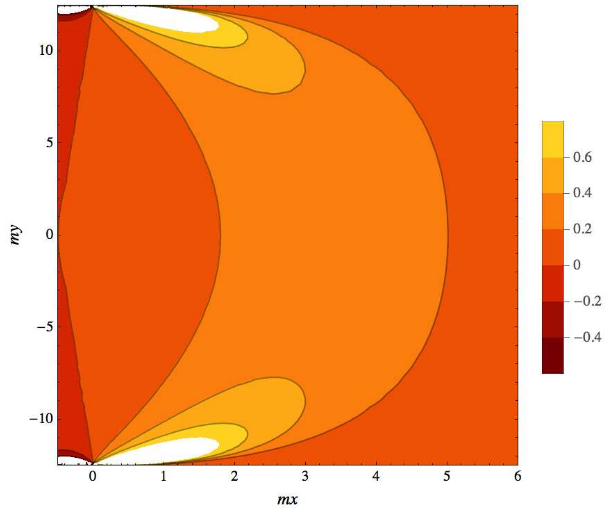


$$\langle\sigma(x,y)\rangle_{W_{aba}} = \frac{{}_\alpha\langle\Omega_a|\mu_{ab}(0,\frac{R}{2})\sigma(x,y)\mu_{ba}(0,-\frac{R}{2})|\Omega_a\rangle_{-\alpha}}{{}_\alpha\langle\Omega_a|\mu_{ab}(0,\frac{R}{2})\mu_{ba}(0,-\frac{R}{2})|\Omega_a\rangle_{-\alpha}} \sim$$

$$\frac{\int_{-\infty}^{+\infty}\frac{d\theta_1 d\theta_2}{(2\pi)^2}\mathcal{F}^\mu_\alpha(\theta_1)F_\sigma(\theta_1|\theta_2)\mathcal{F}^\mu_{-\alpha}(\theta_2)e^{-\frac{m}{2}[(\frac{R}{2}-y)\theta_1^2+(\frac{R}{2}+y)\theta_2^2]+imx(\theta_1-\theta_2)}}{\int_0^\infty \frac{d\theta}{2\pi}\,\mathcal{F}^\mu_\alpha(\theta)\mathcal{F}^\mu_{-\alpha}(\theta)\,e^{-mR\frac{\theta^2}{2}}}$$

$$\sim \langle\sigma\rangle_b + (\langle\sigma\rangle_a - \langle\sigma\rangle_b)\Big[\mathrm{erf}(\chi) - \frac{2}{\sqrt{\pi}}\,\frac{\chi+\sqrt{2mR}\,\frac{\alpha}{\kappa}}{1+mR\alpha^2}\,e^{-\chi^2}\Big]$$

$$\kappa \equiv \sqrt{1-4y^2/R^2} \qquad \chi \equiv \sqrt{\frac{2m}{R}}\,\frac{x}{\kappa}$$



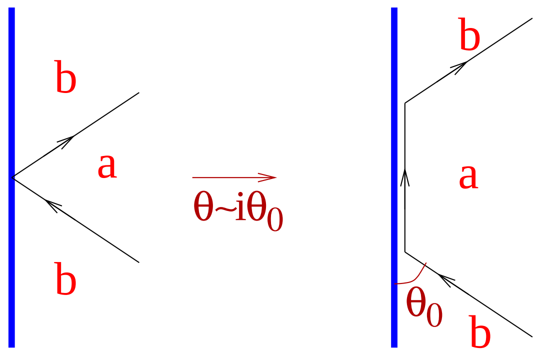
passage probability density:

$$p(x;y) \sim \frac{8\sqrt{2}}{\sqrt{\pi}\,\kappa^3}\left(\frac{m}{R}\right)^{3/2}\frac{\left(x+\frac{R\alpha}{2}\right)^2-(\alpha y)^2}{1+mR\alpha^2}\,e^{-\chi^2}$$

wedge wetting :

$\alpha = 0$: for $T < T_0 < T_c$ boundary bound state $|\Omega'_a\rangle_0$ with energy

$$E'_0 = E_0 + m\cos\theta_0 \qquad \text{Young's law!}$$



resonance angle θ_0 = contact angle

wetting transition = kink unbinding : $\theta_0(T_0) = 0$

wedge wetting :

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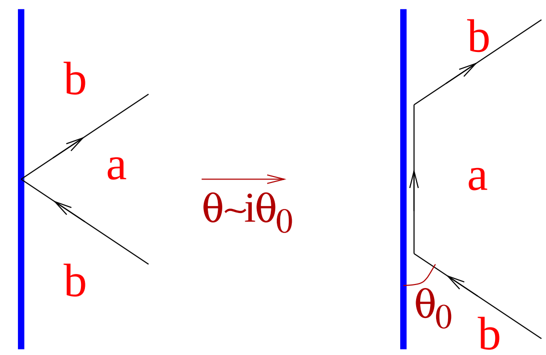


$$E'_0 = E_0 + m\cos\theta_0 \qquad \text{Young's law!}$$

resonance angle θ_0 = contact angle

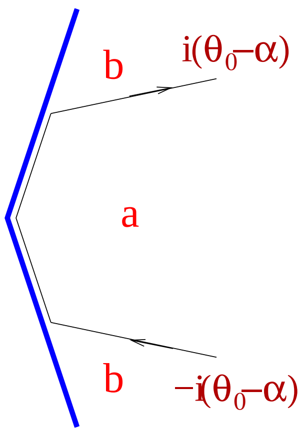
wetting transition = kink unbinding : $\theta_0(T_0) = 0$

$\alpha \neq 0$: $\quad E'_\alpha = E_\alpha + m\cos(\theta_0 - \alpha)$

wedge wetting at T_α such that $\theta_0(T_\alpha) = \alpha$

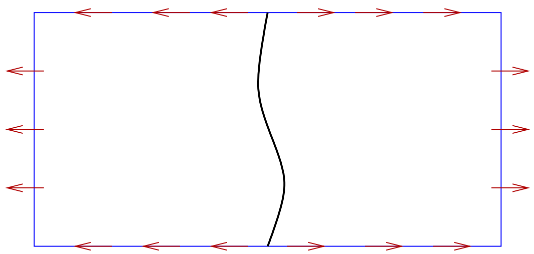
condition known phenomenologically [Hauge, '92]

"wedge covariance" actually is relativistic covariance



Higher dimensions

What done so far relies on the fact that 2D interfaces are trajectories of topological particles (kinks)



2D Ising: kink

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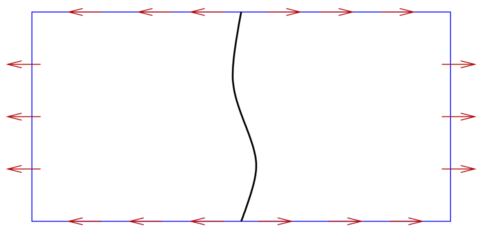

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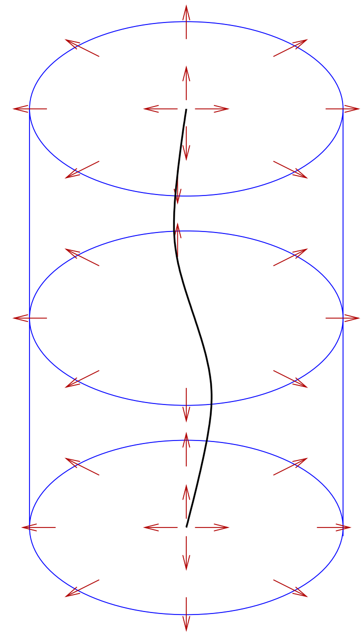


3D XY: vortex

Generalization: (n+1)-dimensional n-vector model

$$\mathcal{H} = -\frac{1}{T}\sum_{<i,j>} \mathbf{s}_i \cdot \mathbf{s}_j \, , \qquad\qquad T < T_c$$

radial boundary conditions produce topological defect lines

$$|B(\pm R/2)\rangle = e^{\pm\frac{R}{2}\omega} \sum_\sigma \int \frac{d\mathbf{p}}{(2\pi)^n \omega}\, a_\sigma(\mathbf{p})\, |\tau(\mathbf{p},\sigma)\rangle + \ldots$$

$$\langle\Phi(\mathbf{x},0)\rangle_{\mathcal{R}} = \frac{\langle B(\frac{R}{2})|\Phi(\mathbf{x},0)|B(-\frac{R}{2})\rangle}{\langle B(\frac{R}{2})|B(-\frac{R}{2})\rangle}$$

$$\sim \left(\frac{2\pi R}{m}\right)^{n/2} \int \frac{d\mathbf{p}_1 d\mathbf{p}_2}{(2\pi)^{2n} m}\, F_\Phi(\mathbf{p}_1|\mathbf{p}_2)\, e^{-\frac{R}{4m}(\mathbf{p}_1^2+\mathbf{p}_2^2)+i\mathbf{x}\cdot(\mathbf{p}_1-\mathbf{p}_2)}$$

$$F_\Phi(\mathbf{p}_1|\mathbf{p}_2) \equiv \frac{\sum_{\sigma_1,\sigma_2} a^*_{\sigma_1}(0) a_{\sigma_2}(0)\, \langle\tau(\mathbf{p}_1,\sigma_1)|\Phi(0,0)|\tau(\mathbf{p}_2,\sigma_2)\rangle}{\sum_\sigma |a_\sigma(0)|^2}$$

$F_{\mathbf{s}\cdot\mathbf{s}}(0|0) = \mathrm{const}$ $\Rightarrow$ $\langle \mathbf{s}\cdot\mathbf{s}(\mathbf{x},0)\rangle_{\mathcal{R}} \propto e^{-\frac{2m}{R}\mathbf{x}^2}$ (passage probability)

$$F_{\mathbf{s}}(\mathbf{p}_1|\mathbf{p}_2) \sim C_n \frac{\mathbf{p}_-}{|\mathbf{p}_-|^{n+1}} + D_n\,|\mathbf{p}_-|^{\alpha_n}\,\mathbf{p}_+\,, \qquad \mathbf{p}_1,\,\mathbf{p}_2 \to 0$$

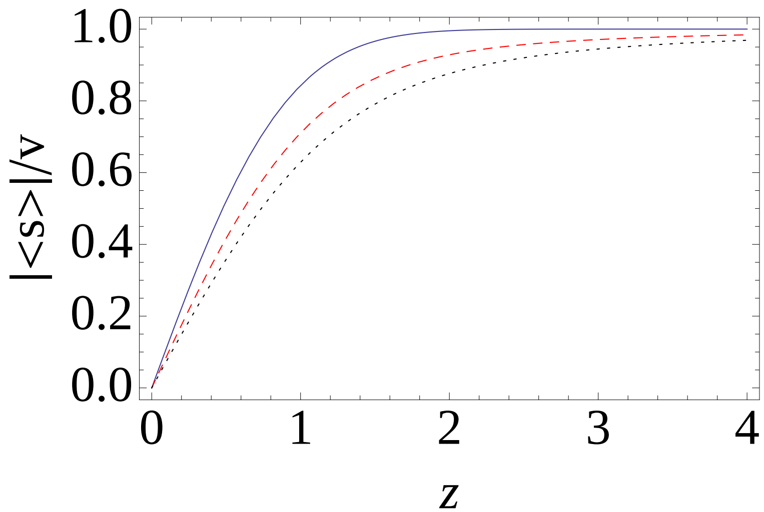
$$\mathbf{p}_\pm \equiv \mathbf{p}_1 \pm \mathbf{p}_2$$

$$\Rightarrow \quad \langle \mathbf{s}(\mathbf{x},0)\rangle_{\mathcal{R}} \sim v\,\frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma(1+\frac{n}{2})}\,{}_1F_1\left(\tfrac{1}{2}, 1+\tfrac{n}{2}; -z^2\right) z\,\hat{\mathbf{x}} \qquad z \equiv \sqrt{\frac{2m}{R}}\,|\mathbf{x}|$$

—— $n = 1$, 2D Ising

- - - $n = 2$, 3D XY

...... $n = 3$, 4D Heisenberg



reduces to $v\,\mathrm{erf}(z)$ for $n = 1$

kinematical singularities are necessary in this case and yield testable predictions

Conclusions

- field theory yields exact results for phase separation in 2D (order parameter, passage probability, branching, wetting)

- due to the limit $R \gg \xi$, most results follow from general low-energy properties of 2D field theory

- integrability essential in establishing presence of bound states, which determines wetting properties

- relativistic nature of particles explains fundamental origin of contact angle and wedge covariance

- in any dimension kinematical singularities in momentum space characterize non-locality of order parameter w.r.t. topological particles and lead to exact and testable predictions