Critical Casimir force scaling function of the mean spherical model

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outline

motivation

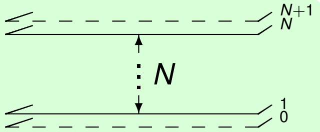
- previous theoretical studies of FS scaling in critical phenomena: very little known below T_c for nonperiodic b.c.
- goal: obtain scaling functions for this case (with: - isotropic on large dist. - short range couplings $\rightsquigarrow$ V. Dohm's talk)
- use mean spherical model (MSM)
  - exactly solvable
  - some pathologies: nevertheless instructive
- however:
  - Barber & Fisher, Ann. Phys. (NY) **77**, 1 (1973): $d = 3$: **scaling violations** for free (realistic) b.c.
  - Chen & Dohm, PRE **67**, 056127 (2003): $d = 3$: clarification of scaling violations take MSM to $2 < d < 3$: **scaling** for free b.c.
- we study in MSM:
  - film geometry: $L \times \infty^{d-1}$
    - ★ $2 < d < 3$: Neumann, Dirichlet (free) b.c.
    - ★ $2 < d \leq 3$: periodic, antiperiodic, ND b.c.
  - FS scaling functions for $T \gtreqless T_c$ of free energy & critical Casimir force

MSM in film geometry

consider

- simple cubic lattice in film geometry, $L \times \infty^{d-1}$ with $L = Na$
- nearest-neighbor interaction (only: isotropic on large distance $\rightsquigarrow$ V. Dohm's talk)

$$\mathcal{H} = a^d \left[\frac{J}{2a^2} \sum_{\langle \boldsymbol{x}, \boldsymbol{x}' \rangle} (S_{\boldsymbol{x}} - S_{\boldsymbol{x}'})^2 + \frac{\mu}{2} \sum_{\boldsymbol{x}} S_{\boldsymbol{x}}^2 \right]$$



constraint: $\sum_{x_\perp} \langle S^2_{(x_\perp, \boldsymbol{x}_\parallel)} \rangle = \frac{N}{a^{d-2}}$ $\rightsquigarrow \mu$(T,N)

b.c. in L direction:

p:	periodic,	$S_{x_{N+1}} = S_{x_1}$	
a:	antiperiodic,	$S_{x_{N+1}} = -S_{x_1}$	
N:	Neumann,	$S_{x_0} = S_{x_1}$,	$S_{x_{N+1}} = S_{x_N}$
D:	Dirichlet (free),	$S_{x_0} = 0$,	$S_{x_{N+1}} = 0$
ND:	mixed,	$S_{x_0} = S_{x_1}$,	$S_{x_{N+1}} = 0$

consider $2 < d \leq 3$: **bulk** transition with $T_c > 0$
no film transition with $T_c > 0$

definitions of FS scaling functions

excess free energy density: $\Delta f = f_{film} - f_{bulk}$

decompose: $\Delta f = \Delta f_{sing} + \Delta f_{reg}$

reduced temperature: $t = \frac{T - T_c}{T_c}, \quad |t| \ll 1$

scaling variable ($\xi_{bulk} = \xi_0 t^{-\nu}$): $s = t(L/\xi_0)^{1/\nu}, \quad \nu = \frac{1}{d-2}$

$$-\infty < s < \infty, \quad L \gg a$$

universal scaling function:
(isotropic, short range)

$$\beta L^d \Delta f_{sing} = 2L^{d-1} f_{surf,sing}(t) + \mathcal{G}(s) + \cdots$$

singular part of Casimir force: $F_{Cas} = -\frac{\partial(L \Delta f_{sing})}{\partial L}$

universal scaling function:

$$\beta L^d F_{Cas} = \mathcal{X}(s)$$
$$= (d-1)\mathcal{G}(s) - (d-2)s\mathcal{G}(s)'$$

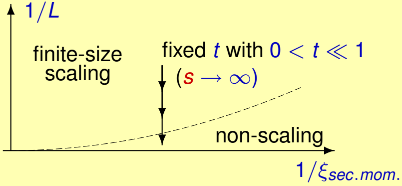
expectations vs. result for $T > T_c$

expectations (see, e.g., Privman, Hohenberg, Aharony, Phase Trans. (1991), Vol.14):

$$\Delta f_{sing} = \underbrace{\frac{1}{L} f_{surf,sing}(t)}_{\text{no contribution to } \mathcal{X}(s)} + \mathcal{O}(e^{-L/\xi})$$

$\rightsquigarrow$ $\mathcal{X}(s) \to 0$ as $s \to \infty$

note however: $\xi = \xi_{sec.mom.} + \Delta\xi$
(see Chen, Dohm, EPJB **10**, 687 (1999))



result for MSM with fixed (Neumann, Dirichlet) b.c.:

$$\Delta f_{sing} = \frac{1}{L} f_{surf,sing}(t) + \underbrace{\frac{1}{L^2} f_2(t) + \mathcal{O}(L^{-3})}_{\text{combined action of constraint + surface free energy}}$$

$\rightsquigarrow$ $\mathcal{X}(s) \to \underbrace{const. \times s}_{\text{unexpected}}$ as $s \to \infty$

example: Dirichlet (free) b.c. for $2<d<3$

$$\mathcal{X}(s) = -\frac{\Gamma(\frac{2-d}{2})}{2(4\pi)^{d/2}}\left[{y_L}^2 - \pi^2 - {y_\infty}^2\right] s - \frac{(d-1)\Gamma(\frac{-d}{2})}{2(4\pi)^{d/2}}\left[{y_L}^d - {y_\infty}^d\right]$$
$$-\frac{\Gamma(\frac{3-d}{2})}{2(4\pi)^{(d-1)/2}}{y_L}^{d-1} - \frac{\pi^2(d-1)\Gamma(\frac{2-d}{2})}{2(4\pi)^{d/2}}{y_L}^{d-2}$$
$$-\frac{d-1}{2^{d+1}\pi}\int_0^\infty dz\left(\frac{\pi}{z}\right)^{(d+1)/2} e^{-z{y_L}^2/\pi^2}\left\{e^z[K(z)-1]-\sqrt{\frac{\pi}{z}}+1-\sqrt{\pi z}\right\}$$

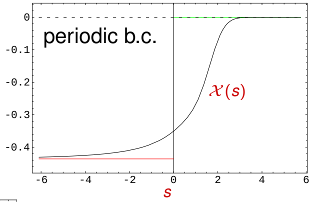
with $y_L(s)$ and $y_\infty(s)$ from $y_\infty \equiv \begin{cases} s^{1/(d-2)} & s>0, \\ 0 & s\le 0, \end{cases}$ and

constraint $\Gamma(\frac{2-d}{2})({y_L}^{d-2} - s) = \sqrt{\pi}\,\Gamma(\frac{3-d}{2}){y_L}^{d-3} - 2(4\pi)^{d/2}\mathcal{E}_d(y_L)$

with $\mathcal{E}_d(y_L) = \frac{1}{2^{d+1}\pi^2}\int_0^\infty dz\left(\frac{\pi}{z}\right)^{(d-1)/2} e^{-z{y_L}^2/\pi^2}\left\{e^z[K(z)-1]-\sqrt{\frac{\pi}{z}}+1\right\}$

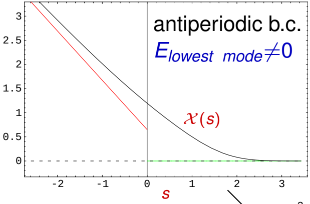
$$K(z) \equiv \sum_{n=-\infty}^{\infty} e^{-n^2 z}$$

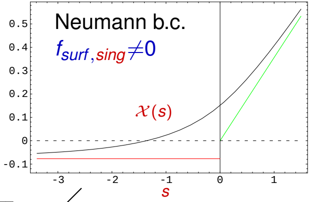
$d=2.5$: $\mathcal{X}(s)$ for various boundary conditions

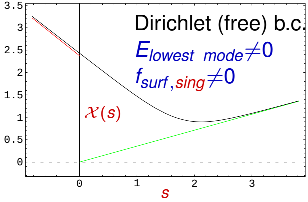


d=3: Dantchev
PRE **53**, 2104 (1996)
PRE**58**, 1455 (1998)

2<d<3: Chen & Dohm
PRE **67**, 056127 (2003)







$d=3$: unexpected scaling for Neumann-Dirichlet B.C.

$d=3$:
- scaling violations for Dirichlet (free) and Neumann b.c.
- scaling holds for periodic, antiperiodic, ND mixed b.c.

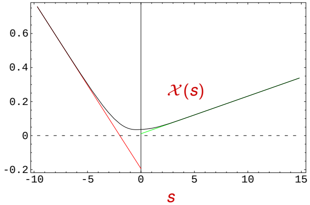
result for Neumann-Dirichlet b.c.($E_{3a} \approx -0.237167$):

$$\mathcal{X}(s) = -\frac{1}{4} E_{3a} {y_L}^2 + \frac{1}{8\pi} \left({y_L}^2 - {y_\infty}^2\right) s - \frac{1}{6\pi} \left({y_L}^3 - {y_\infty}^3\right) - \frac{1}{8\pi} \left[\mathrm{Li}_3(-e^{-2y_L}) + 2y_L \mathrm{Li}_2(-e^{-2y_L})\right]$$

with

$$y_L \equiv \operatorname{arcosh}\left(\tfrac{1}{2} e^{s-\pi E_{3a}}\right)$$

$$y_\infty \equiv \begin{cases} s, & s > 0 \\ 0, & s \le 0 \end{cases}$$



summary

results:

- exact results within MSM (with: - isotropic on large dist., - short range couplings)
  for $\mathcal{G}(s)$ and $\mathcal{X}(s)$ for $T \geq T_c$ and $T < T_c$ for nonperiodic b.c.

- finite-size scaling of Δf_{sing} and F_{Cas} verified for
  - 2<d<3: periodic (known), antiperiodic, NN, ND, DD (all expected) b.c.
  - d=3: periodic (known), antiperiodic (expected), ND (unexpected) b.c.

- unexpected linear rise of $\mathcal{X}(s)$ for
  - $s \to -\infty$ for non-zero energy of lowest mode
  - $s \to +\infty$ from combined action of constraint + surface free energy

- $d = 3$: scaling violations for Dirichlet (free), Neumann b.c.; at T_c
  - $\Delta f_{sing} \propto L^{-3} \ln L$ (instead of L^{-3})
  - $F_{Cas} \propto L^{-3} \ln L$ (instead of L^{-3})

open problems:

- which of found features apply to realistic systems?