The effect of boundary conditions and dimensionality on the critical Casimir force

R. Zandi, A. Shackell, J. Rudnick, M. Kardar, L. Chayes

Wetting by a Superfluid Film

Critical Fluctuation-Induced Thinning of ^{4}He Films near the Superfluid Transition

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(Received 15 December 1998)

We report dielectric constant measurements showing critical fluctuation-induced thinning of ^{4}He films near the superfluid transition. The films are adsorbed on a stack of copper electrodes suspended at different heights above bulk liquid. We calibrate the measurements by assuming that the film thickness away from the transition region at different heights is accurately given by theory. The thinning is found to be consistent with finite-size scaling, if the value of the scaling function for each thickness is normalized by its value at the minimum.
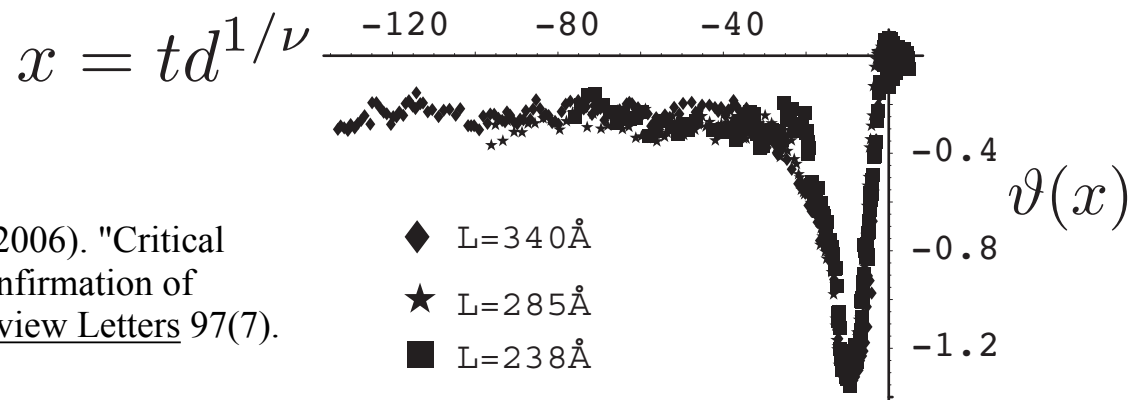

mass, capacitance

He (vapor)
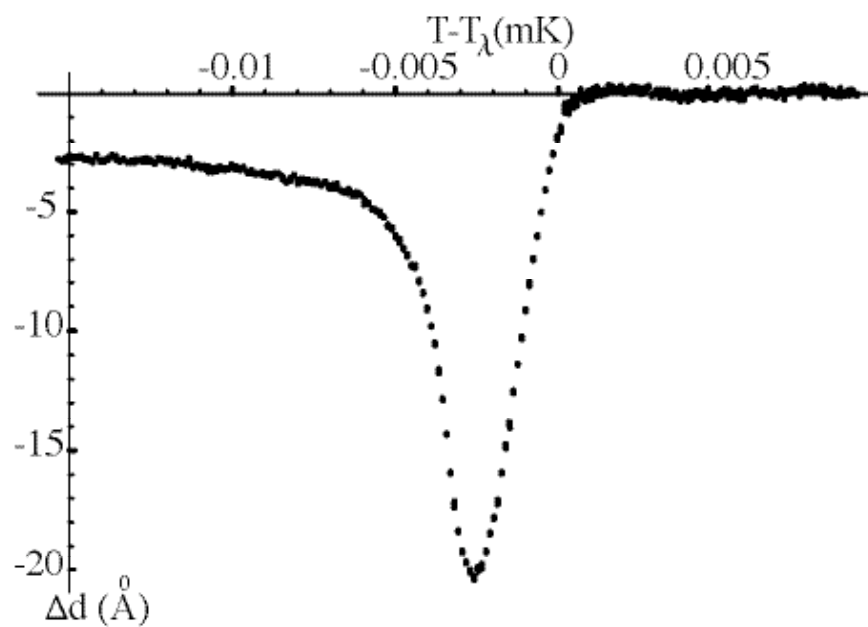
H

He (liquid)
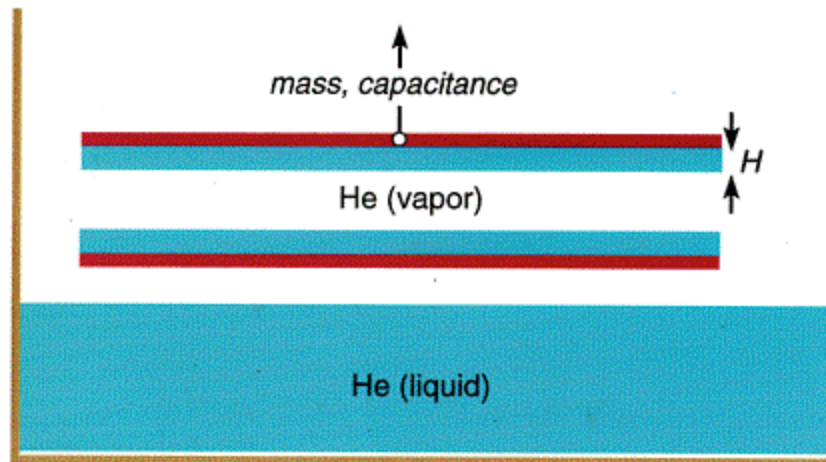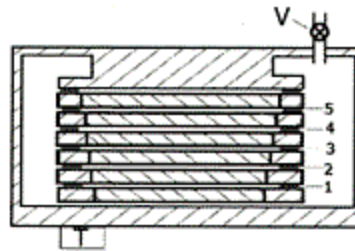
Thinning of a Superfluid film

- The film is thinner at the transition, and in the superfluid phase

$$x = td^{1/\nu}$$

$\vartheta(x)$

-120   -80   -40

-0.4

-0.8

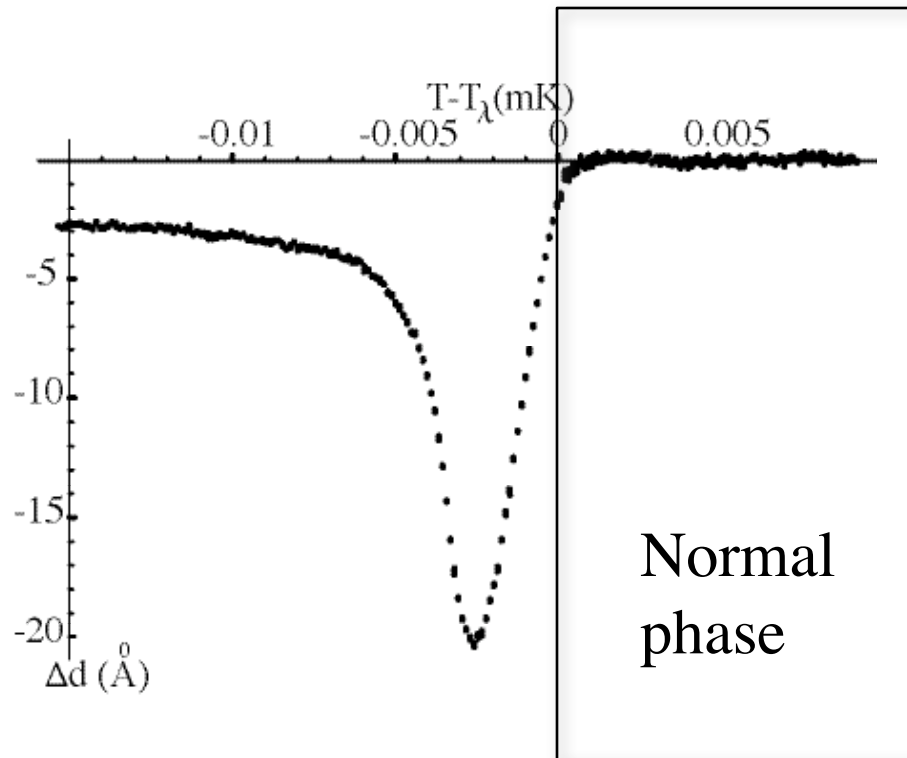-1.2

◆ L=340Å

★ L=285Å

■ L=238Å
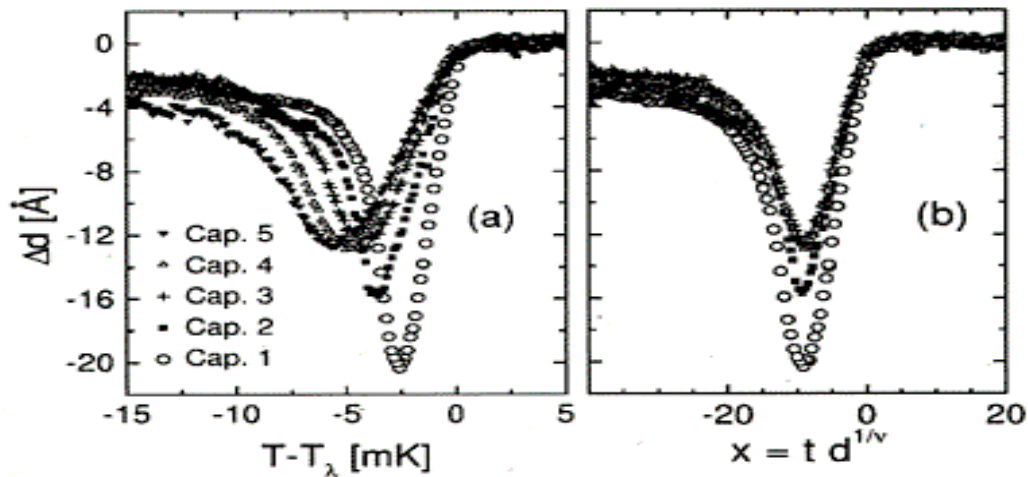
Ganshin, A., S. Scheidemantel, et al. (2006). "Critical Casimir force in He-4 films: Confirmation of finite-size scaling." Physical Review Letters 97(7).

Garcia, R. and M. H. W. Chan (1999). "Critical fluctuation-induced thinning of He-4 films near the superfluid transition." *Physical Review Letters* **83**(6): 1187-1190.
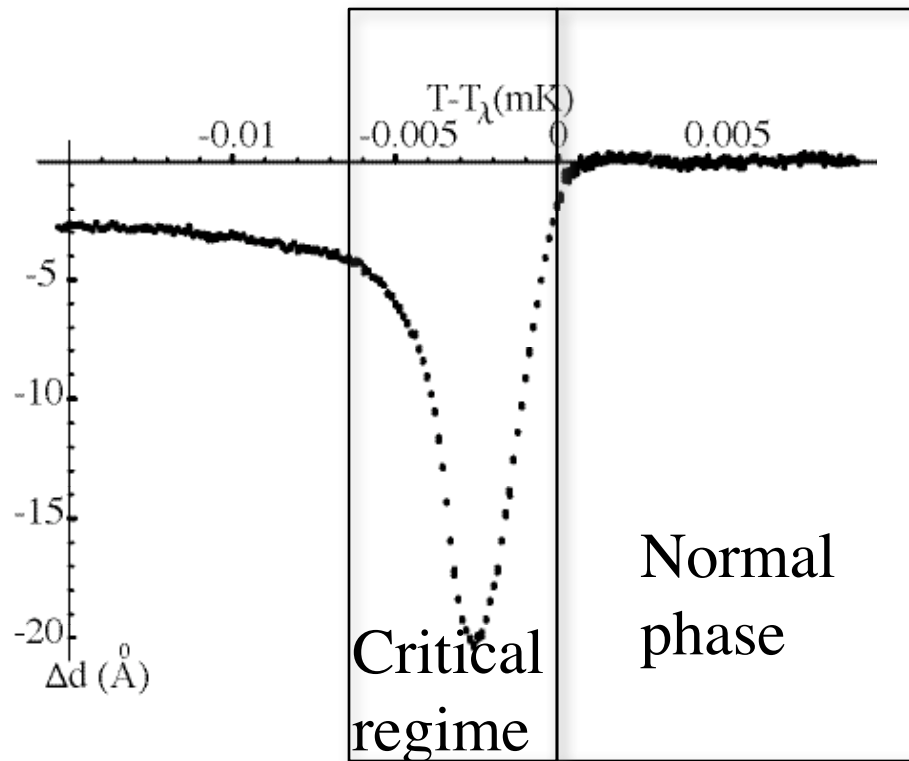
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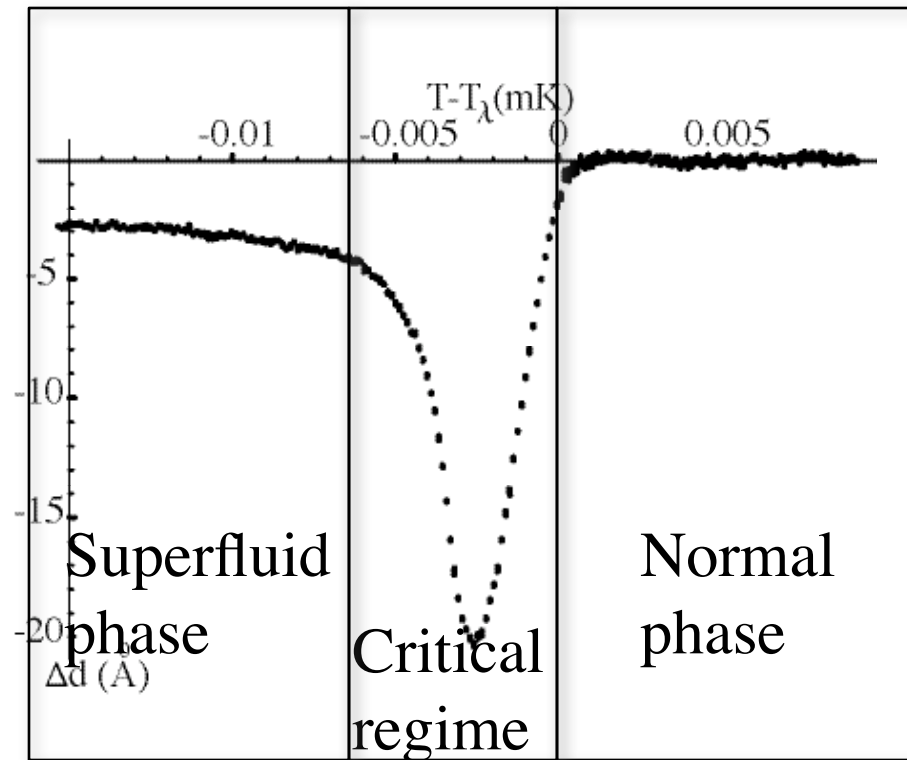
Garcia, R. and M. H. W. Chan (1999). "Critical fluctuation-induced thinning of He-4 films near the superfluid transition." *Physical Review Letters* **83**(6): 1187-1190.

Garcia, R. and M. H. W. Chan (1999). "Critical fluctuation-induced thinning of He-4 films near the superfluid transition." *Physical Review Letters* **83**(6): 1187-1190.

Krech, M. (1999). "Fluctuation-induced forces in critical fluids." Journal of Physics-Condensed Matter **11** (37): R391-R412.
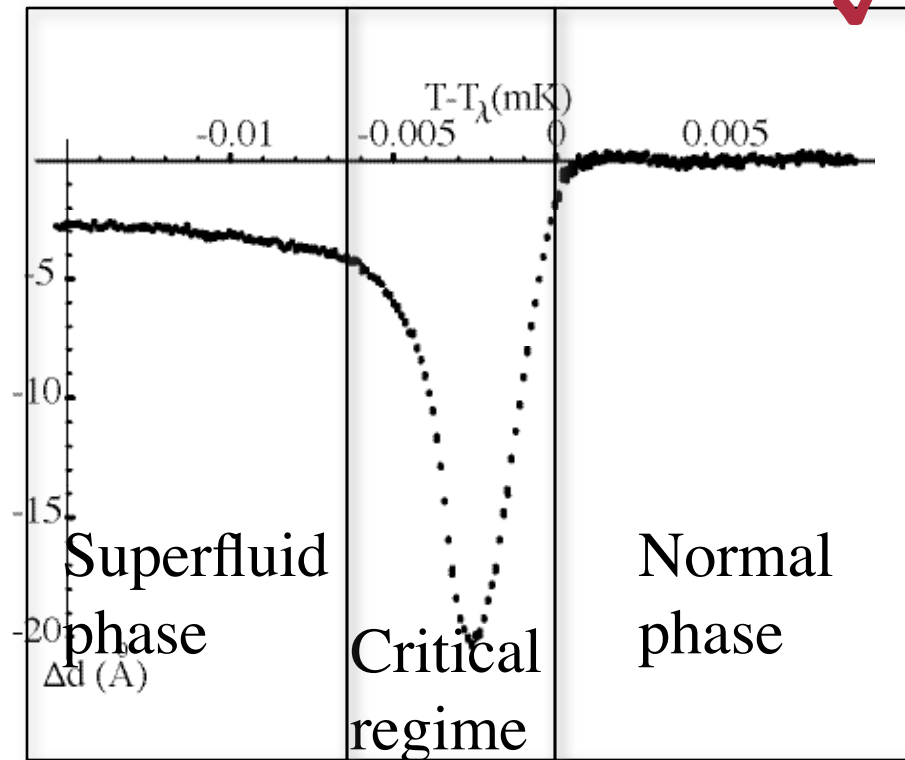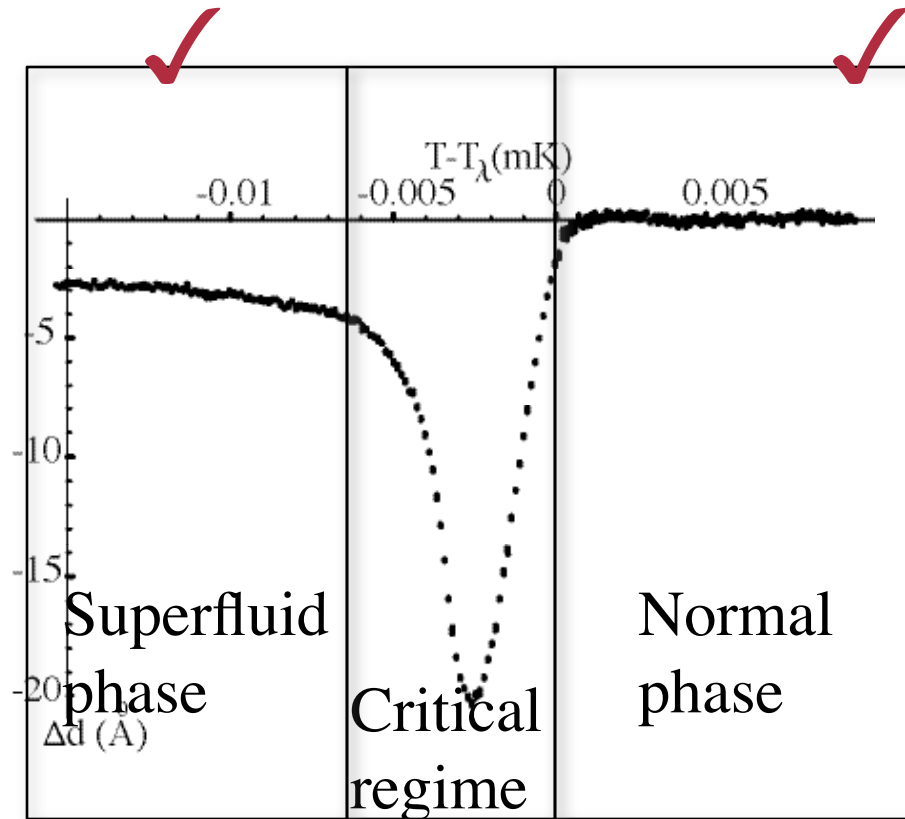
Garcia, R. and M. H. W. Chan (1999). "Critical fluctuation-induced thinning of He-4 films near the superfluid transition." *Physical Review Letters* **83**(6): 1187-1190.

Zandi, R., J. Rudnick and M. Kardar, (2004). "Casimir forces, surface fluctuations, and thinning of superfluid film." <u>Physical Review Letters</u> 93 (15).

Krech, M. (1999). "Fluctuation-induced forces in critical fluids." <u>Journal of Physics-Condensed Matter</u> **11** (37): R391-R412.

Garcia, R. and M. H. W. Chan (1999). "Critical fluctuation-induced thinning of He-4 films near the superfluid transition." *Physical Review Letters* **83**(6): 1187-1190.
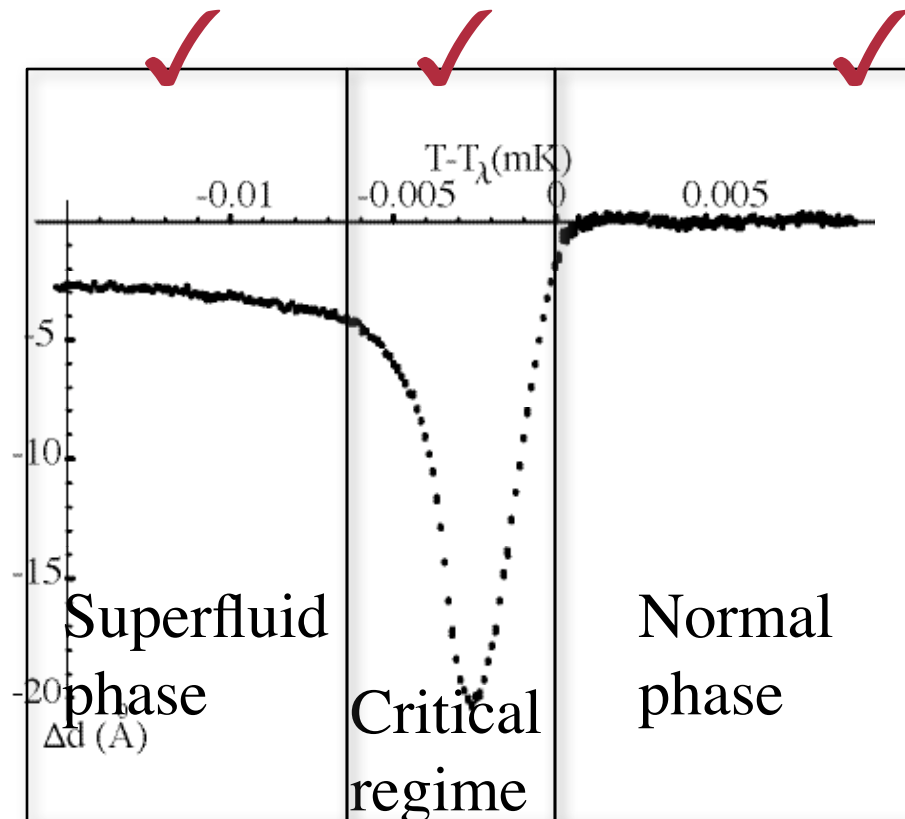
Zandi, R., J. Rudnick and M. Kardar, (2004). "Casimir forces, surface fluctuations, and thinning of superfluid film." <u>Physical Review Letters</u> 93 (15).

Krech, M. (1999). "Fluctuation-induced forces in critical fluids." <u>Journal of Physics-Condensed Matter</u> **11** (37): R391-R412.

Superfluid phase

Critical regime

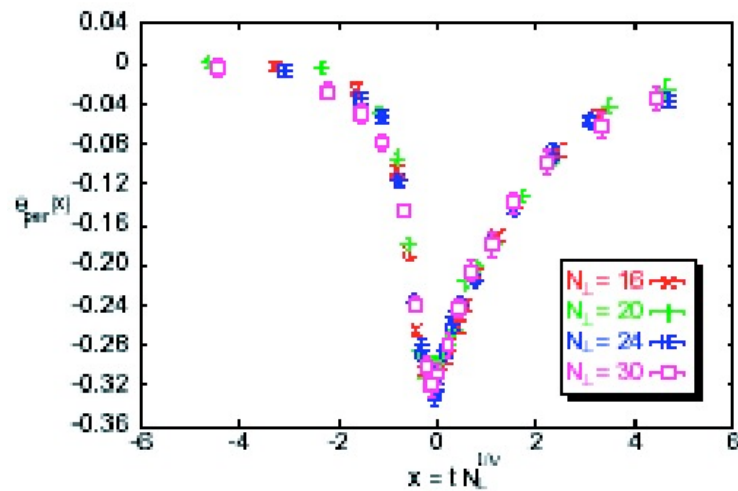Normal phase

$T-T_\lambda$ (mK)

Δd (Å)

A. Maciolek et. al. PRE **76** (2007)
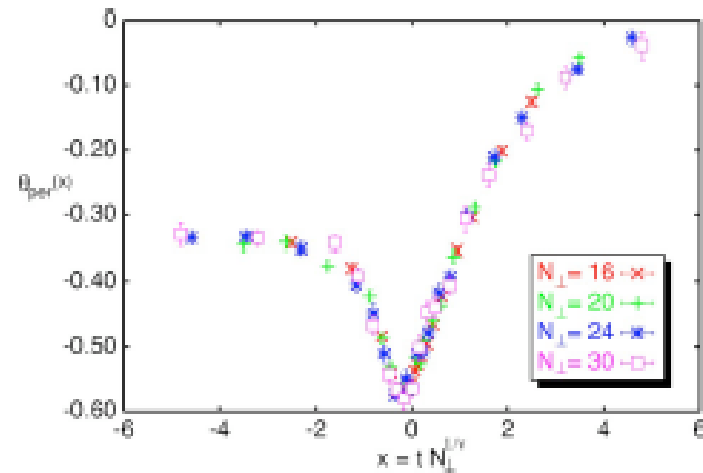
A. Hucht, PRL **99**, 185301 (2007)

R. Zandi, et al., PRE **76** (2007)

Dantchev, D. and M. Krech (2004). "Critical Casimir force and its fluctuations in lattice spin models: Exact and Monte Carlo results." *Physical Review E* **69**(4).
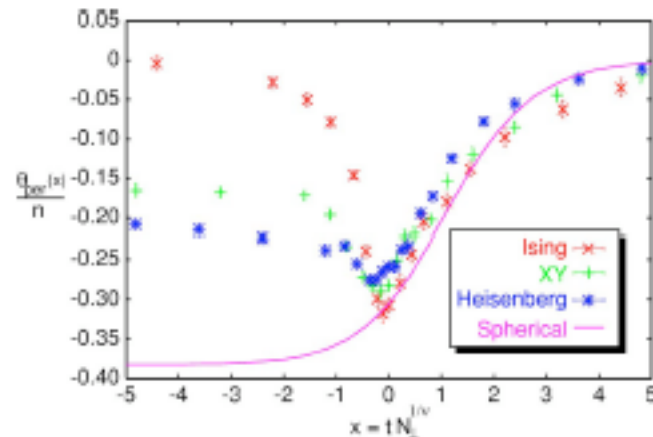
Ising-like

xy (superfluid)

n=1,n=2, n=3, n=∞

Williams, G. A. (2004). "Vortex fluctuations in the critical casimir effect of superfluid and superconducting films." *Physical Review Letters* **92**(19).
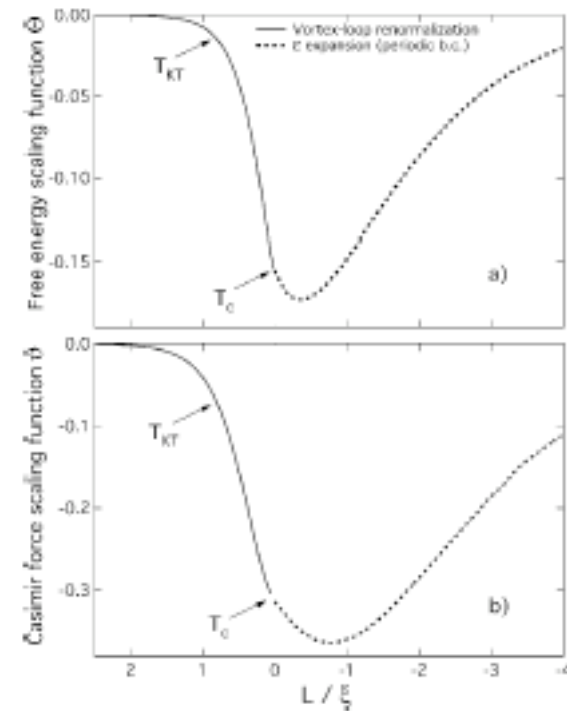

FIG. 2. (a) Free-energy scaling function versus L/ξ, where ξ is the bulk correlation length, taken to be positive for $T < T_c$ and negative for $T > T_c$. (b) Casimir force scaling function.

What's so special about Dirichlet boundary conditions?

Dirichlet boundary conditions tend to suppress ordering in a film: According to Ginzburg and Landau, the ordering temperature is suppressed by an amount proportional to $(\pi/L)^2$ where L is the film thickness

When Dirichlet boundary conditions apply, changing film thickness is like changing temperature in the vicinity of the critical point
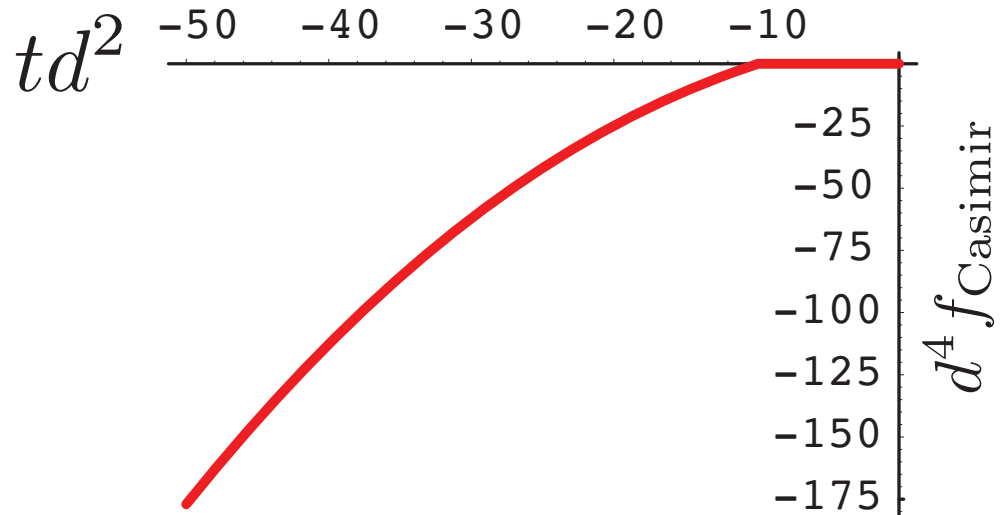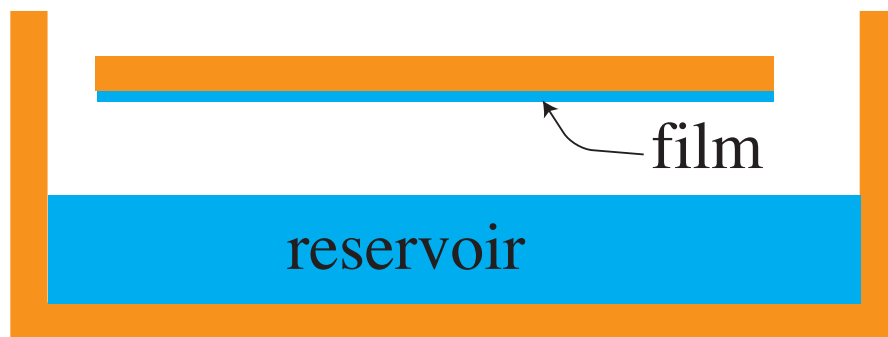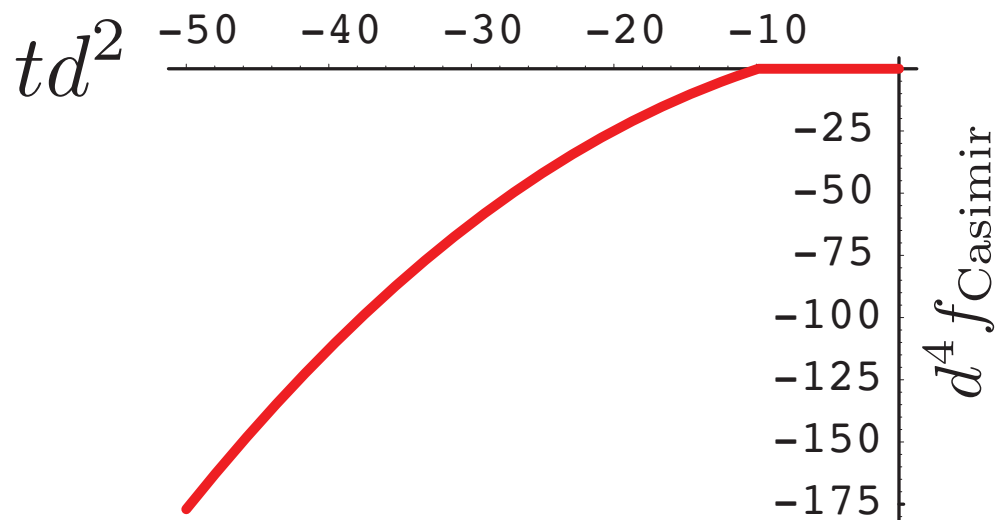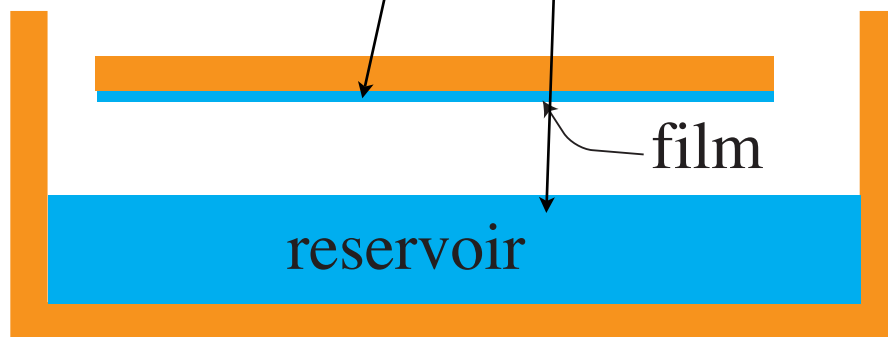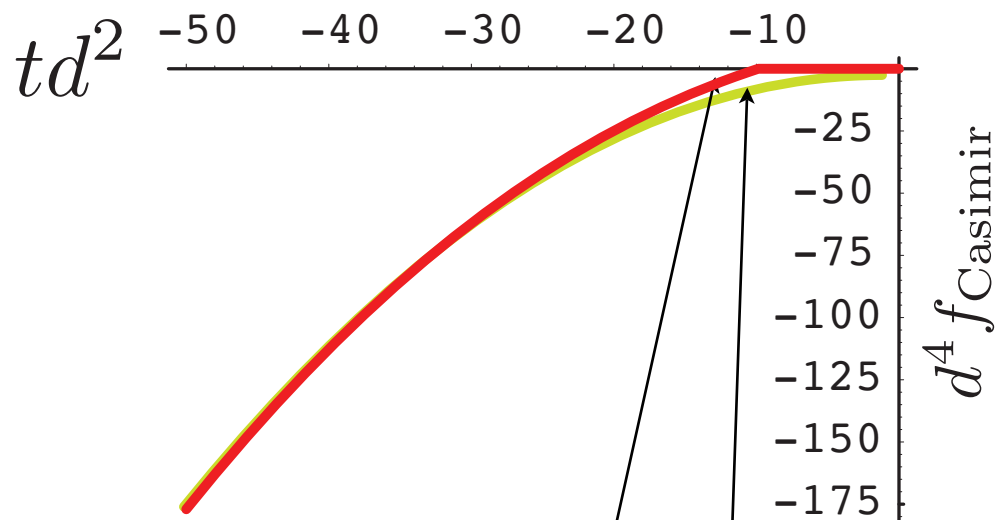
Taking the difference:
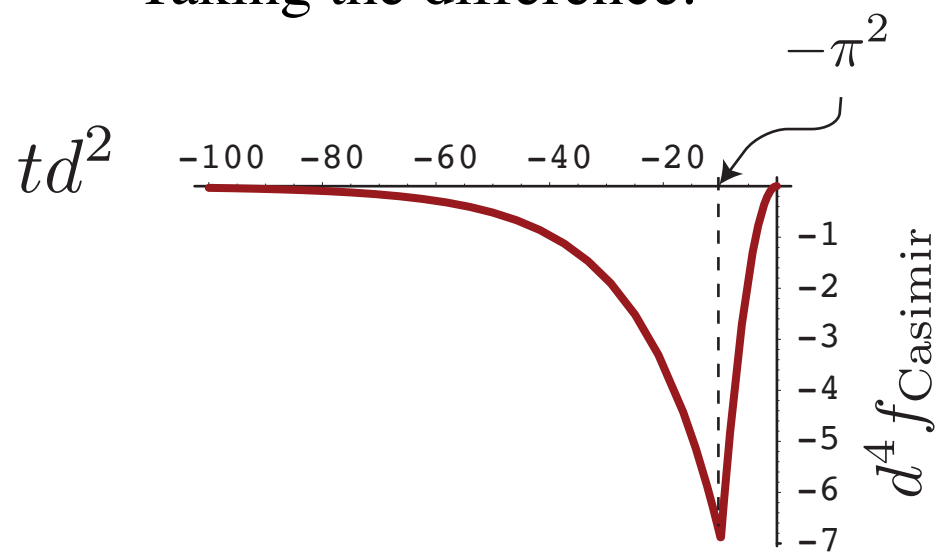
Taking the difference:
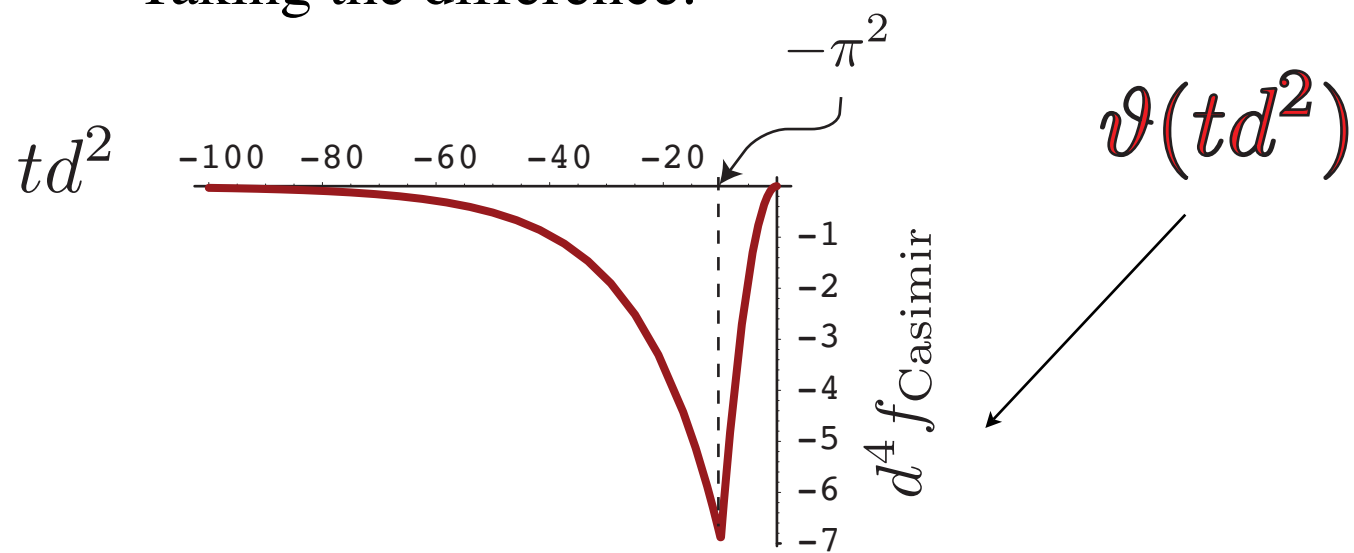
The general question:

What influence does the combination of boundary conditions and dimensionality exert on the critical casimir force?

Focusing on the Ising model, we look at three cases in which exact solutions are available

1. The one dimensional Ising model (zero dimensional film)
2. The two dimensional Ising model (one dimensional film)
3. The four dimensional O(1) model (*three* dimensional film)

We consider three kinds of boundary conditions: periodic, Dirichlet and free

The one dimensional Ising model

Film

$\downarrow \uparrow \uparrow \downarrow$

Bulk

.... $\uparrow \downarrow \downarrow \uparrow \downarrow \uparrow \uparrow \downarrow \uparrow \downarrow \downarrow \downarrow \uparrow \uparrow \downarrow \uparrow$ ....
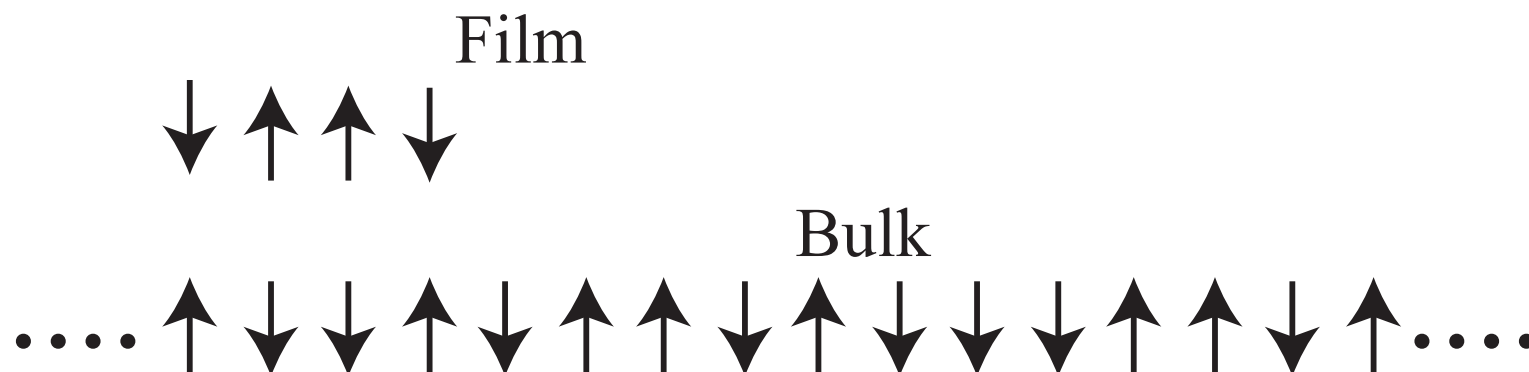
General scaling form of the critical Casimir force

$$F_{\mathrm{Casimir}} = \frac{1}{L^d}\mathcal{F}(\tau L^{1/\nu})$$

For a one-dimensional system:

$$F_{\mathrm{Casimir}} = \frac{1}{L}\mathcal{F}(\tau L^{1/\nu})$$

or

$$\frac{1}{L}\mathcal{G}(L/\xi)$$

In the case of the one-dimensional Ising model, starting with the transfer matrix

$$\mathbf{T} = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}$$

with eigenvectors

$$|e\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|o\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and corresponding eigenvalues

$$\lambda_e = 2\cosh \beta J$$

$$\lambda_o = 2\sinh \beta J$$

then

$$\mathbf{T} = |e\rangle \lambda_e \langle e| + |o\rangle \lambda_o \langle o|$$

In the case of periodic boundary conditions

$$
\begin{aligned}
\mathcal{Z}(L) &= \operatorname{Tr} \mathbf{T}^L \\
&= \lambda_e^L + \lambda_o^L
\end{aligned}
$$

and for the free energy, $A(L)$

$$
\begin{aligned}
A(L) &= -k_B T \ln \mathcal{Z}(L) \\
&= -L k_B T \ln \lambda_e - k_B T \ln \left[1 + \left(\frac{\lambda_o}{\lambda_e} \right)^L \right]
\end{aligned}
$$

Given the correlation length, ξ, where

$$
\xi = 1 / \ln(\lambda_e / \lambda_o)
$$

$$
A(L) = f_B L - k_B T \ln \left(1 + e^{-L/\xi} \right)
$$

Then

$$\frac{\partial A(L)}{\partial L} - f_B \;\; = \;\; \frac{k_B T}{\xi} \frac{e^{-L/\xi}}{1 + e^{-L/\xi}}$$

$$= \;\; \frac{k_B T}{L} \left\{ \frac{L}{\xi} \frac{e^{-L/\xi}}{1 + e^{-L/\xi}} \right\}$$

Then

$$\frac{\partial A(L)}{\partial L} - f_B \;=\; \frac{k_B T}{\xi}\frac{e^{-L/\xi}}{1+e^{-L/\xi}}$$

$$=\; \frac{k_B T}{L}\left\{\frac{L}{\xi}\frac{e^{-L/\xi}}{1+e^{-L/\xi}}\right\}$$
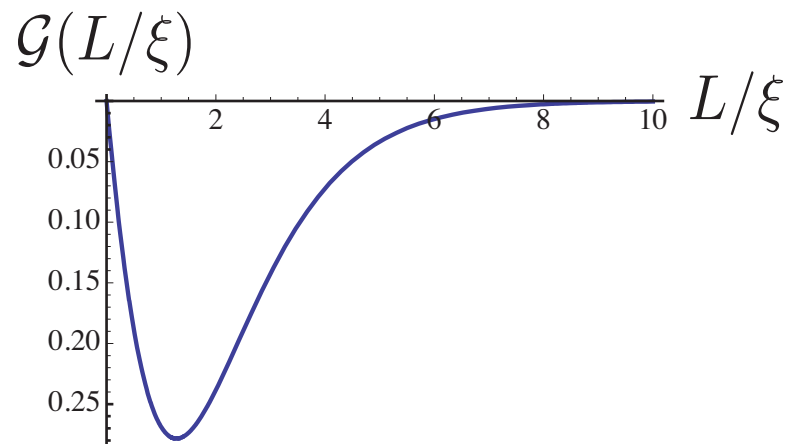
$$-\mathcal{G}(L/\xi)$$

Then

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$$=\; \frac{k_B T}{L} \left\{ \frac{L}{\xi} \frac{e^{-L/\xi}}{1 + e^{-L/\xi}} \right\}$$

$$-\mathcal{G}(L/\xi)$$

$\mathcal{G}(L/\xi)$

For free boundary conditions

$$\mathcal{Z} = (1\ 1)\,\mathbf{T}^L \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= 2\langle e|\mathbf{T}^L|e\rangle$$

$$= 2\lambda_e^L$$

which means that

$$\frac{\partial A(L)}{\partial L} - f_B = 0$$

For free boundary conditions

$$\mathcal{Z} \;=\; (1\ 1)\,\mathbf{T}^L \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

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$$=\; 2\lambda_e^L$$

which means that

$$\frac{\partial A(L)}{\partial L} - f_B = 0$$

No critical Casimir force!

The continuous one-dimensional O(1) model

Starting with the effective Hamiltonian

$$\mathcal{H}(m(x)) = \int \left\{ \left(\frac{dm(x)}{dx} \right)^2 + rm(x)^2 + um(x)^4 \right\} dx$$

the partition function is given by

$$\mathcal{Z} = \int \mathcal{D}m(x) \exp\left[-\mathcal{H}(m(x)) \right]$$

Here, the eigenvalues of the corresponding transfer matrix satisfy

$$-\frac{d^2 \Psi_l(m)}{dm^2} + (rm^2 + um^4)\Psi_l(m) = \lambda_l \Psi_{(}m)$$

with associated eigenvalues

$$e^{-\lambda_l w}$$

The continuous one-dimensional O(1) model

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with associated eigenvalues

width over which **T** operates

$$e^{-\lambda_l w}$$

The continuous version of the transfer matrix product

$$\langle m| \prod_{x=x_1}^{x_2} \mathbf{T}(x)|m'\rangle = \sum_l \Psi_l(m)\Psi_l(m')e^{-\lambda_l(x_2-x_1)}$$

In the case of periodic boundary conditions
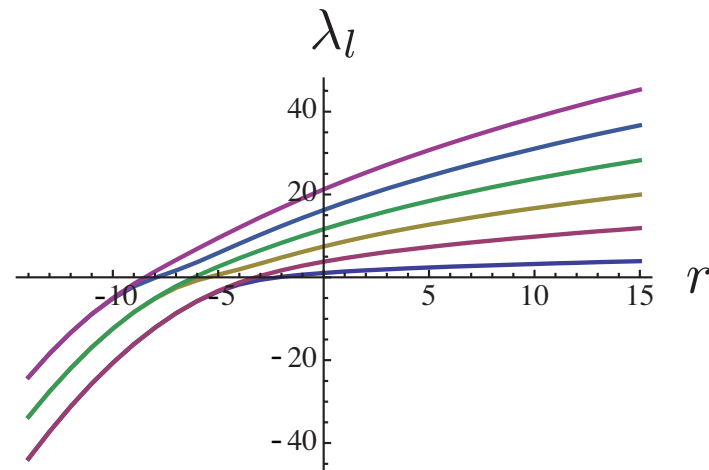
$$\mathcal{Z}(L) = \sum_l e^{-\lambda_l L}$$

For Dirichlet boundary conditions
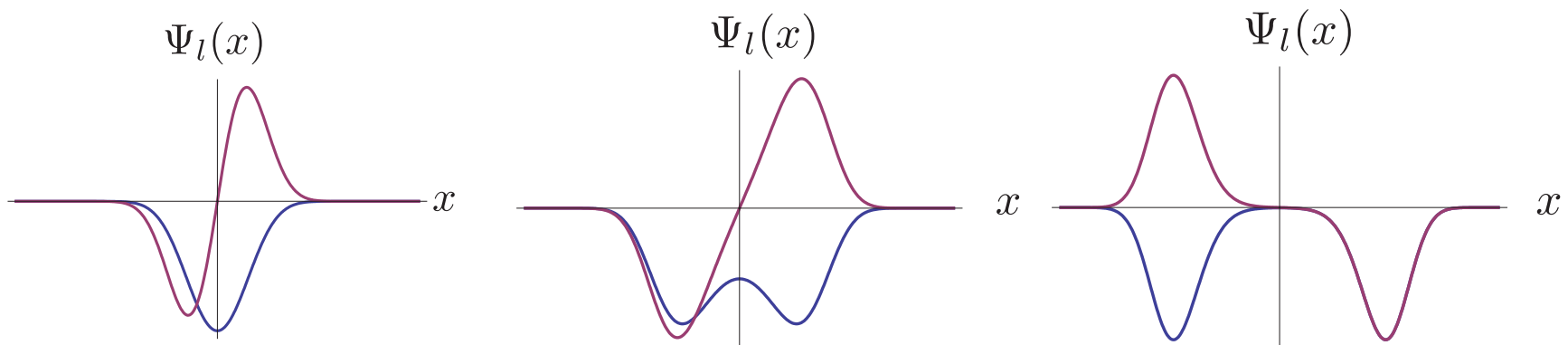
$$\mathcal{Z}(L) = \sum_l e^{-\lambda_l L}\Psi_l(0)^2$$

And for free boundary conditions

$$\mathcal{Z}(L) = \sum_l e^{-\lambda_l L}\left(\int_{-\infty}^{\infty}\Psi_l(x)dx\right)^2$$

The eigenvalues of the Schroedinger-like equation

The eigenfunctions associated with the two lowest eigenvalues

The "critical point" is at $r = -\infty$

$$\xi(r) \to \frac{1}{\lambda_2(r) - \lambda_1(r)}$$

Periodic boundary conditions:

$$\mathcal{Z}(L) \to e^{-\lambda_1 L} + e^{-\lambda_2 L} + \dots$$

Dirichlet boundary conditions:

$$\begin{aligned}
\mathcal{Z}(L) &\to e^{-\lambda_1 L}\Psi_1(0)^2 + e^{-\lambda_2 L}\Psi_2(0)^2 + \dots \\
&= e^{-\lambda_1 L}\Psi_1(0)^2 + \dots
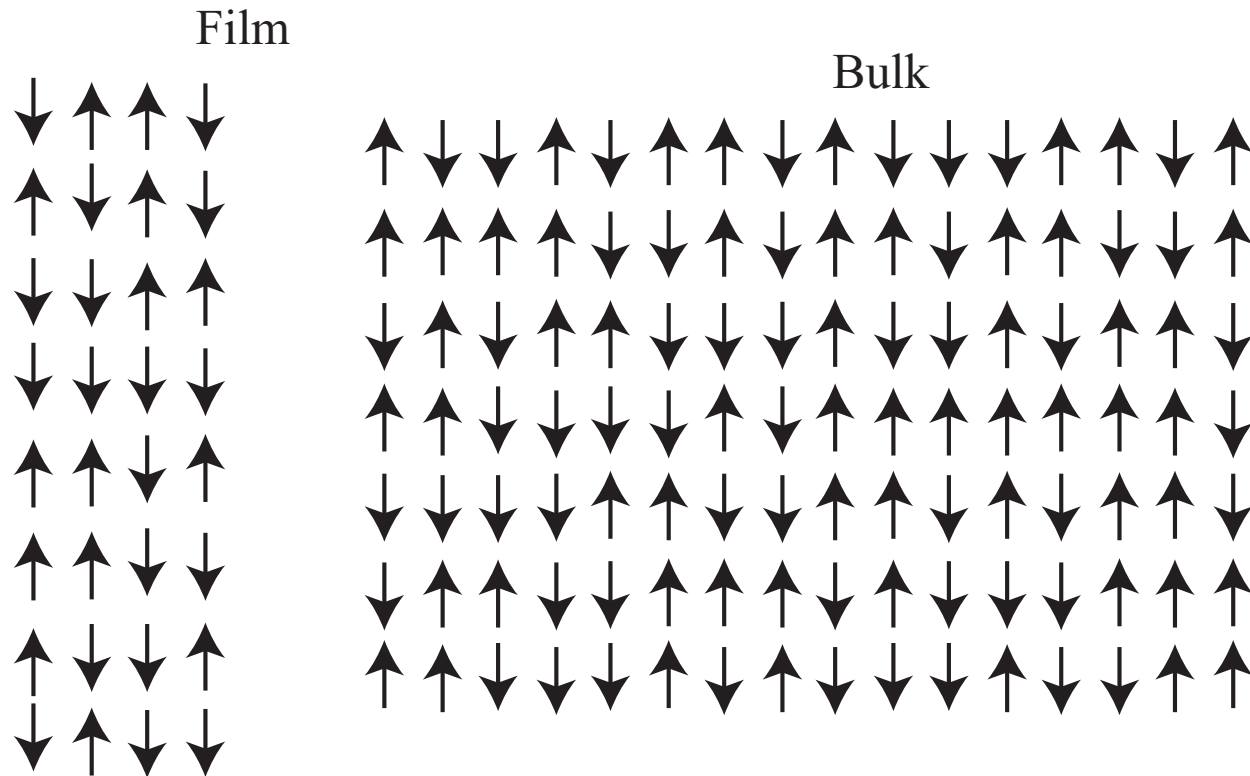\end{aligned}$$

Free boundary conditions:

$$\begin{aligned}
\mathcal{Z}(L) &\to e^{-\lambda_1 L}\left(\int_{-\infty}^{\infty}\Psi_1(x)dx\right)^2 + e^{-\lambda_2 L}\left(\int_{-\infty}^{\infty}\Psi_2(x)dx\right)^2 + \dots \\
&= e^{-\lambda_1 L}\left(\int_{-\infty}^{\infty}\Psi_1(x)dx\right)^2 + \dots
\end{aligned}$$

In the scaling limit ($r \rightarrow -\infty$) the only boundary conditions yielding a critical Casimir force are periodic, with

$$\mathcal{G}(L/\xi) = -\frac{L}{\xi}\frac{e^{-L/\xi}}{1 + e^{-L/\xi}}$$

The same result holds for higher spin versions of the one dimensional Ising model

The two dimensional Ising model

Film

Bulk

In the case of free boundary conditions

Surface ordering and finite-size effects in liquid-crystal films

Hao Li, Maya Paczuski, Mehran Kardar, and Kerson Huang

$$-\beta f_{\text{sing}} = \frac{1}{n}\int_0^1 \frac{d\omega}{\pi\sqrt{1-\omega^2}}\ln(f_+\lambda_+^{n-2}+f_-\lambda_-^{n-2})$$

$$f_\pm = [(1-Z_S)^2+4Z_S\omega^2]^2 V_\pm^2 + 16 Z_S^2 Z_2^2 \omega^2(1-\omega^2) V_\mp^2 \pm 8 V_+ V_- Z_S Z_2 \omega \sqrt{1-\omega^2}\,[(1-Z_S)^2+4Z_S\omega^2]\;,$$

$$V_\pm = \left[\frac{1}{2}\left[1\pm\frac{\sqrt{g}\left[\dfrac{\tau^2}{n^2}+\dfrac{\tau}{n}\dfrac{Z_2(1+Z_1)}{\sqrt{Z_1(1-Z_2^2)}}+\left[\dfrac{1+Z_2^2}{1-Z_2^2}\right]\omega^2\right]}{\left[\left[\dfrac{\tau^2}{n^2}+\omega^2\right]g+1\right]^{1/2}\left[\dfrac{\tau^2}{n^2}+\omega^2\right]^{1/2}}\right]\right]^{1/2},$$

$$\lambda_\pm = 1+2g\left[\frac{\tau^2}{n^2}+\omega^2\right]$$

$$\pm 2\left\{\left[\left[\frac{\tau^2}{n^2}+\omega^2\right]g+1\right]\left[\frac{\tau^2}{n^2}+\omega^2\right]g\right\}^{1/2}$$

$$\tau = n\frac{1-Z_1-Z_2(1+Z_1)}{2\sqrt{Z_1(1-Z_2^2)}}$$

$$g = \frac{\sinh(2\beta J_H)}{\sinh(2\beta J_V)}$$

$$Z_1 = \tanh(\beta J_H),\ \ Z_2 = \tanh(\beta J_V),$$

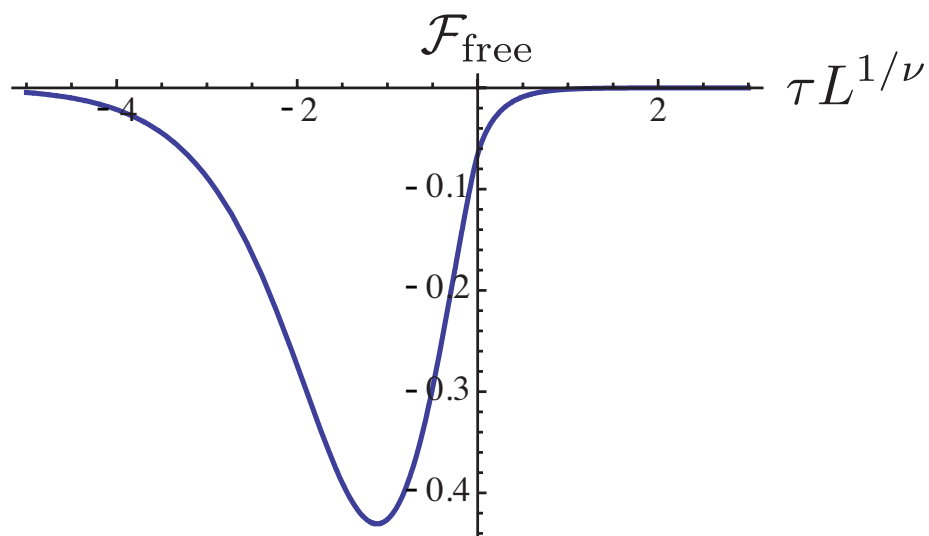$$Z_S = \tanh(\beta J_S)$$

$\mathcal{F}_{\text{free}}$

$$t = \tau L^{1/\nu}$$

$$= \frac{1}{\pi n^2} \int_{-\infty}^{\infty} d\Omega \sqrt{t^2 + \Omega^2}$$

$$\left[\frac{\left(1 + \frac{t}{\sqrt{t^2+\Omega^2}}\right) e^{2\sqrt{t^2+\Omega^2}} - \left(1 - \frac{t}{\sqrt{t^2+\Omega^2}}\right) e^{-2\sqrt{t^2+\Omega^2}}}{\left(1 + \frac{t}{\sqrt{t^2+\Omega^2}}\right) e^{2\sqrt{t^2+\Omega^2}} + \left(1 - \frac{t}{\sqrt{t^2+\Omega^2}}\right) e^{-2\sqrt{t^2+\Omega^2}}} - 1 \right]$$

In the case of periodic boundary conditions

Bounded and Inhomogeneous Ising Models. I. Specific-Heat Anomaly of a Finite Lattice

Arthur E. Ferdinand* and Michael E. Fisher

$$Z_{mn}(T) = \tfrac{1}{2}(2\sinh 2K)^{\frac{1}{2}mn} \sum_{i=1}^{4} Z_i(K) \qquad K = J/kT$$
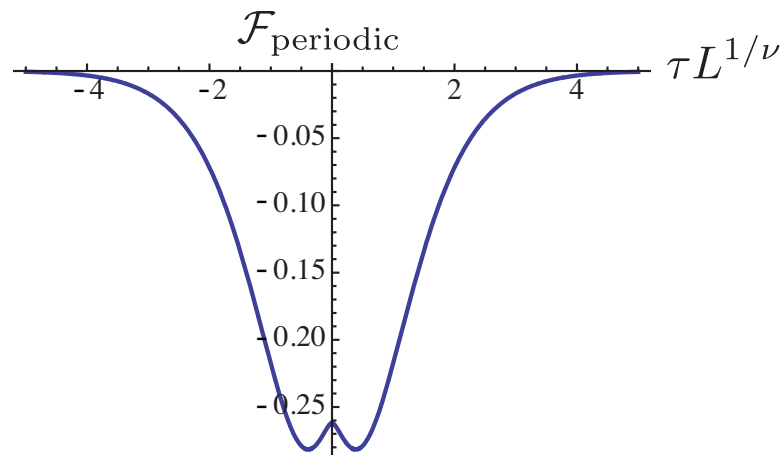
$$Z_1 = \prod_{r=0}^{n-1} 2\cosh\tfrac{1}{2}m\gamma_{2r+1}, \quad Z_2 = \prod_{r=0}^{n-1} 2\sinh\tfrac{1}{2}m\gamma_{2r+1},$$

$$Z_3 = \prod_{r=0}^{n-1} 2\cosh\tfrac{1}{2}m\gamma_{2r}, \quad Z_4 = \prod_{r=0}^{n-1} 2\sinh\tfrac{1}{2}m\gamma_{2r},$$
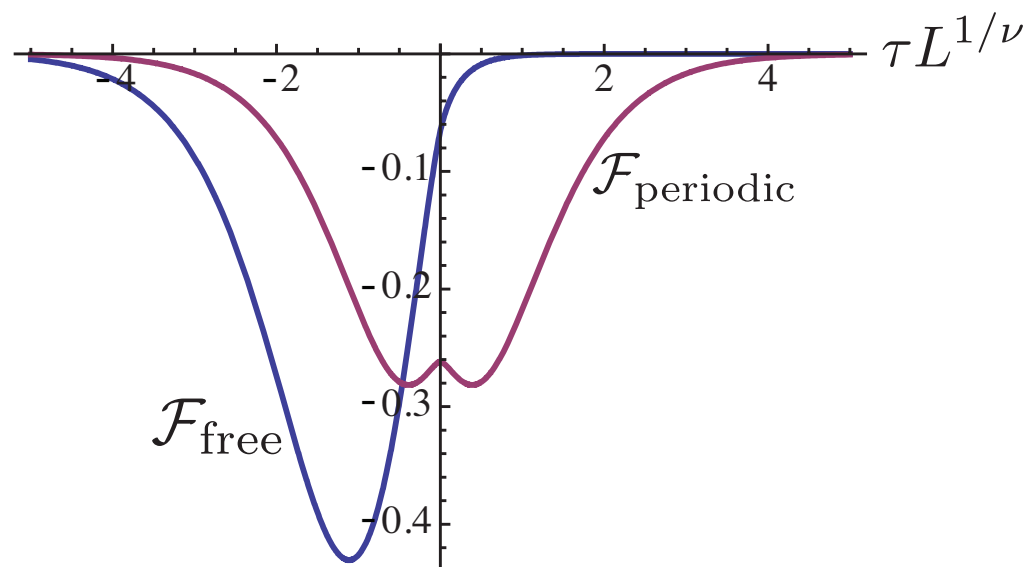
$$\cosh\gamma_l = c_l = \cosh 2K \coth 2K - \cos(l\pi/n)$$

$$\mathcal{F}_{\mathbf{periodic}} = \frac{1}{\pi m^2} \int_{-\infty}^{\infty} d\Omega \sqrt{t^2 + \Omega^2} \left[\tanh \sqrt{t^2 + \Omega^2} - 1 \right]$$

$$\boxed{t = \tau L^{1/\nu}}$$

Both Casimir forces

A four dimensional "bulk" and a three dimensional "film"

The critical behavior of the bulk is, to within logarithmic corrections, described by mean field theory.

However, the critical behavior of the film is non-classical.

A complication: the dominant contribution to the renormalized version of the effective Hamiltonian for the bulk system has the Ginzburg-Landau-Wilson form with a fourth order coupling constant that is quite small. In principle, this is the "starting" effective Hamiltonian of the film.

How do we evaluate the partition function—and especially the Casimir force—of the non-classical film?

Transformation from a continuous spin to a discrete model

Given an effective Hamiltonian on a lattice

$$\mathcal{H} = \sum_l \frac{1}{2} r s_l^2 + \sum_{l,k \ \text{n.n.}} \frac{1}{2}(s_l - s_k)^2 + \sum_l u s_l^4$$

and associated partition function

$$\mathcal{Z} = \int \prod_l ds_l \exp(-\mathcal{H})$$

the partition function can be recast in terms of a product of transfer matrices

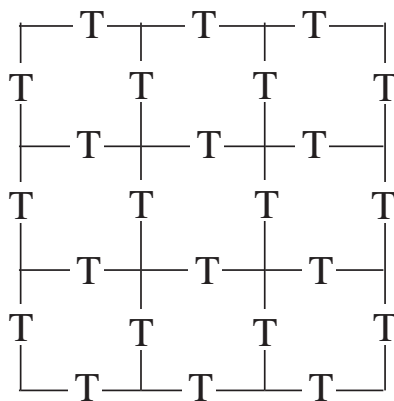$$\mathcal{Z} = \int \prod_l ds_l \prod_{l,k \ \text{n.n.}} \mathbf{T}(s_l, s_k)$$

where

$$\mathbf{T}(s_l, s_k) = \exp\left[-\frac{r}{4d}(s_l^2 + s_k)^2 - \frac{1}{2}(s_l - s_k)^2 - \frac{u}{2d}(s_l^4 + s_k^4)\right]$$
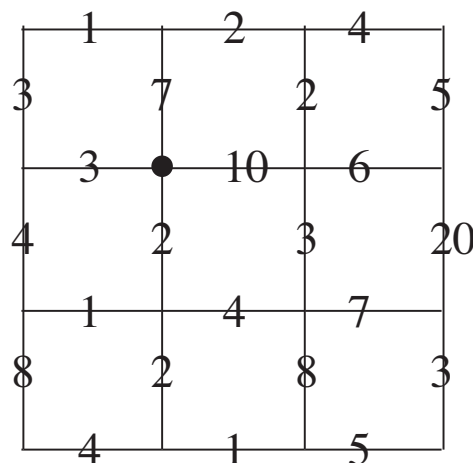
We can also write

$$\mathbf{T}(s_l, s_k) = \sum_j \psi_j(s_l)\lambda_j\psi_j(s_k)$$

Figuratively, the lattice looks like this:

If we associated the *j*'s in the eigenfunction expansion of the transfer matrix with the bonds, for a particular realization of this approach to the calculation of the partition function, then one term in the multiple sum for that quantity looks like this:
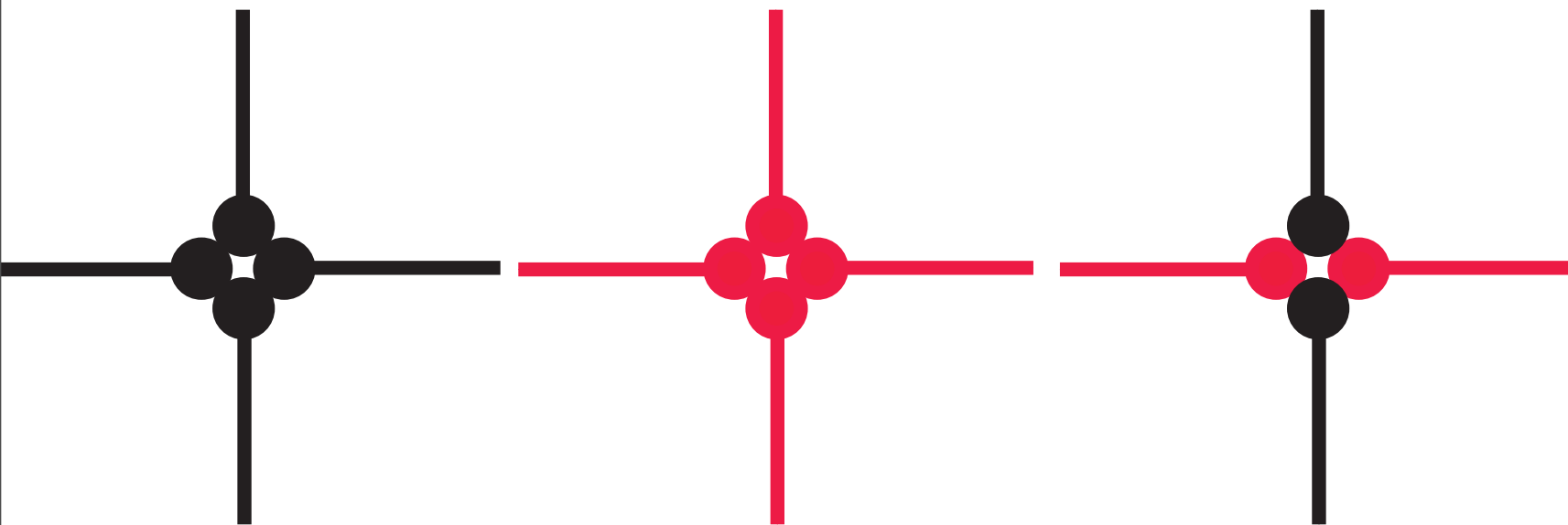

The indicated vertex carries the factor

$$\int_{-\infty}^{\infty} \psi_3(s)\psi_7(x)\psi_{10}(s)\psi_2(s)\,ds$$

A truncated version of the model

Keep only the two largest eigenvalues of the transfer matrix. Then, there are two types of bond and, in d dimensions, $d+1$ types of vertex. For example in two dimensions, the three possible kinds of vertex are
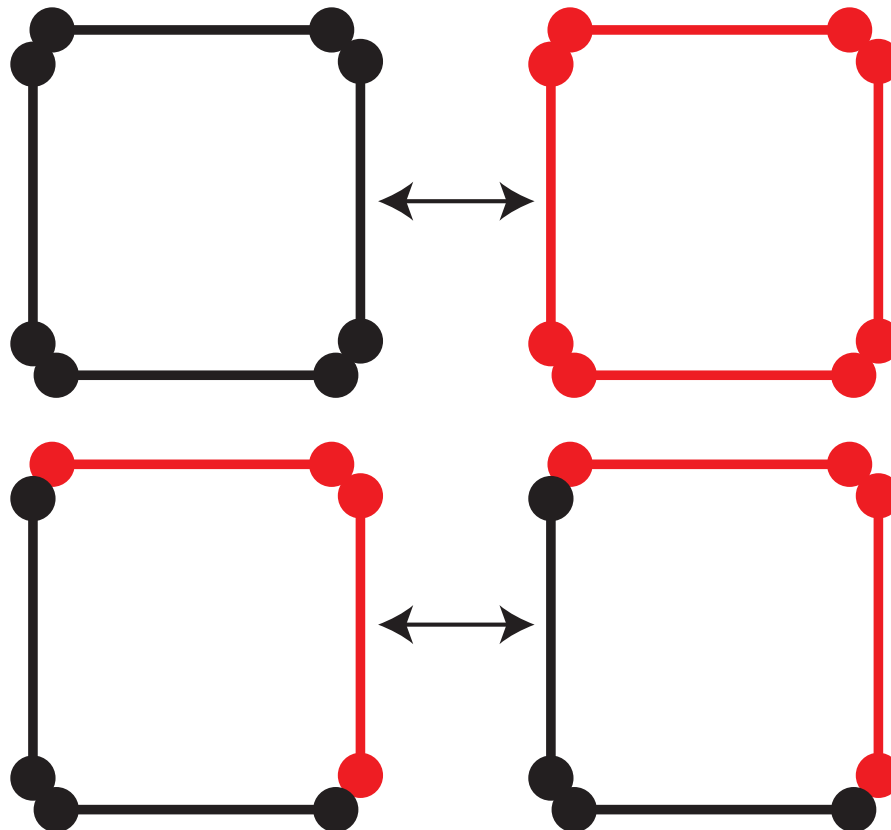
$$\int_{-\infty}^{\infty} \psi_1(x)^4 dx, \ \int_{-\infty}^{\infty} \psi_2(x)^4 dx, \ \text{and} \ \int_{-\infty}^{\infty} \psi_1(x)^2 \psi_2(x)^2 dx$$

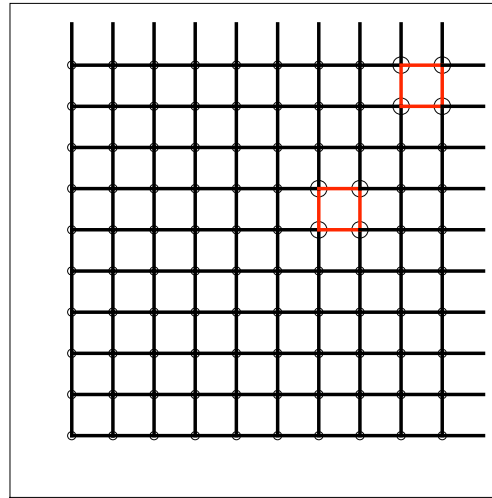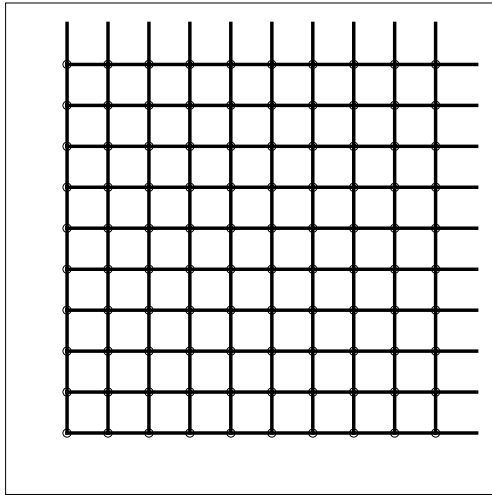Because the eigenfunction ψ_2 has odd parity, there can only be an even number of it at a given vertex.
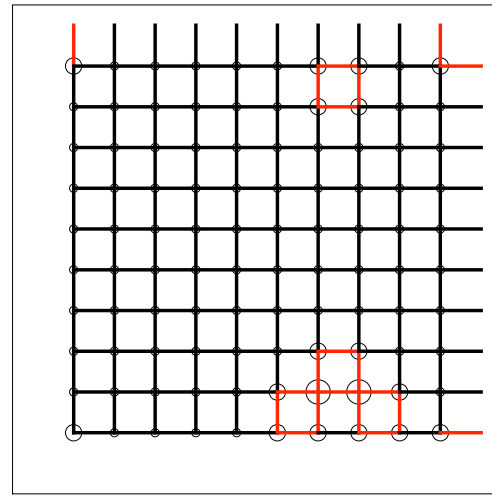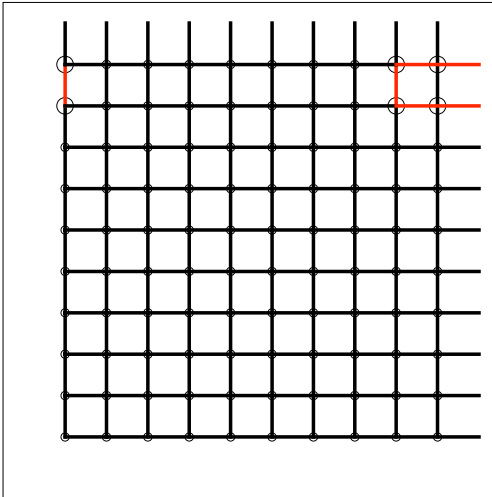
One possible approach in 2D:TMRG (W. Lay and J. Rudnick, PRL **88** (5), 057203 (2002))

The Monte Carlo method: "bond-flipping," plaquette by plaquette.
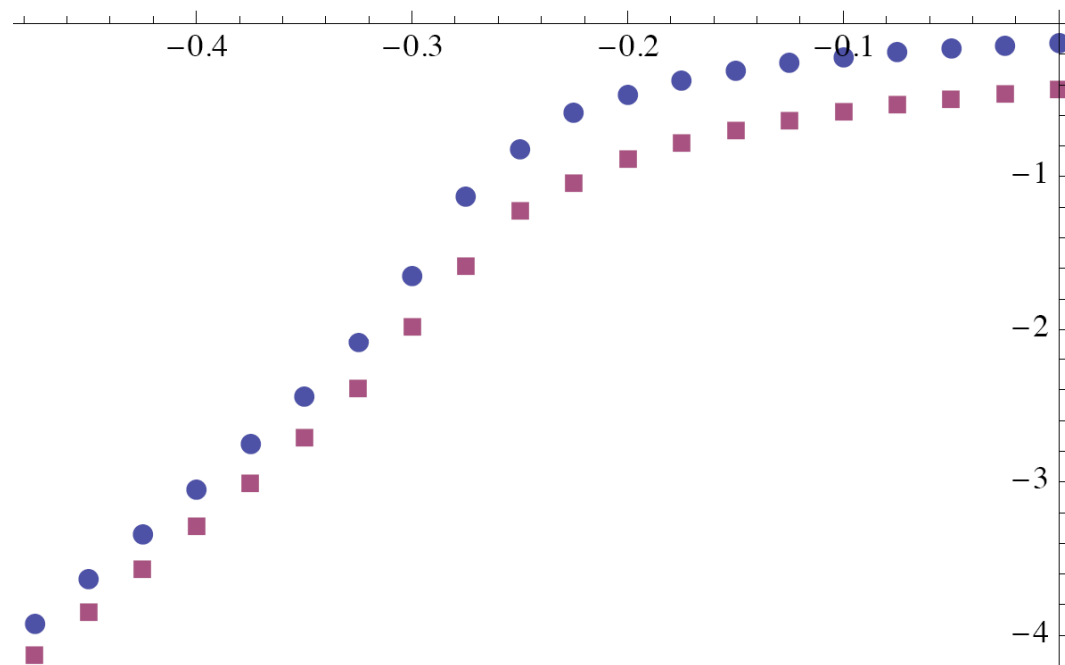
Note: <u>two</u> kinds of lines and <u>three</u> kinds of vertex
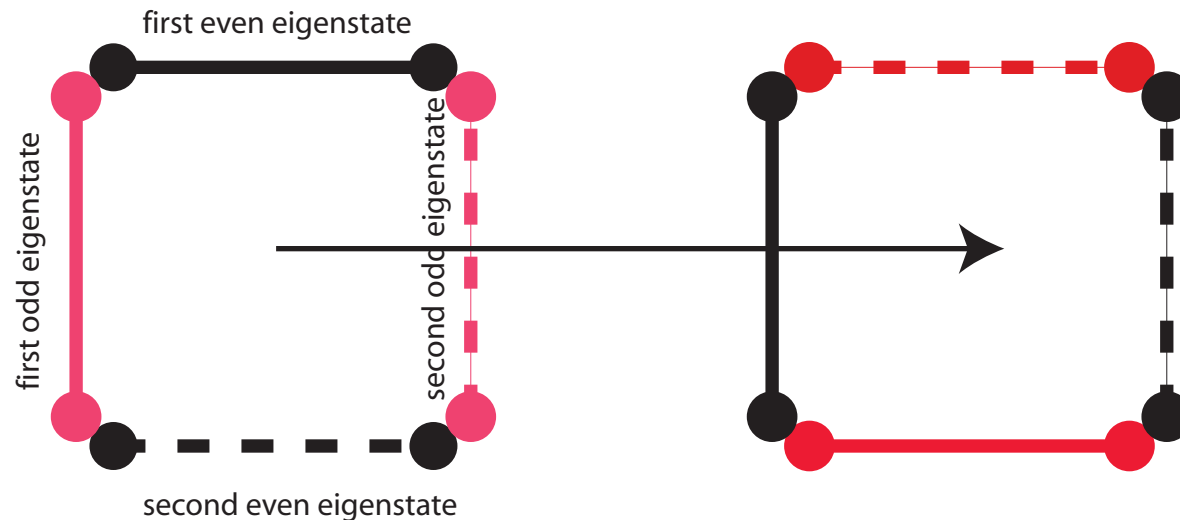
The entropy, defined as $\langle s_i^2 \rangle$ (squares) and $\langle s_i s_j \rangle$ (circles)

Keeping the four largest eigenvalues of the transfer matrix

Now there are four kinds of bond and 17 vertices—and a complication. For some of the vertices, the contribution to the partition function is negative.
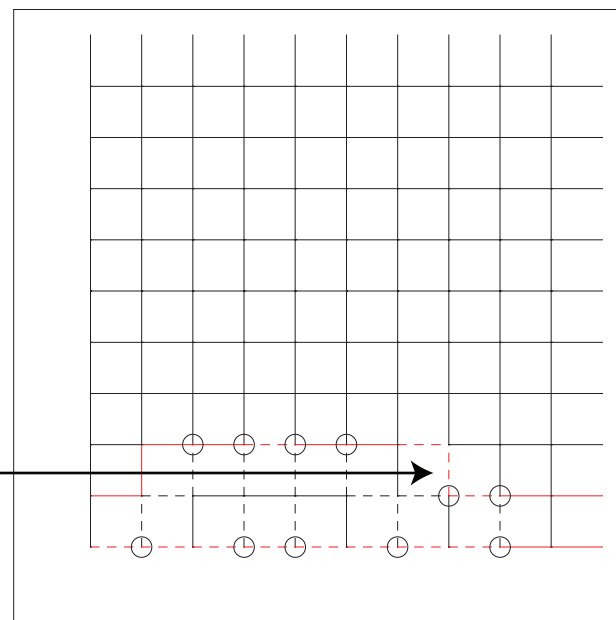
Example of a plaquette "move."

However, some of the 17 possible vertex values contribute a negative factor to the partition function, and a plaquette move can turn a configuration that contributes positively to the partition function into a configuration that yields a negative contribution.
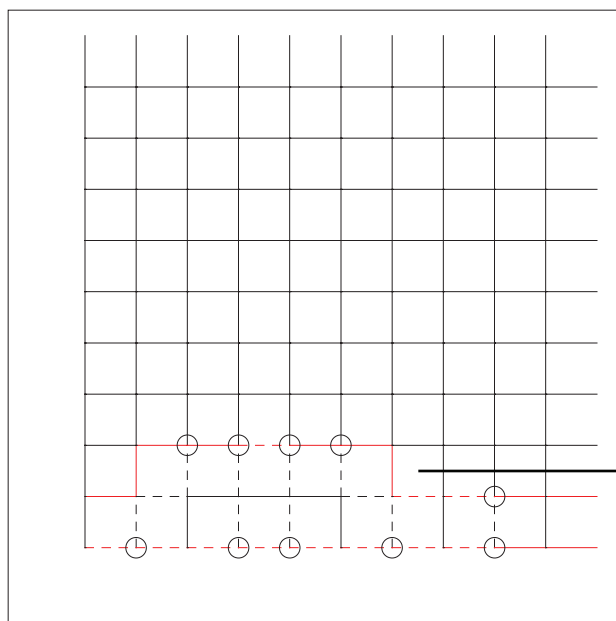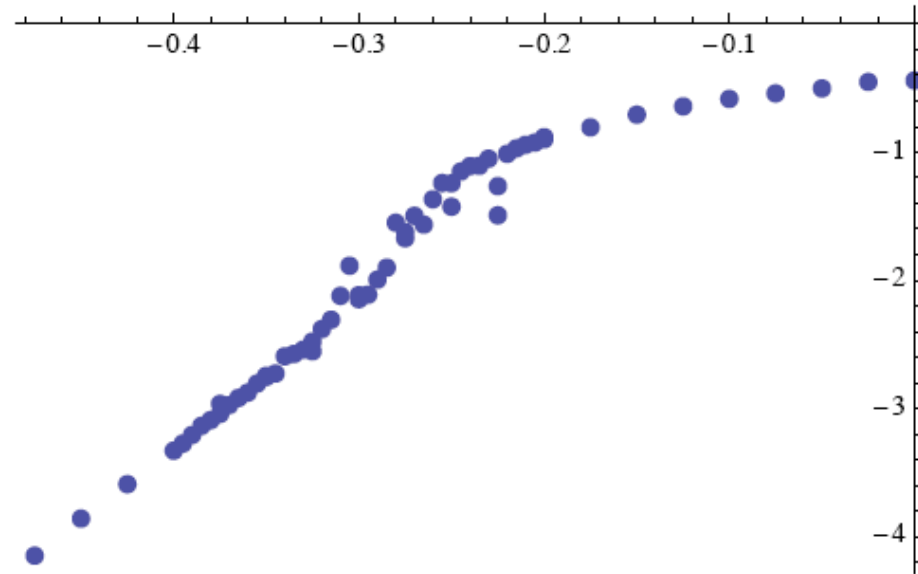

10 negative vertices   11 negative vertices

The solution: evaluate properties for negative and positive configurations separately

The entropy, defined in terms of $\langle s_i^2 \rangle$, as a function of reduced temperature, r.
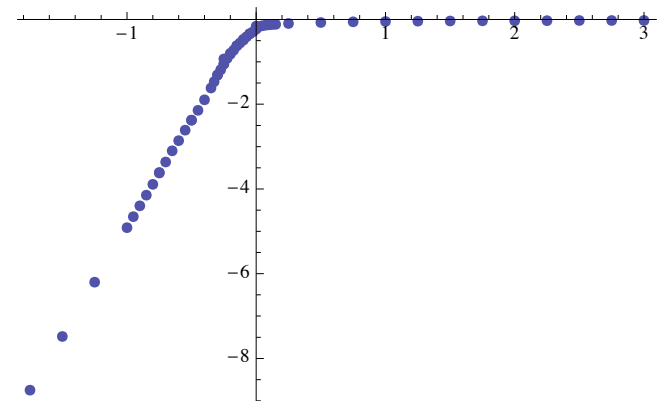
The calculation in a three dimensional system

If we keep the two largest eigenvalues, there are two bonds and four vertices. If we keep the four largest eigenvalues there are four bonds and 44 vertices.

Sample configuration
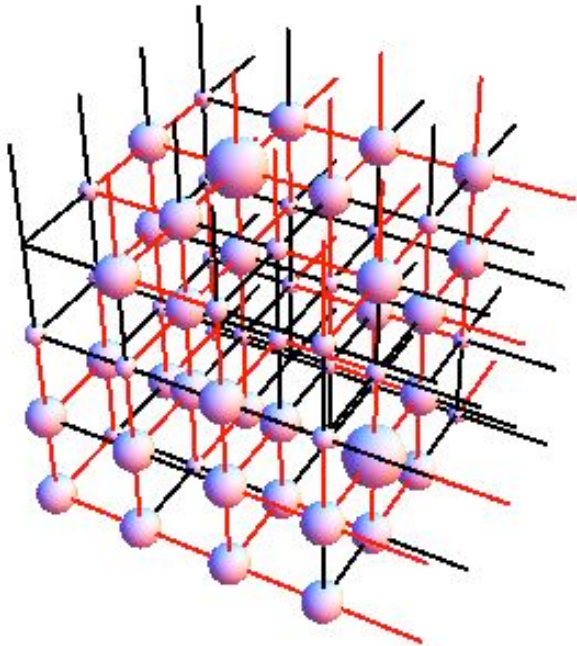
Entropy function

Approach to the calculation of the Casimir force

•First, write the order parameter in the film in terms of a mean field profile multiplied by an amplitude that varies in the d-1 dimensional region occupied by that film

•Then, formulate the change in the effective Hamiltonian of the film induced by a change in the thickness of the film

•This gives rise to a quantity that can be determined by a Monte Carlo calculation

•Finally, subtract the result for that quantity from the mean field free energy per unit volume of the bulk system

Writing
$$\psi(x, y, z, w) = A(y, x, w)p(x)$$

We have for the GLW effective Hamiltonian

$$
\begin{aligned}
\mathcal{H} \quad = \quad & \int dx\, dy\, dz\, dw \left\{ \frac{1}{2} A(y,z,w)^2 \left(\frac{dp(x)}{dx} \right)^2 + \frac{r}{2} A(y,z,w)^2 p(x)^2 \right. \\
& \left. + \frac{1}{2} p(x)^2 \left[\left(\frac{\partial A(y,z,w)}{\partial y} \right)^2 + \left(\frac{\partial A(y,z,w)}{\partial z} \right)^2 + \left(\frac{\partial A(y,z,w)}{\partial w} \right)^2 \right] + \frac{u}{4} p(x)^4 A(y,z,w)^4 \right\}
\end{aligned}
$$

Defining

$$
\begin{aligned}
P_1 \quad &= \quad \frac{1}{L} \int_0^L p(x)^2 \, dx \\
P_2 \quad &= \quad \int_0^L \left(\frac{dp(x)}{dx} \right)^d \, dx \\
P_3 \quad &= \quad \frac{1}{L} \int_0^L p(x)^4 \, dx
\end{aligned}
$$

The effective Hamiltonian becomes

$$
\begin{aligned}
\mathcal{H} \quad = \quad & \int dy\, dz\, dw \left\{ \frac{1}{2} A(y,z,w)^2 \left(rP_1 + P_2 \right) + \frac{1}{2} P_1 \left[\left(\frac{\partial A(y,z,w)}{\partial y} \right)^2 + \right. \right. \\
& \left. \left. \left(\frac{\partial A(y,z,w)}{\partial z} \right)^2 + \left(\frac{\partial A(y,z,w)}{\partial w} \right)^2 \right] + \frac{u}{4} P_3 A(y,z,w)^4 \right\}
\end{aligned}
$$

Sequence of profiles for varying film thickness
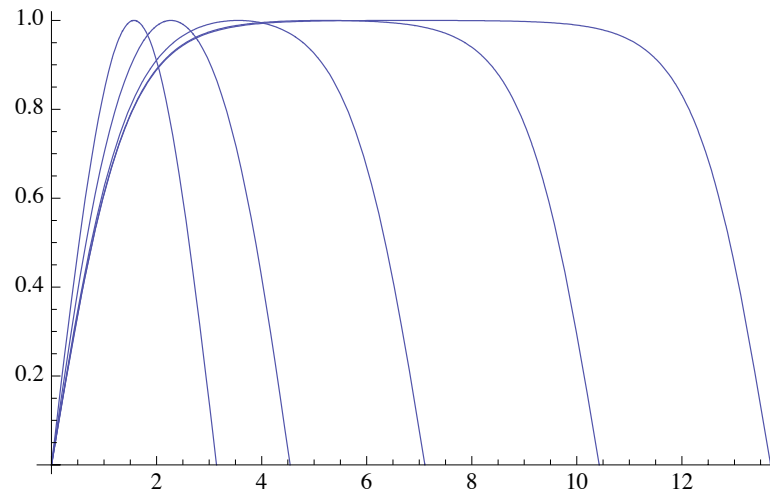
The *L*-derivative of the effective Hamiltonian is

$$
\begin{aligned}
\frac{\partial \mathcal{H}}{\partial L} \;=\;& \int dy \; dz \; dw \Bigg\{ \frac{1}{2} A(y,z,w)^2 \left(r \frac{dP_1}{dL} + \frac{dP_2}{dL} \right) + \frac{1}{2} \frac{dP_1}{dL} \left[\left(\frac{\partial A(y,z,w)}{\partial y} \right)^2 \right. \\
& + \left(\frac{\partial A(y,z,w)}{\partial z} \right)^2 + \left. \left(\frac{\partial A(y,z,w)}{\partial w} \right)^2 \right] + \frac{u}{4} \frac{dP_3}{dL} A(y,z,w)^4 \Bigg\}
\end{aligned}
$$

and the Casimir force is given by

$$
- \langle \partial \mathcal{H} / \partial L \rangle + f_B
$$

where f_B is the mean field bulk free energy

Casimir force, as a function of unrenormalized reduced temperature, *r*, for a 10x10x10 film