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Critical Casimir Forces between Homogeneous and Chemically Striped Surfaces

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In collaboration with: M. Tröndle, S. Dietrich (MPI-IS, Stuttgart)

Critical Casimir effect

- In statistical physics, Critical Casimir effect is the analogue of the Casimir effect in QED
- Casimir effect arises when a long-ranged fluctuating field is confined
- A fluid near a critical point, $\xi \to \infty \Rightarrow$ long-ranged fluctuations
- A confined fluid close to criticality $\Rightarrow$ Critical Casimir effect:
  M. E. Fisher, P.-G. de Gennes, *C. R. Acad. Sc. Paris* **287** (1978), 207

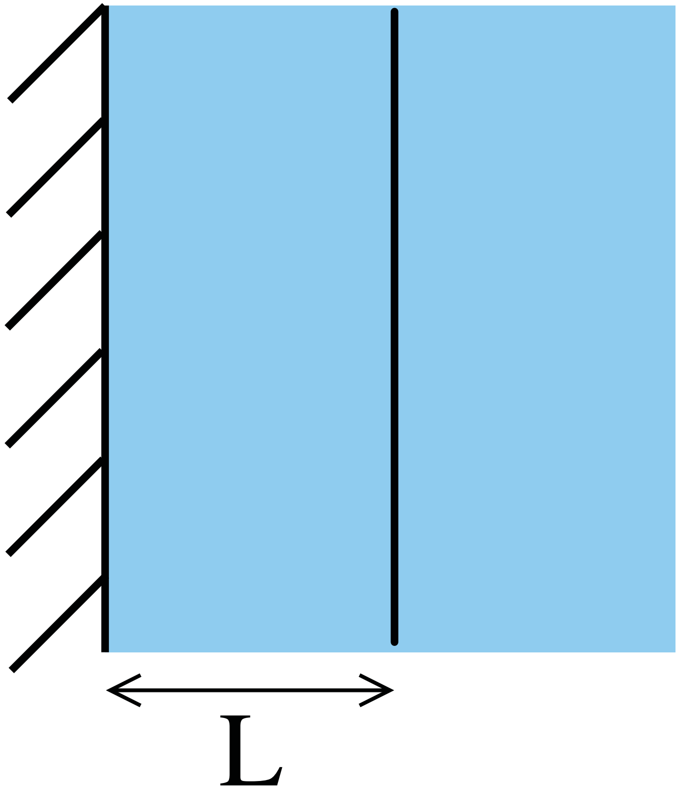
Reviews:

M. Krech, *J. Phys. : Condens. Matter* **11**, R391 (1999)

A. Gambassi, *J. Phys.: Conf. Ser.* **161**, 012037 (2009)

Critical Casimir effect

Fluid confined between surfaces



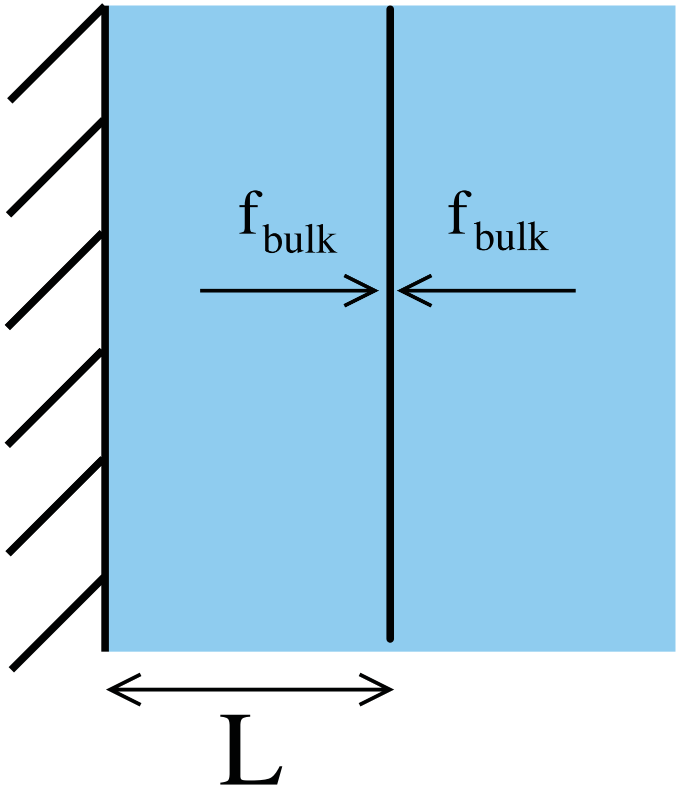
Free energy F per area A:

$$\frac{F}{A} = Lf_{\text{bulk}}(T) + f_{\text{surf}}(T) + \frac{1}{\beta} f_{\text{ex}}(L, T)$$

$$-\frac{\delta(F/A)}{\delta L} = -f_{\text{bulk}}(T) - \frac{1}{\beta}\frac{\delta f_{\text{ex}}(L, T)}{\delta L}$$

Critical Casimir effect

Fluid confined between surfaces



Free energy F per area A:

$$\frac{F}{A} = Lf_{\text{bulk}}(T) + f_{\text{surf}}(T) + \frac{1}{\beta} f_{\text{ex}}(L, T)$$

$$-\frac{\delta(F/A)}{\delta L} = -f_{\text{bulk}}(T) - \frac{1}{\beta} \frac{\delta f_{\text{ex}}(L, T)}{\delta L}$$

Critical Casimir force per area A and $\beta^{-1} = k_B T$:

$$F_C = -\frac{\delta f_{\text{ex}}(L, T)}{\delta L}$$

Critical Casimir Force

Free energy F per area A

$$\frac{F}{A} = L f_{\text{bulk}}(T) + f_{\text{surf}}(T) + \frac{1}{\beta} f_{\text{ex}}(L, T)$$

According to Finite-size scaling:

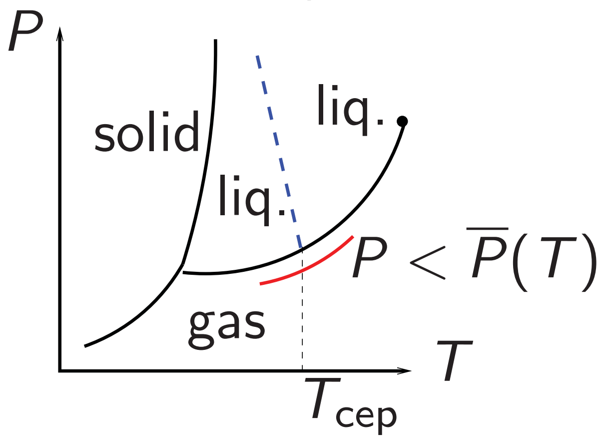
$$F_C \equiv -\frac{\delta f_{\text{ex}}(L, T)}{\delta L} = \frac{1}{L^3}\theta(\tau), \qquad \tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$$

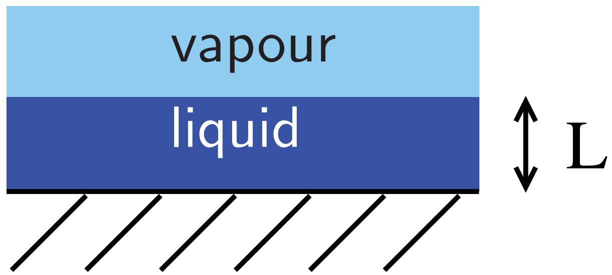
Scaling function $\theta(\tau)$ is <u>universal</u>
Depends on:

- Universality class of bulk phase transition
- Boundary conditions (surface Universality Class)
- Shape of boundaries

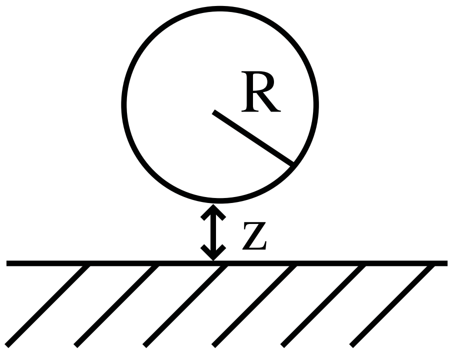
Experimental evidence

- Wetting layers (binary liquid mixture, ^4He)[1]





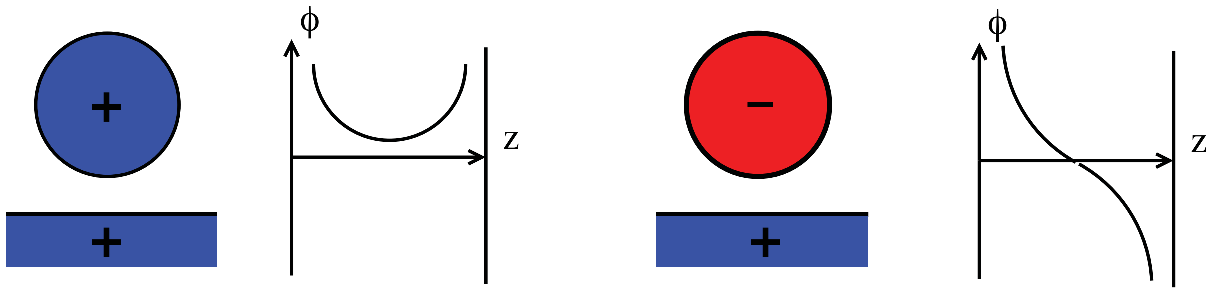
- Colloidal particle in front of a substrate[2]



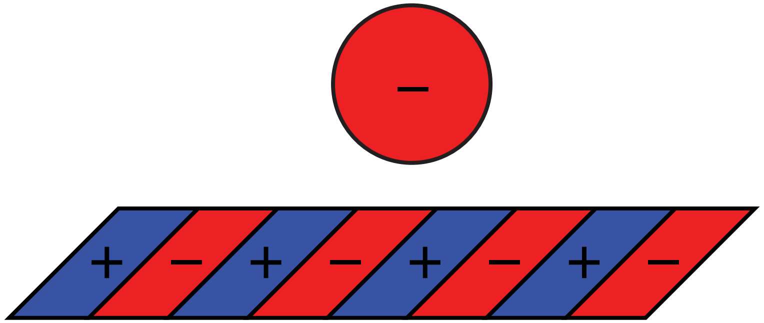
[1] M. Fukuto, Y. F. Yano, P. S. Pershan, 2005; S. Rafaï, D. Bonn, J. Meunier, 2007; R. Garcia, M. H. W. Chan, 2002; R. Garcia, M. H. W. Chan, 1999; A. Ganshin, S. Scheidemantel, R. Garcia, M. H. W. Chan, 2000
[2] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, C. Bechinger, 2008

Casimir force: direct measurement

- Binary liquid mixture $A + B$ at critical concentration $c_{A,c}$: continuous demixing phase transition
- Order parameter: $\phi = c_A - c_{A,c}$
- Ising Universality class
- Surfaces can be treated so to prefer one component:



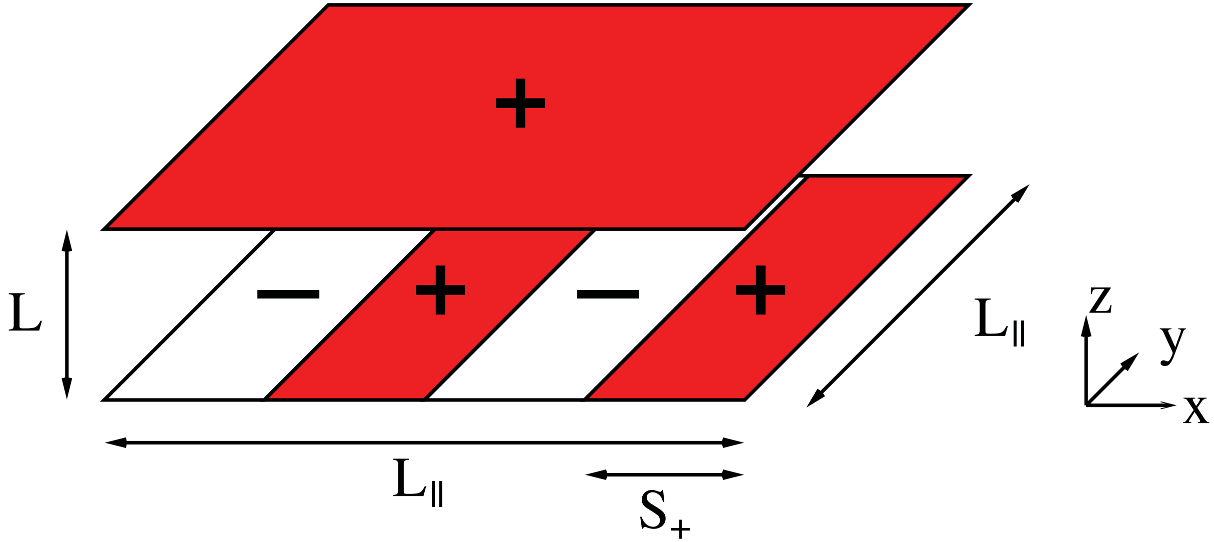
Substrate can be chemically structured[1]



[1] F. Soyka, O. Zvyagolskaya, C. Hertlein, L. Helden, C. Bechinger, 2008

Geometry

- Film geometry with a homogeneous wall and a striped surface



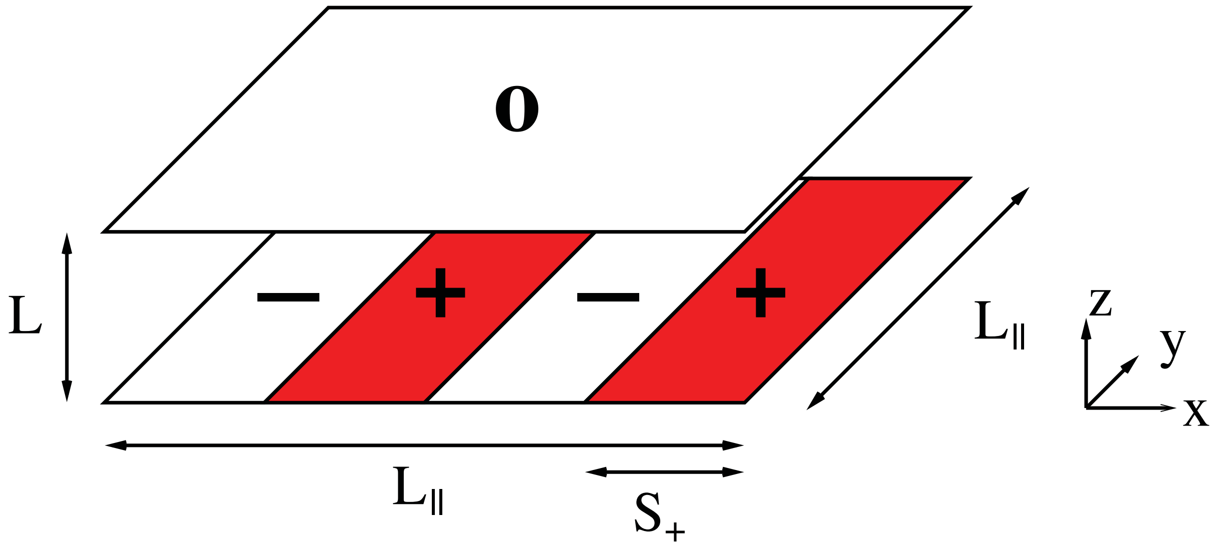
- 3D system $L \times L_\parallel \times L_\parallel$, we extrapolate $\rho \equiv L/L_\parallel \to 0$
- Additional dependence on the Casimir force

$$F_C = \frac{1}{L^3}\theta\left(\tau, \kappa = S_+/L\right), \qquad \tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$$

- Upper surface: fixed b.c. $+$

Geometry

- Film geometry with a homogeneous wall and a striped surface

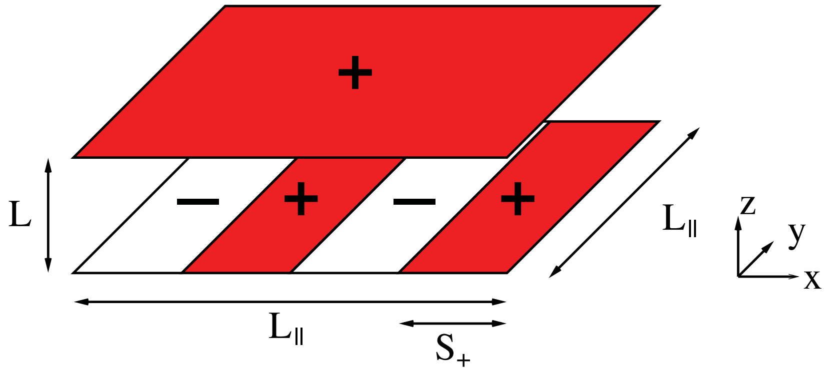


- 3D system $L \times L_{\|} \times L_{\|}$, we extrapolate $\rho \equiv L/L_{\|} \to 0$
- Additional dependence on the Casimir force ($S_+ = S_-$)

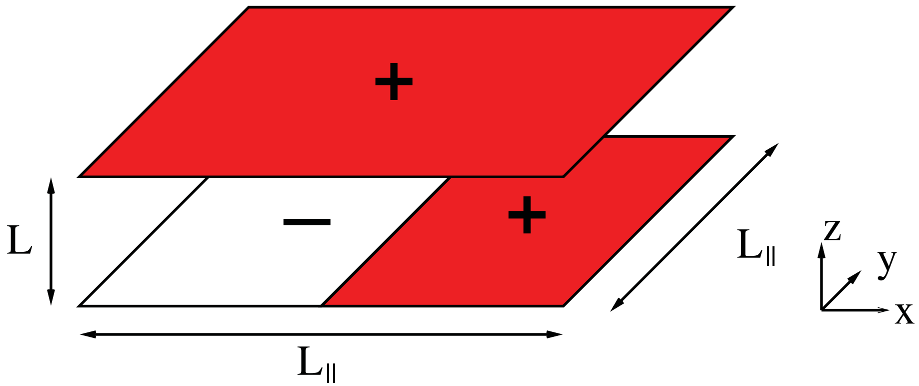
$$F_C = \frac{1}{L^3}\theta\left(\tau, \kappa = S_+/L\right), \qquad \tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$$

- Upper surface: open b.c.

Periodic stripes: limiting cases



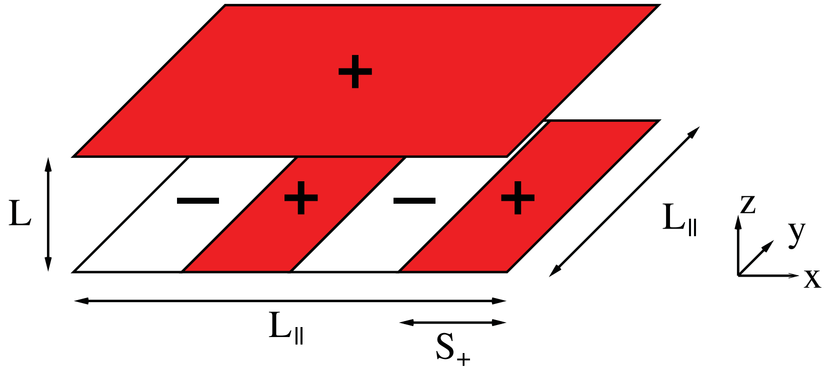
In the limit $\rho \equiv L/L_{\|} \to 0$, for $\kappa \equiv S_+/L \to \infty$:



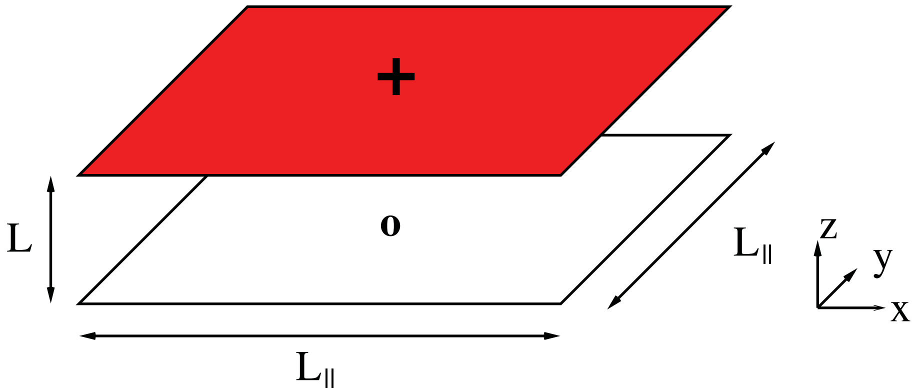
Single chemical step $\Rightarrow$ Mean value $(++)$ and $(+-)$[1]

[1] FPT, S. Dietrich, *JSTAT* P11003 (2010)

Periodic stripes: limiting cases

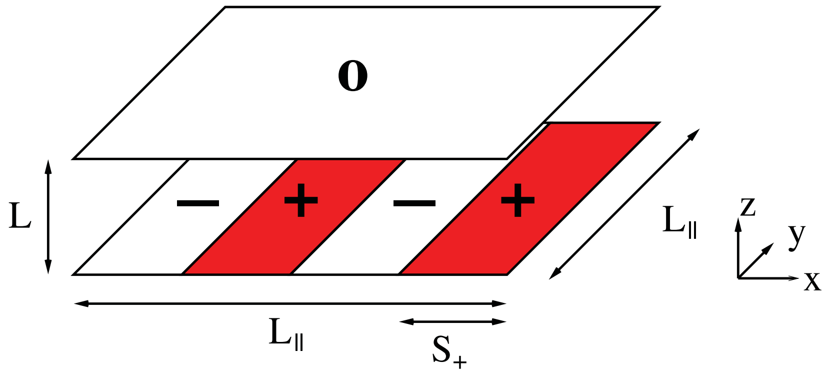


In the limit $\rho \equiv L/L_{\|} \to 0$, for $\kappa \equiv S_{+}/L \to 0$:

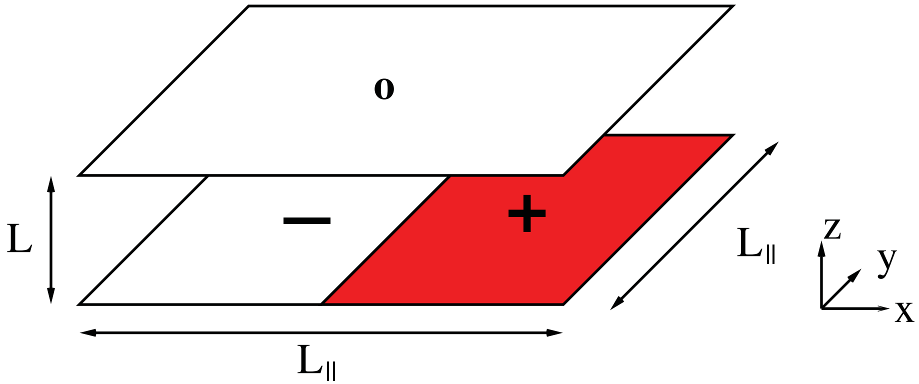


Effective Dirichlet b.c. on the lower surface

Periodic stripes: limiting cases

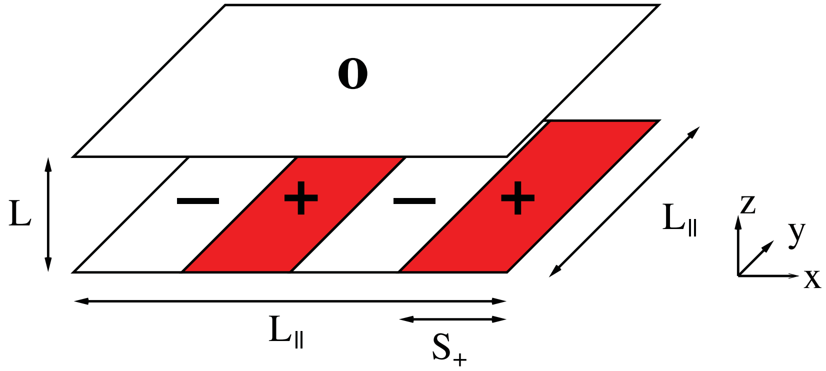


In the limit $\rho \equiv L/L_{\|} \to 0$, for $\kappa \equiv S_{+}/L \to \infty$:

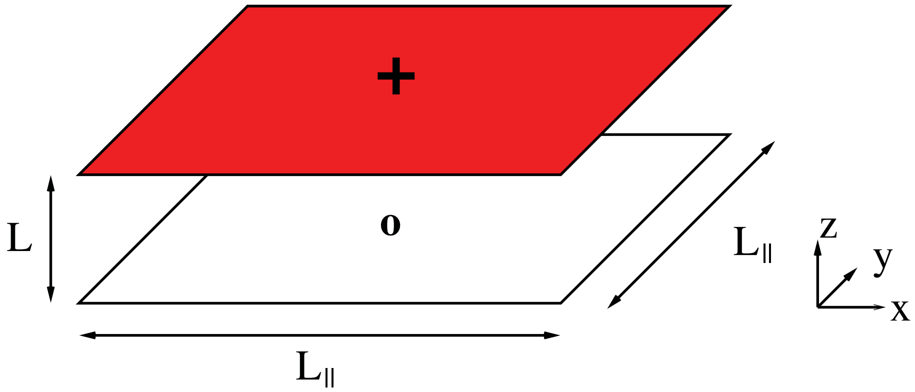


$\Rightarrow$ Mean value $(+o)$ and $(-o)$

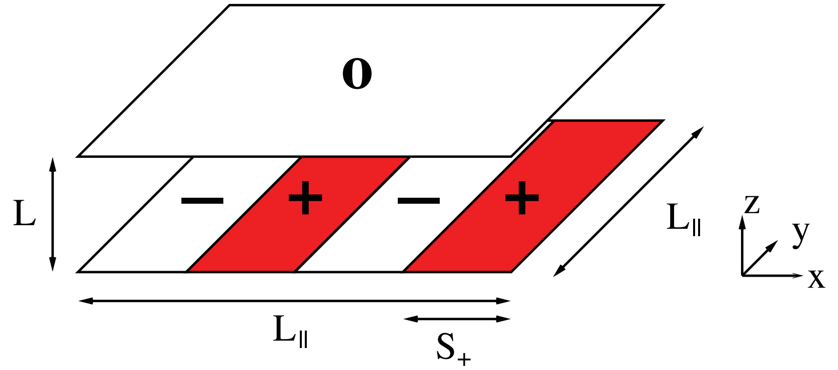
Periodic stripes: limiting cases



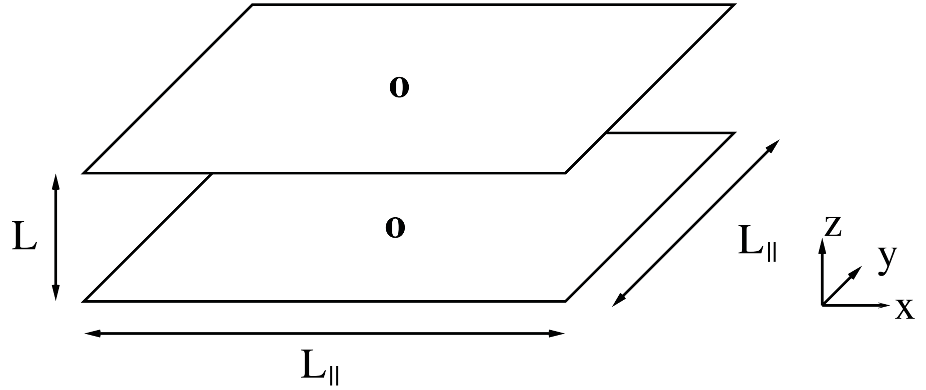
In the limit $\rho \equiv L/L_{\|} \to 0$, for $\kappa \equiv S_{+}/L \to \infty$:



Periodic stripes: limiting cases



In the limit $\rho \equiv L/L_{||} \to 0$, for $\kappa \equiv S_+/L \to 0$:



Dirichlet b.c. on the both surfaces

Method

- The critical Casimir force F_C is obtained as

$$\frac{\delta(F/L_{\parallel}^2)}{\delta L} = f_{\text{bulk}}(T) - \frac{1}{\beta}F_C(L,T)$$

- Monte Carlo simulations + numerical integration on a lattice model

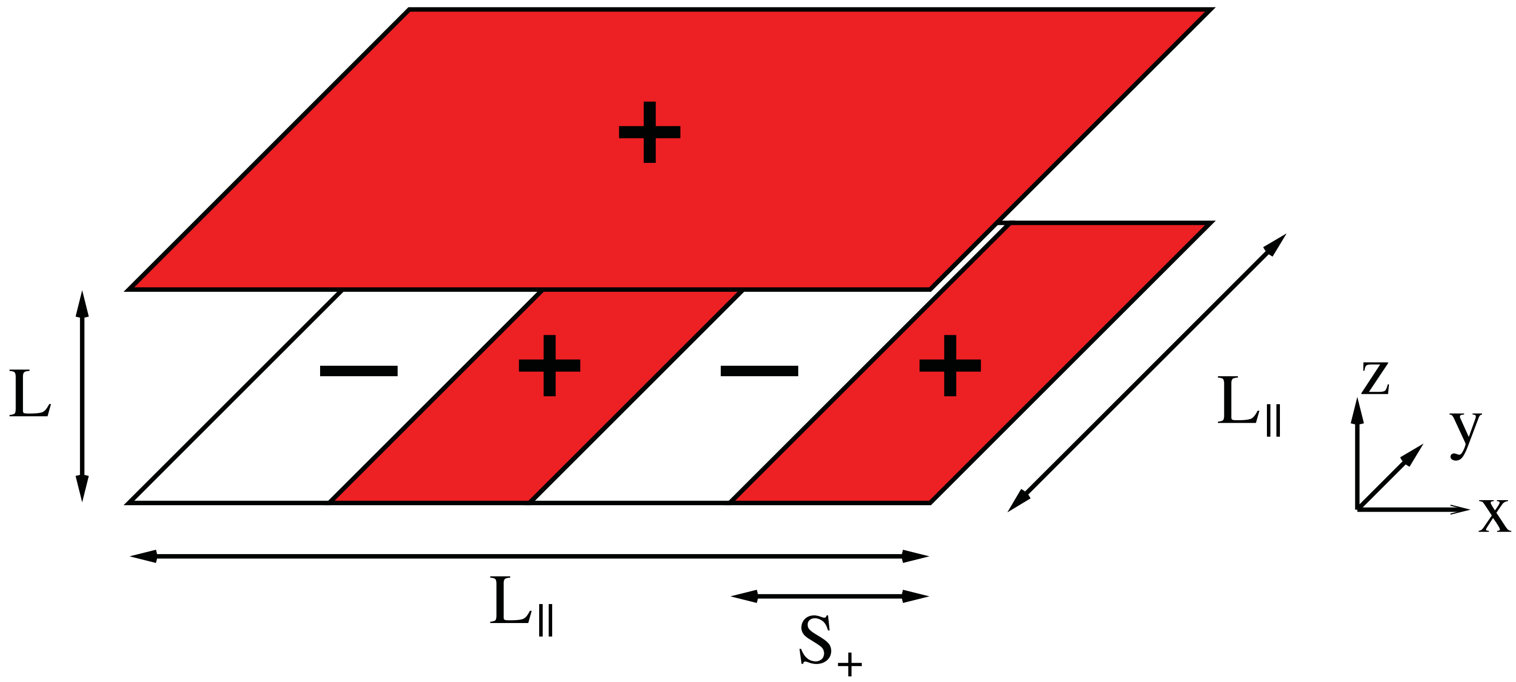
$$\mathcal{H} = -\beta\sum_{\langle ij\rangle} S_i S_j + D\sum_i S_i^2, \qquad S_i = \pm 1, 0$$

At $D = 0.656(20)$[1] the leading scaling corrections are suppressed

- In order to calculate $\delta(F/L_{\parallel}^2)/\delta L$ we use two methods:
  - Coupling parameter approach[2] at T_c
  - Integration over β[3] off criticality
- Mean-Field Theory calculation

[1] M. Hasenbusch, *Phys. Rev. B* **82**, 174433 (2010)
[2] O. Vasilyev, A. Gambassi, A. Maciołek, S. Dietrich, *Europhys. Lett.* **80**, 60009 (2007)
[3] A. Hucht, *Phys. Rev. Lett.* **99**, 185301 (2007)

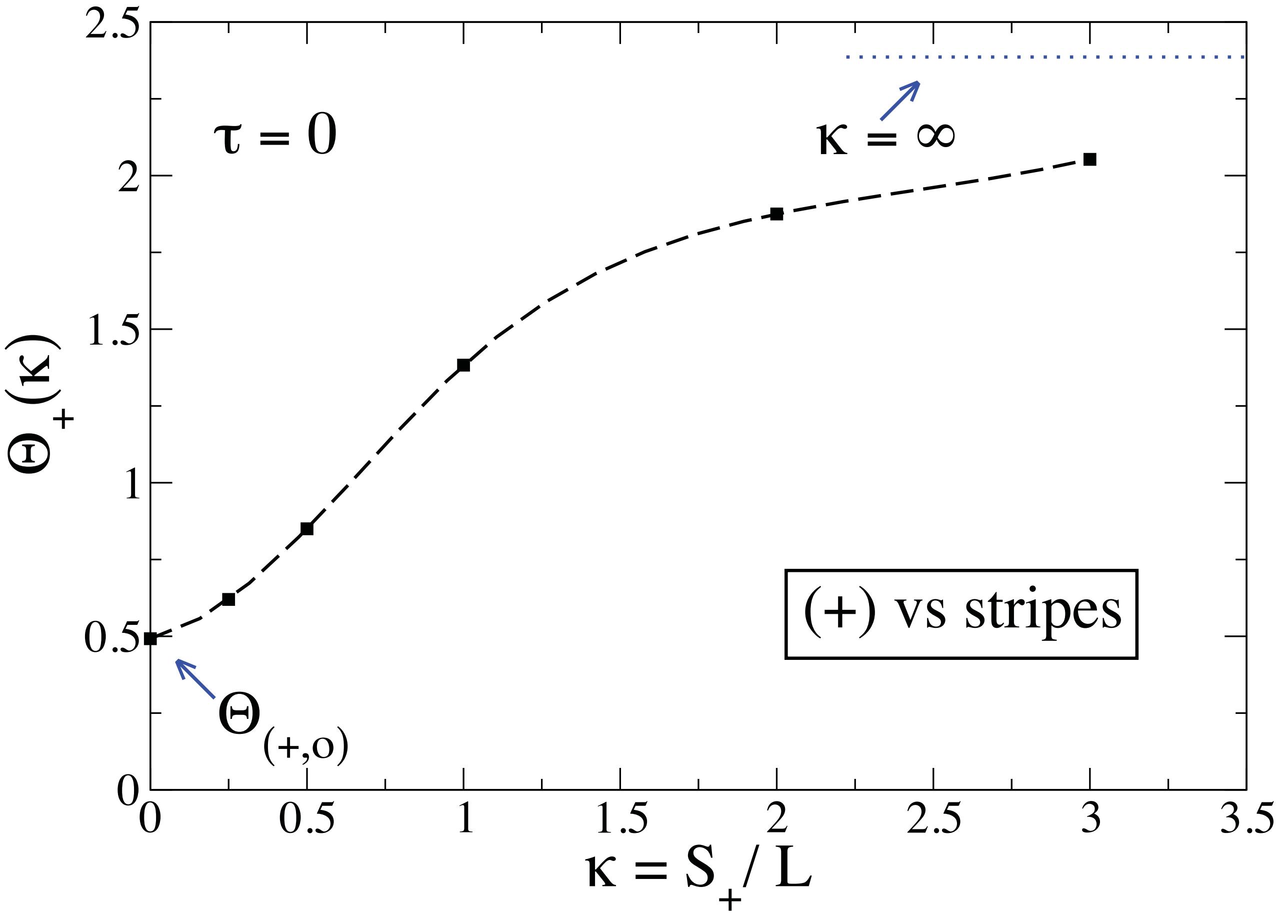
Results: (+) vs stripes



Critical Casimir Force:

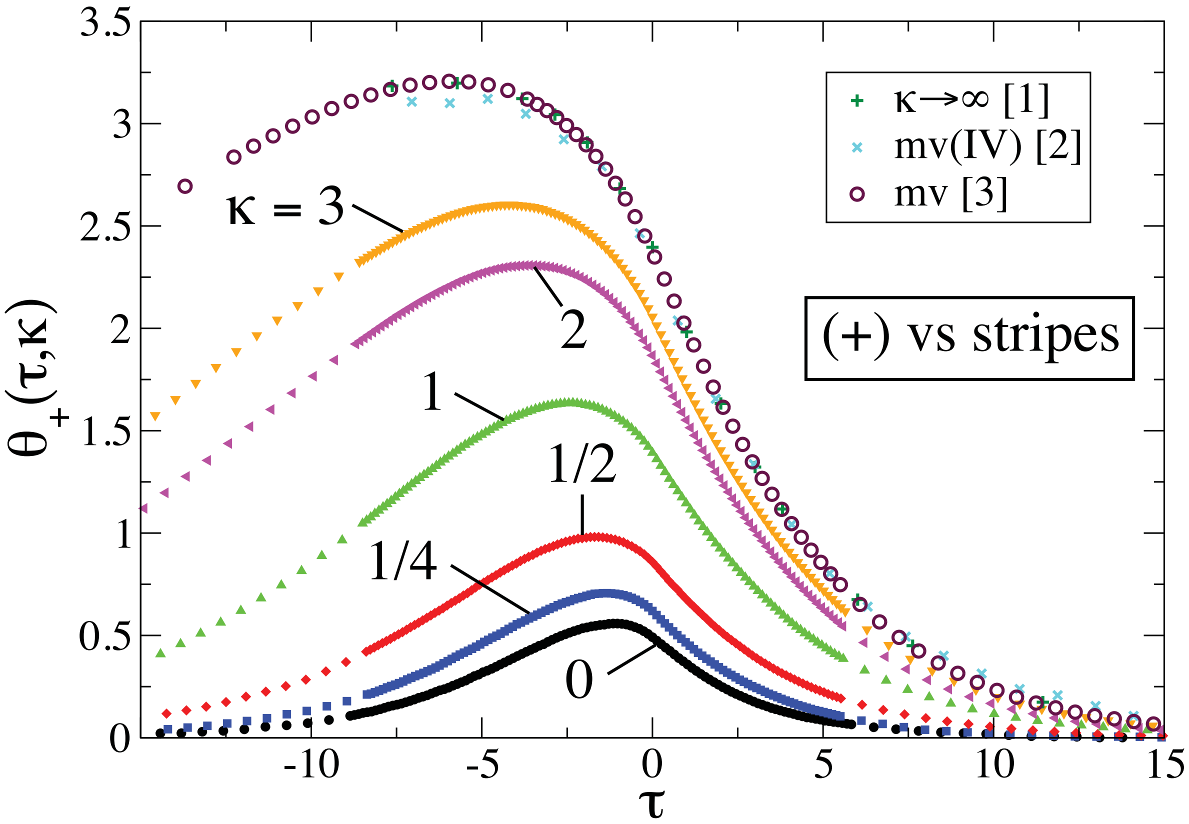
$$F_C = \frac{1}{L^3}\theta\left(\tau, \kappa = S_+/L\right), \qquad \tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$$

MC results: critical Casimir Amplitude (+) vs stripes



Critical amplitude $\Theta(\kappa = S_+/L) \equiv \theta(\tau = 0, \kappa)$, $\tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$

MC results: universal scaling function (+) vs stripes



$$F_C = \frac{1}{L^3}\theta(\tau,\kappa), \qquad \tau \propto \left(\frac{T-T_c}{T_c}\right) L^{1/\nu}, \ \kappa \equiv S_+/L$$

[1] FPT, S. Dietrich, *JSTAT* P11003 (2010)

[2] O. Vasilyev, A. Gambassi, A. Maciołek, S. Dietrich, *Phys. Rev. E* **79**, 041142 (2009)

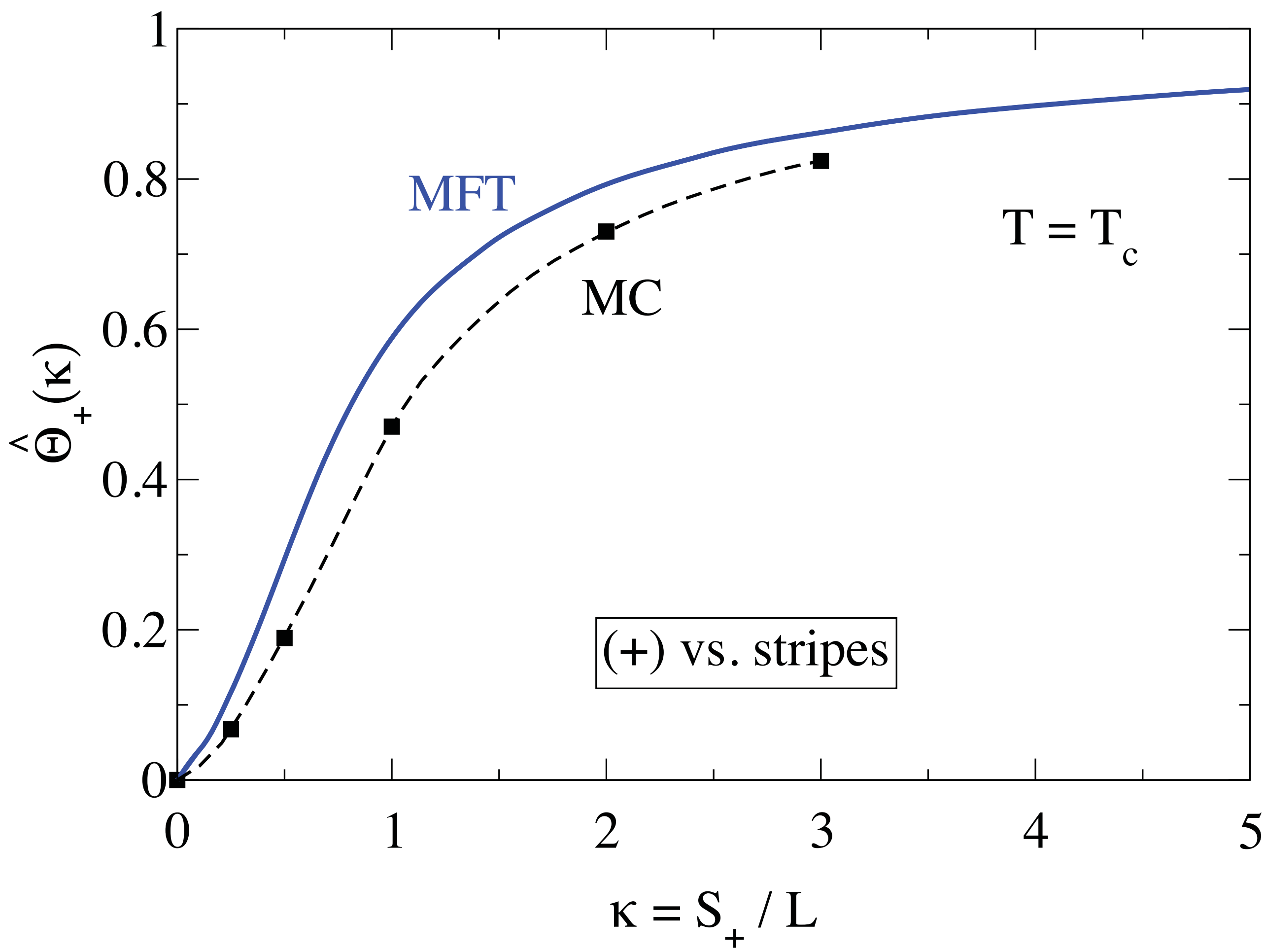
[3] M. Hasenbusch, *Phys. Rev. B* **82**, 104425 (2010)

Comparison with Mean-Field Theory

- Mean-Field Theory allows to determine the critical Casimir force scaling functions $\theta(\tau, \kappa)$ up to a prefactor
- Useful to normalize the results by an overall amplitude (e.g., $|\Theta_{(++)}|$)
- At $T = T_c$ we use an alternative normalization:

$$\hat{\Theta}(\kappa) \equiv \frac{\Theta(\kappa) - \Theta(\kappa \to 0)}{\Theta(\kappa \to \infty) - \Theta(\kappa \to 0)} \to \begin{cases} 0, & \kappa \to 0, \\ 1, & \kappa \to \infty. \end{cases}$$

Comparison with Mean-Field Theory: (+) vs stripes



Normalization: $\hat{\Theta}(\kappa) \equiv \frac{\Theta(\kappa) - \Theta(\kappa \to 0)}{\Theta(\kappa \to \infty) - \Theta(\kappa \to 0)}$

Comparison with Mean-Field Theory

- Mean-Field Theory allows to determine the critical Casimir force scaling functions $\theta(\tau,\kappa)$ up to a prefactor

- Useful to normalize the results by an overall amplitude (e.g., $|\Theta_{(++)}|$)

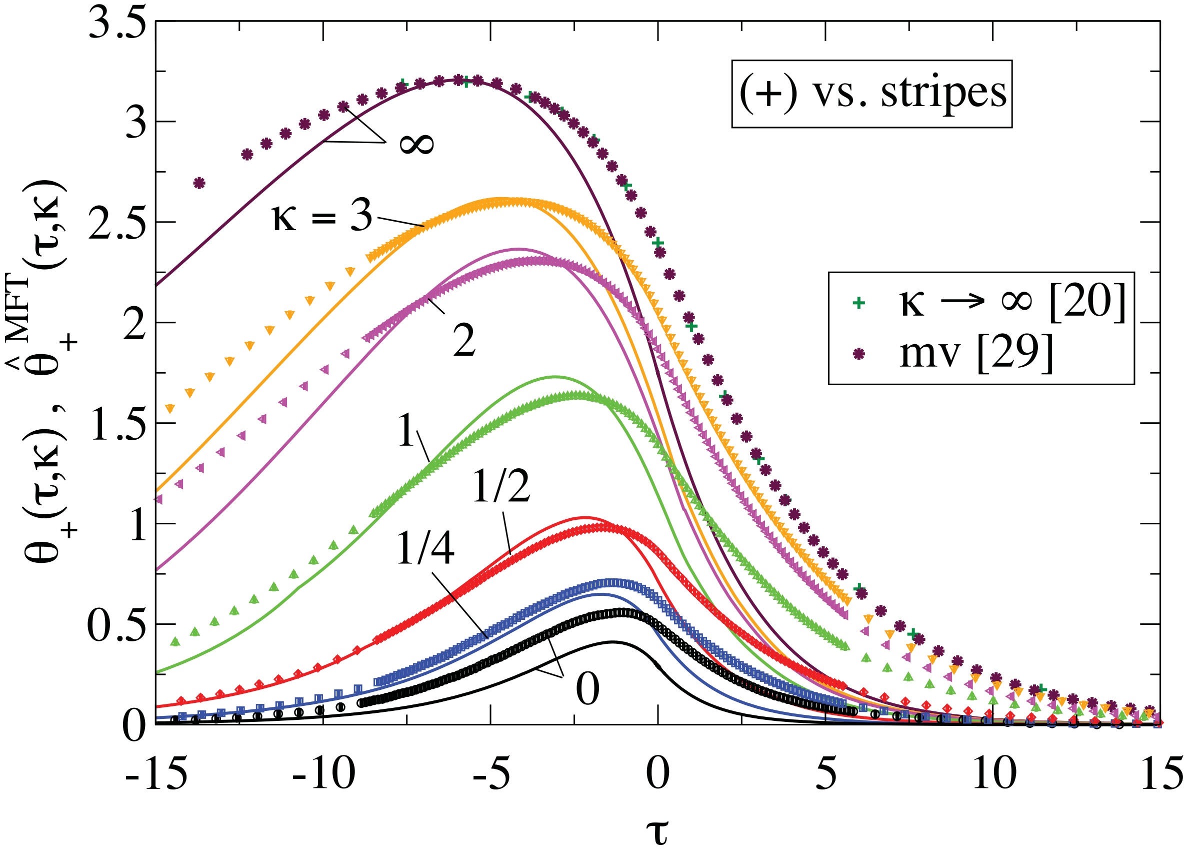
- In order to compare MFT and MC results, it is useful to rescale both the amplitude and the argument τ[1]

$$\hat{\theta}^{\mathrm{MFT}}_{+/o}(\tau,\kappa) \equiv \frac{\theta_{+/o}(\tau_{\mathrm{max},+/o},\kappa\to\infty)}{\theta^{\mathrm{MFT}}_{+/o}(\tau^{\mathrm{MFT}}_{\mathrm{max},+/o},\kappa\to\infty)}\theta^{\mathrm{MFT}}_{+/o}\left(\frac{\tau^{\mathrm{MFT}}_{\mathrm{max},+/o}}{\tau_{\mathrm{max},+/o}}\tau,\kappa\right)$$

with τ_{max} position of the maximum
$\Rightarrow$ For $\kappa\to\infty$ both the position and the value of the maximum match the MC results

[1] T. F. Mohry, A. Maciołek, and S. Dietrich, *J. Chem. Phys.* **136**, 224902 (2012)

Comparison with Mean-Field Theory: (+) vs stripes

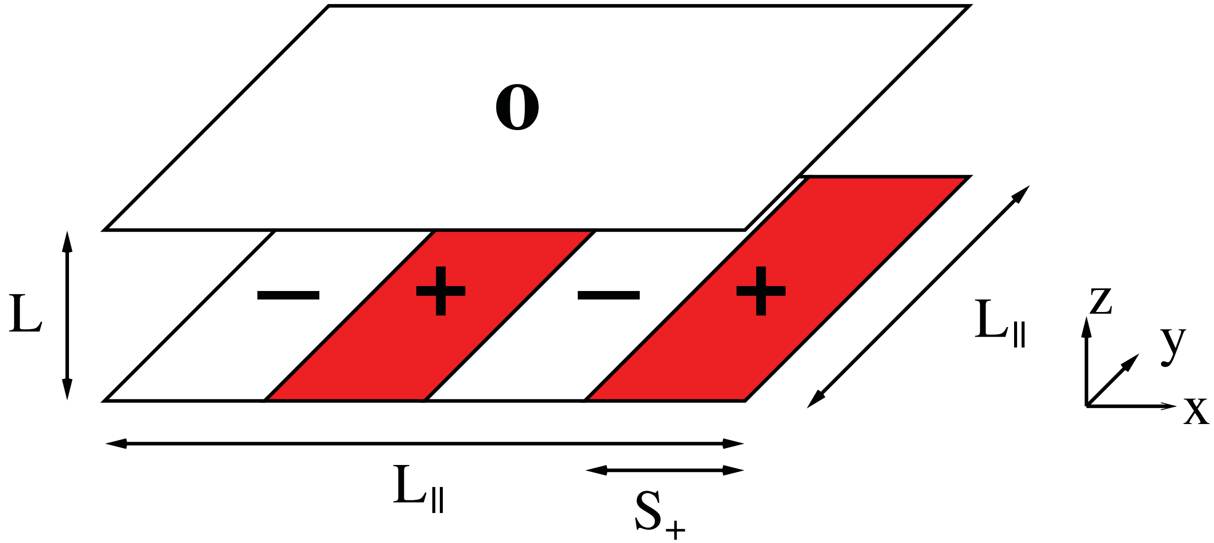


Normalization: $\hat{\theta}^{\mathrm{MFT}}_{+/o}(\tau,\kappa) \equiv \frac{\theta_{+/o}(\tau_{\mathrm{max},+/o},\kappa\to\infty)}{\theta^{\mathrm{MFT}}_{+/o}(\tau^{\mathrm{MFT}}_{\mathrm{max},+/o},\kappa\to\infty)}\theta^{\mathrm{MFT}}_{+/o}\left(\frac{\tau^{\mathrm{MFT}}_{\mathrm{max},+/o}}{\tau_{\mathrm{max},+/o}}\tau,\kappa\right)$

[1] FPT, S. Dietrich, *JSTAT*, P11003 (2010)

[2] M. Hasenbusch, *Phys. Rev. B* **82**, 104425 (2010)

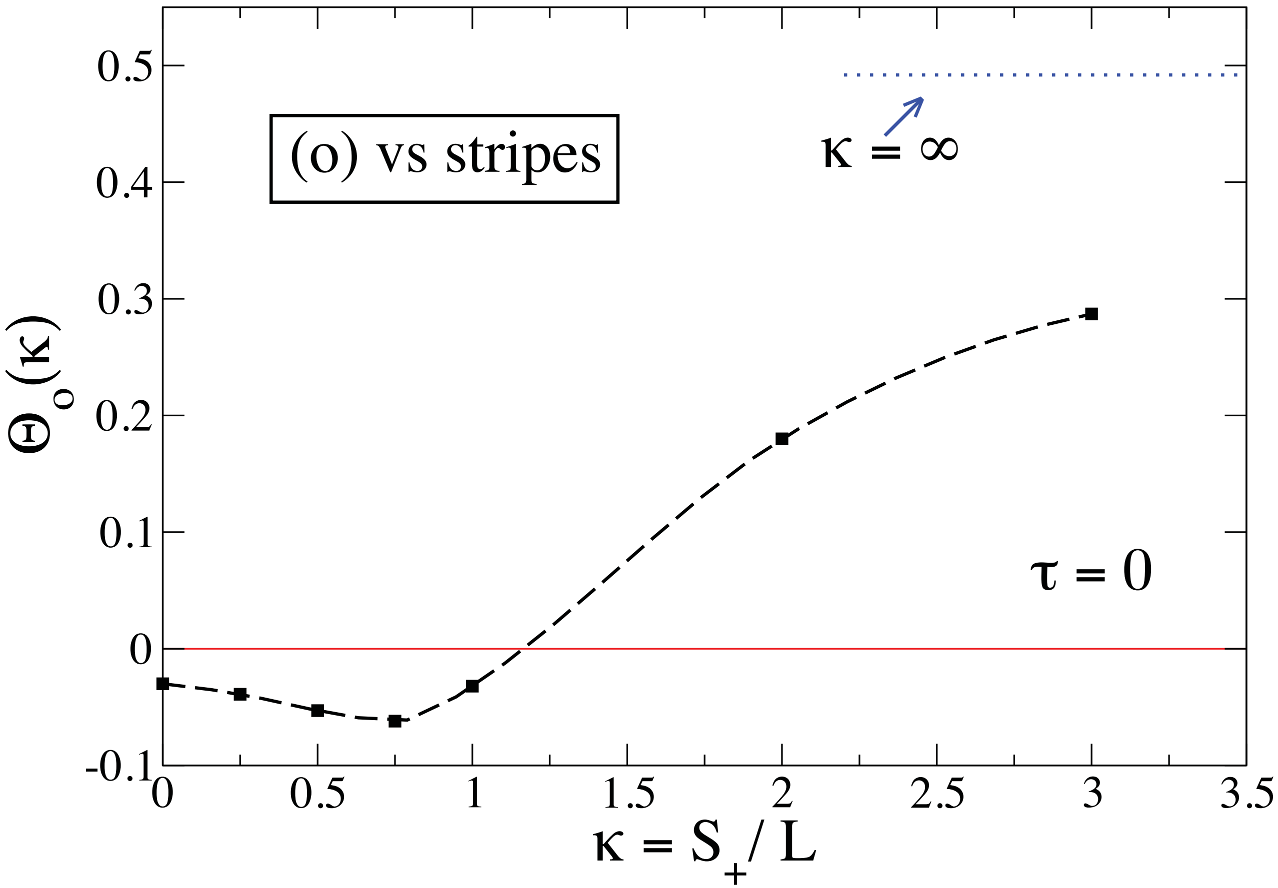
Results: (o) vs stripes



Critical Casimir Force

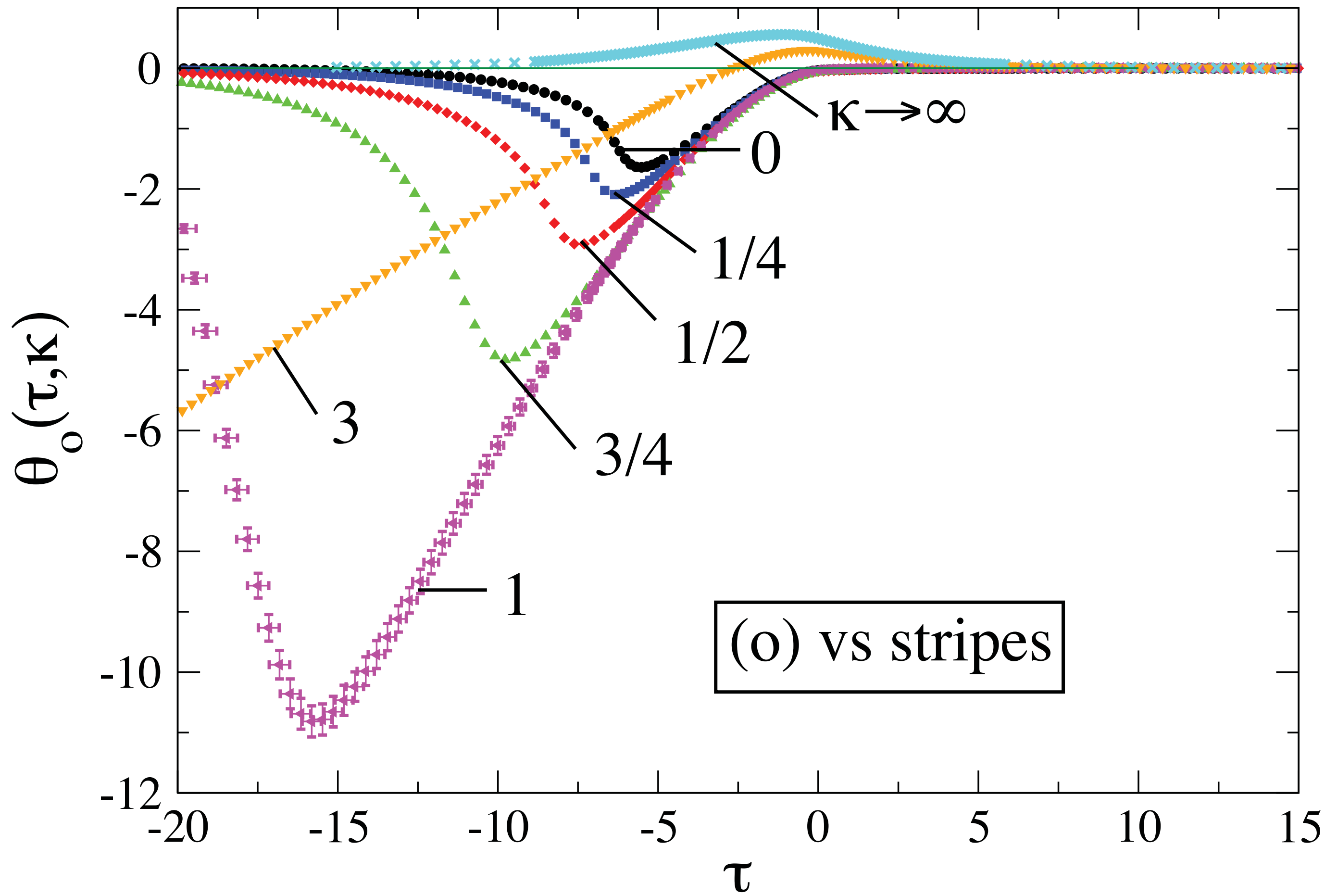
$$F_C = \frac{1}{L^3}\theta\left(\tau, \kappa = S_+/L\right), \qquad \tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$$

Critical Casimir Amplitude: (o) vs stripes



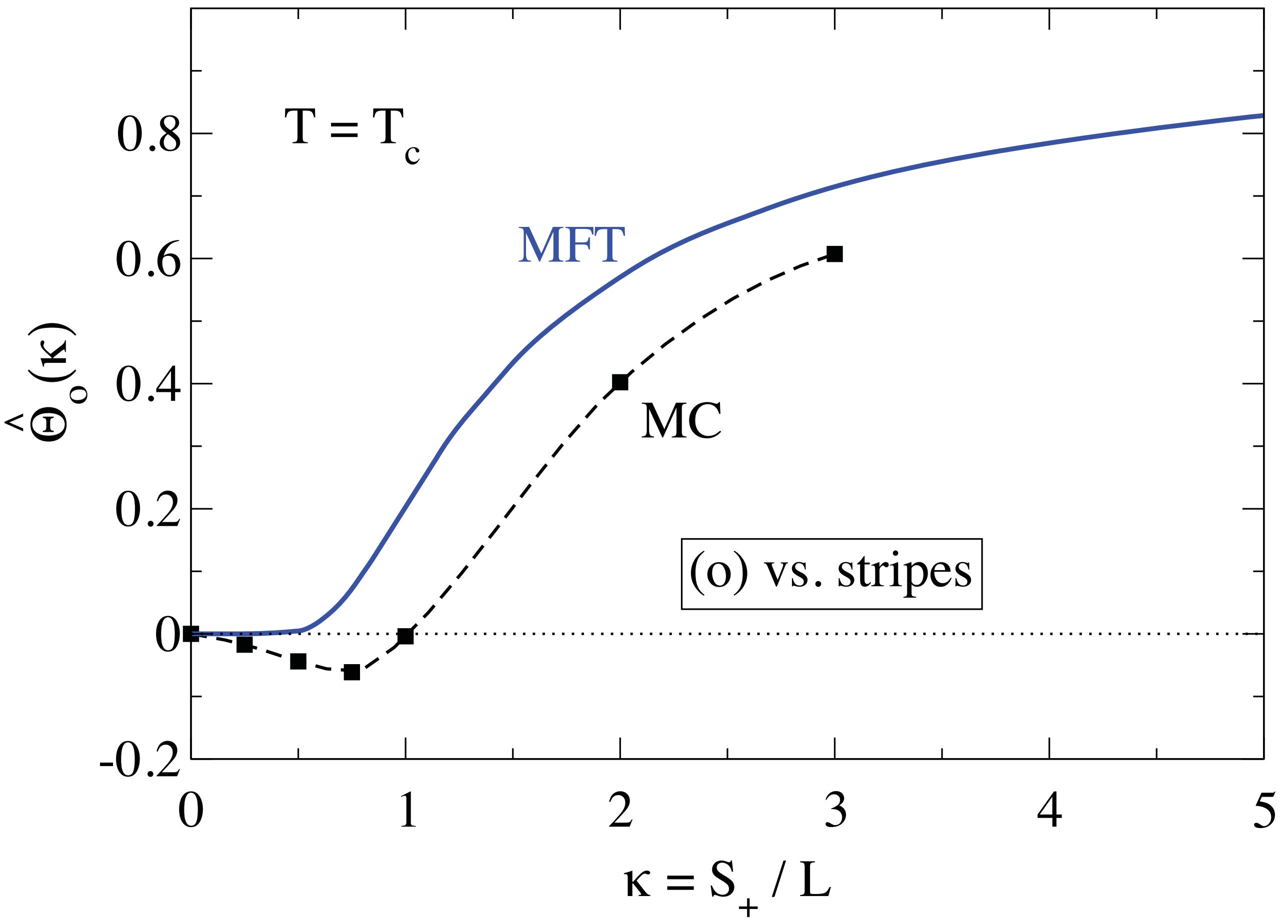
Critical amplitude $\Theta(\kappa = S_+/L) \equiv \theta(\tau = 0, \kappa)$, $\tau \propto \left(\frac{T - T_c}{T_c}\right) L^{1/\nu}$

Universal scaling function: (o) vs stripes



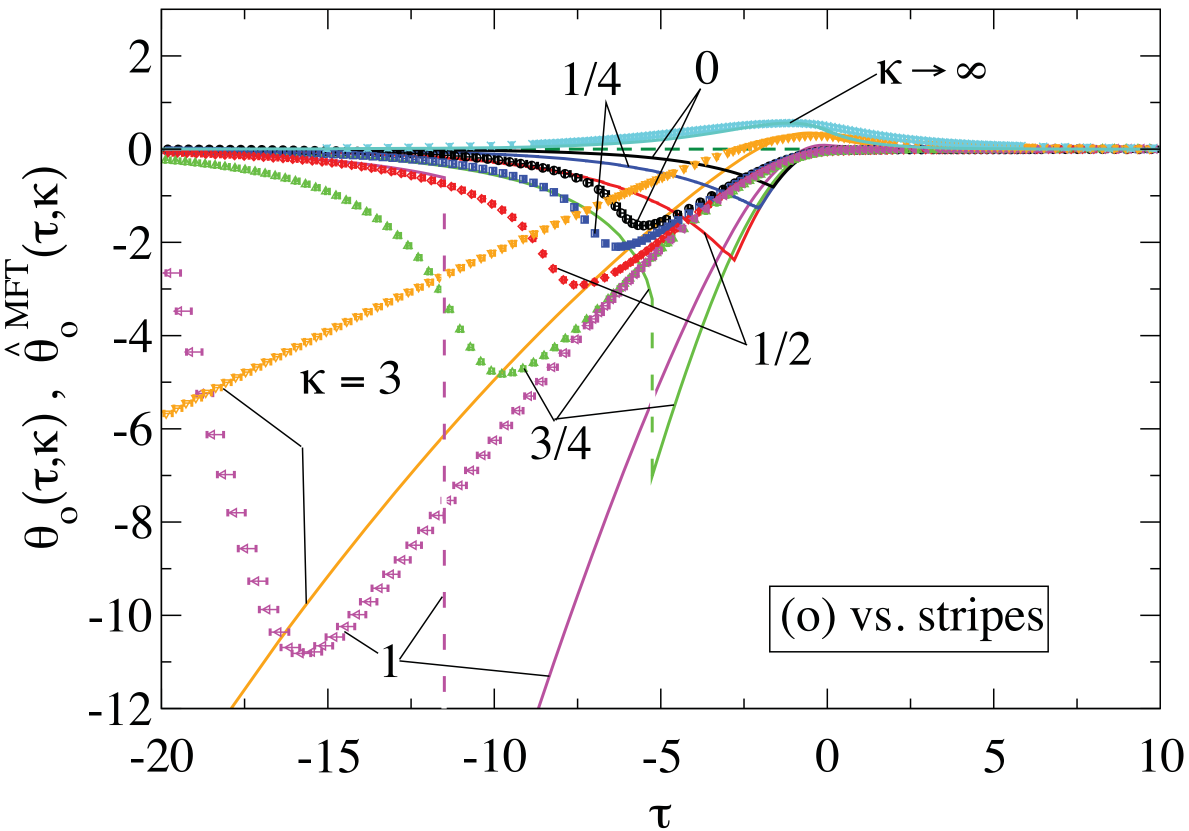
$$F_C = \frac{1}{L^3}\theta(\tau,\kappa), \qquad \tau \propto \left(\frac{T-T_c}{T_c}\right) L^{1/\nu},\ \kappa \equiv S_+/L$$

Comparison with Mean-Field Theory: (o) vs stripes



Normalization: $\hat{\Theta}(\kappa) \equiv \frac{\Theta(\kappa)-\Theta(\kappa\to 0)}{\Theta(\kappa\to\infty)-\Theta(\kappa\to 0)}$

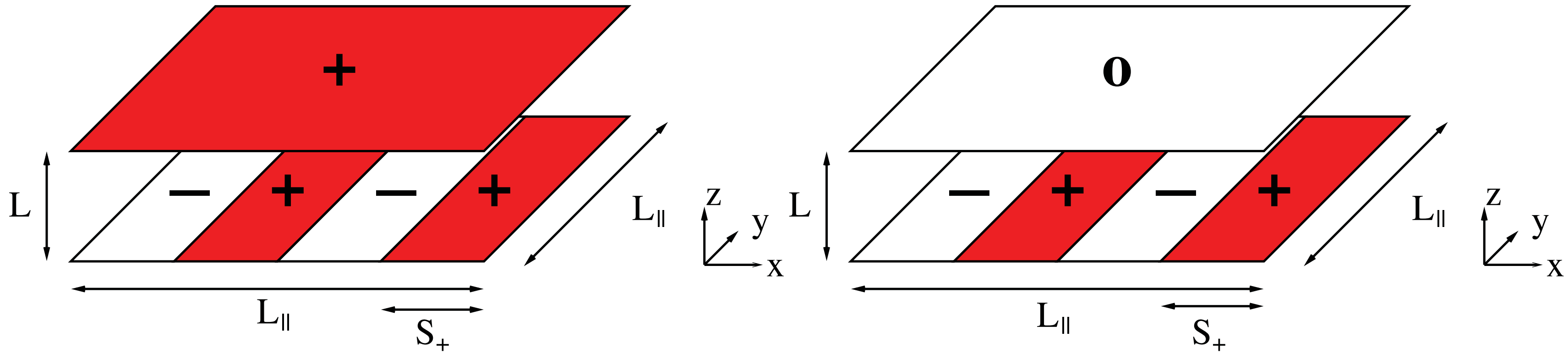
Comparison with Mean-Field Theory: (o) vs stripes



Normalization: $\hat{\theta}^{\text{MFT}}_{+/o}(\tau,\kappa) \equiv \frac{\theta_{+/o}(\tau_{\text{max},+/o},\kappa\to\infty)}{\theta^{\text{MFT}}_{+/o}(\tau^{\text{MFT}}_{\text{max},+/o},\kappa\to\infty)}\theta^{\text{MFT}}_{+/o}\left(\frac{\tau^{\text{MFT}}_{\text{max},+/o}}{\tau_{\text{max},+/o}}\tau,\kappa\right)$

Summary

- We have determined the critical Casimir force for geometries



- For $(+)$ vs stripes:
  - force always repulsive
  - force is monotonic increasing in $\kappa = S_+/L$
  - rescaled MFT in good agreement with MC results
- For (o) vs stripes:
  - force attractive for $\kappa \lesssim 1.2$
  - force changes sign for $\kappa \gtrsim 1.2$: a stable point of equilibrium at $\kappa = 3$
  - force is non-monotonic in $\kappa = S_+/L$
  - rescaled MFT shows qualitative differences with MC results

Ref: FPT, M. Tröndle, S. Dietrich: `arXiv:1303.6104`