Thermal Simulations, Open Boundary Conditions and Switches

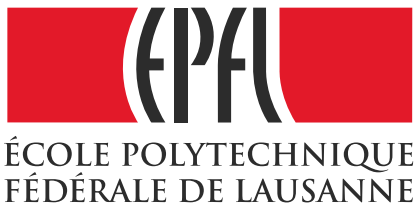
Adrien Florio[1]

in collaboration with

Yannis Burnier, Olaf Kaczmarek[2] and Lukas Mazur[2]

[1]EPFL, [2]Bielefeld University

21st of June 2017, Granada

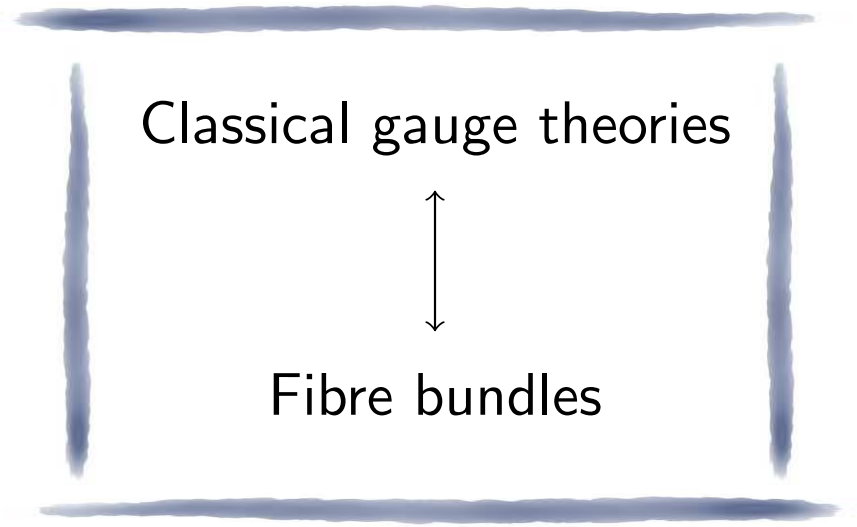


Topology and Freezing

Open-Boundary Conditions in Space

Switches

Some Topology



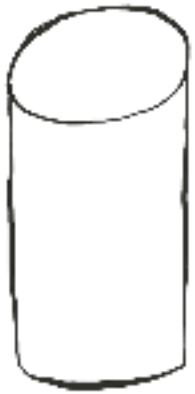
Some Topology

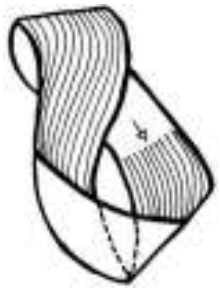
Classical gauge theories

↕

Fibre bundles

→ **Can be 'twisted'!**





Cohomology and Classification

Cohomology and Classification

de Rham's Theorem $\longrightarrow$ $\frac{\partial}{\partial x}$

Cohomology and Classification

de Rham's Theorem

$$\frac{\partial}{\partial x}$$

Characteristic classes

$$\mathbb{P}[\mathcal{F}]$$

Cohomology and Classification

$SU(N)$ bundles in $4D$ $\longleftrightarrow$ 2^{nd} Chern class:

$$q = -\frac{1}{8\pi^2}\mathbf{Tr}\left(F \wedge F\right)$$

Cohomology and Classification

$SU(N)$ bundles in $4D$ $\longleftrightarrow$ 2^{nd} Chern class:

$$q = -\frac{1}{8\pi^2}\mathbf{Tr}\left(F \wedge F\right)$$

Topological charge: $Q = -\frac{1}{16\pi^2}\int_M F_{\mu\nu}\tilde{F}^{\mu\nu}$

Remarks

- For compact spaces $Q \in \mathbb{Z}$
- For non-compact spaces $Q \in \mathbb{R}$
- **Continuum** story

Refs: [Avis,Isham 1978] [DeWitt,Hart,Isham 1979]

Topological Freezing

Continuum limit

Distinct topological sectors emerge

~~Accessible~~ by small motions in conf. space

$t_{autocorrelation}(Q) >> 0$

Topological Freezing

Continuum limit

Distinct topological sectors emerge

~~Accessible~~ by small motions in conf. space

$t_{autocorrelation}(Q) >> 0$

A Solution: OBC

Remarks

- For compact spaces $Q \in \mathbb{Z}$
- For non-compact spaces $Q \in \mathbb{R}$
- **Continuum** story

Refs: [Avis,Isham 1978] [DeWitt,Hart,Isham 1979]

A Solution: OBC

Remarks

- For compact spaces $Q \in \mathbb{Z}$
- For non-compact spaces $Q \in \mathbb{R}$
- **Continuum** story

$\mathbb{T}^4$

Refs: [Avis,Isham 1978] [DeWitt,Hart,Isham 1979]

A Solution: OBC

Remarks

- For compact spaces $Q \in \mathbb{Z}$
- For non-compact spaces $Q \in \mathbb{R}$
- **Continuum** story

Refs: [Avis,Isham 1978] [DeWitt,Hart,Isham 1979]

$\mathbb{T}^4$

↓

Open-up the torus!

A Solution: OBC

[Luescher, Schaeffer 2011]: $F_{0\mu}(x)|_{x_0=0} = F_{0\mu}(x)|_{x_0=l_0} = 0$

$\downarrow$ $T \neq 0$

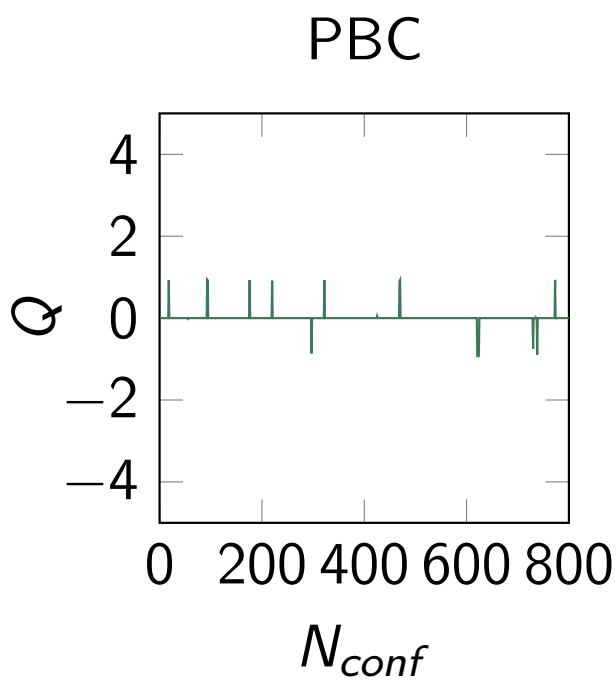
Spatial OBC: $F_{i\mu}(x)|_{x_i=0} = F_{i\mu}(x)|_{x_i=l_i} = 0$

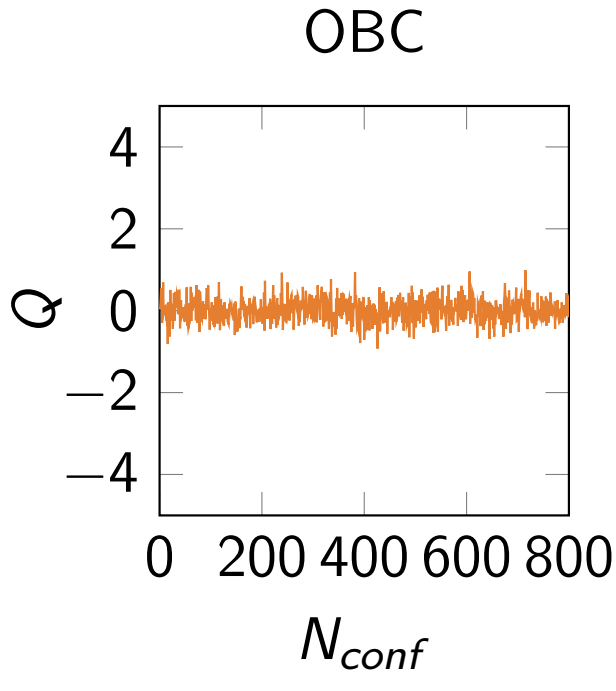
A Solution: OBC

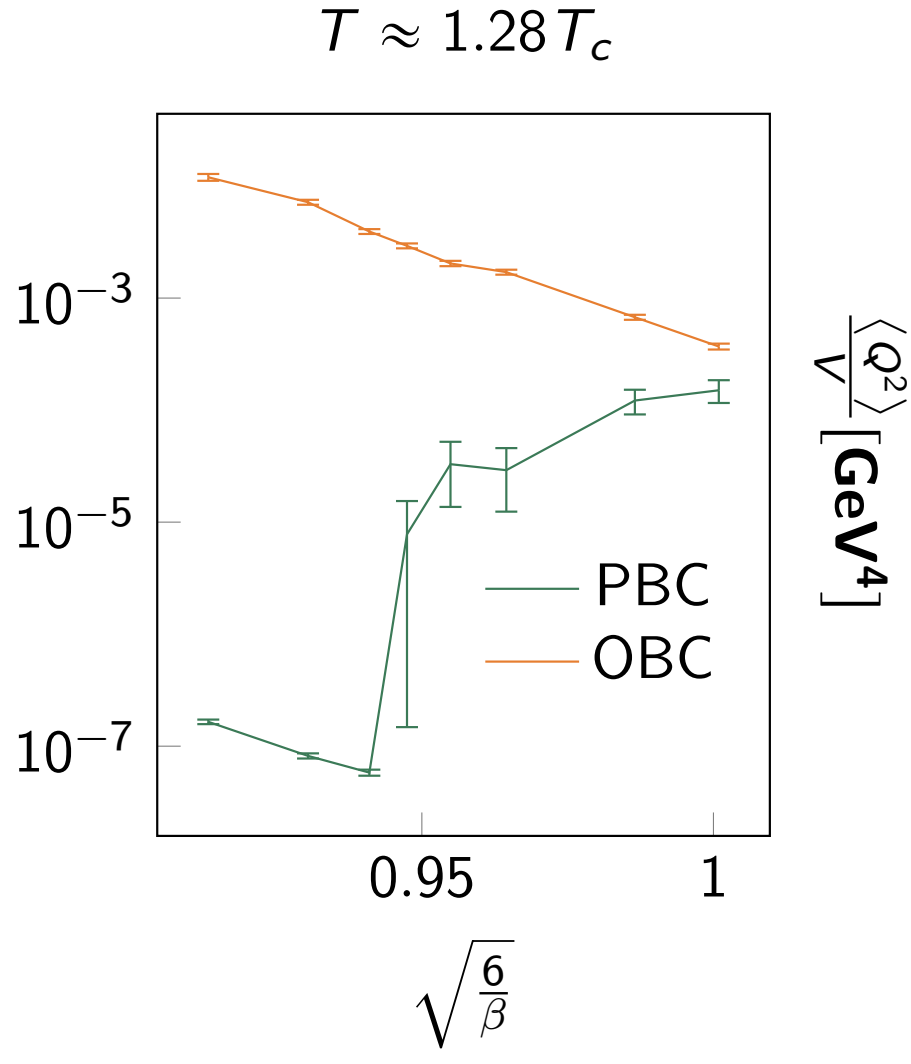
[Luescher, Schaeffer 2011]: $F_{0\mu}(x)|_{x_0=0} = F_{0\mu}(x)|_{x_0=l_0} = 0$

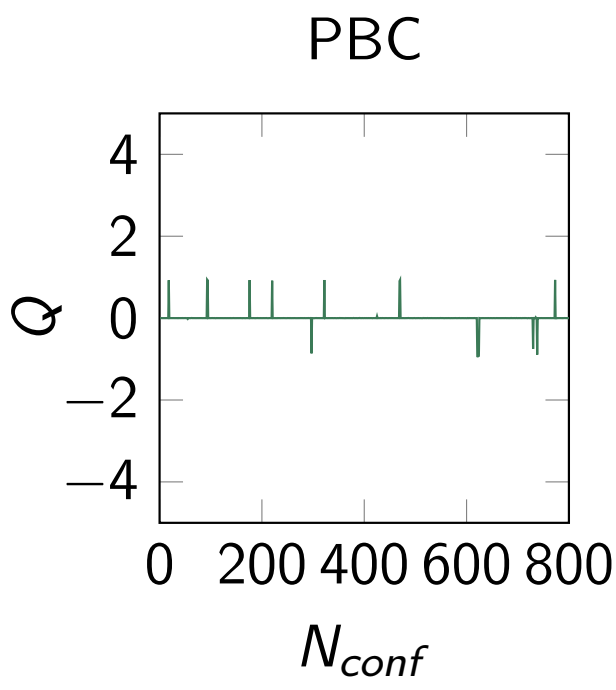
$T \neq 0$

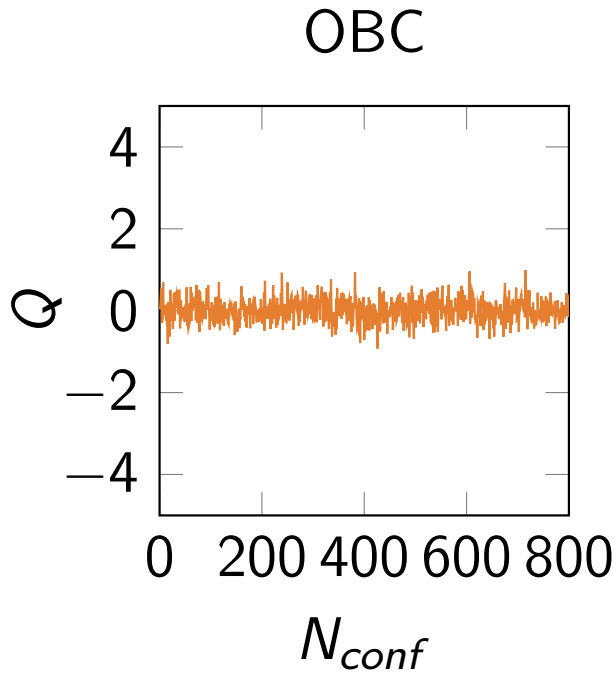
Spatial OBC: $F_{i\mu}(x)|_{x_i=0} = F_{i\mu}(x)|_{x_i=l_i} = 0$


PBC
4
2
0
−2
−4
Q
0
200
400
600
800
N_{conf}

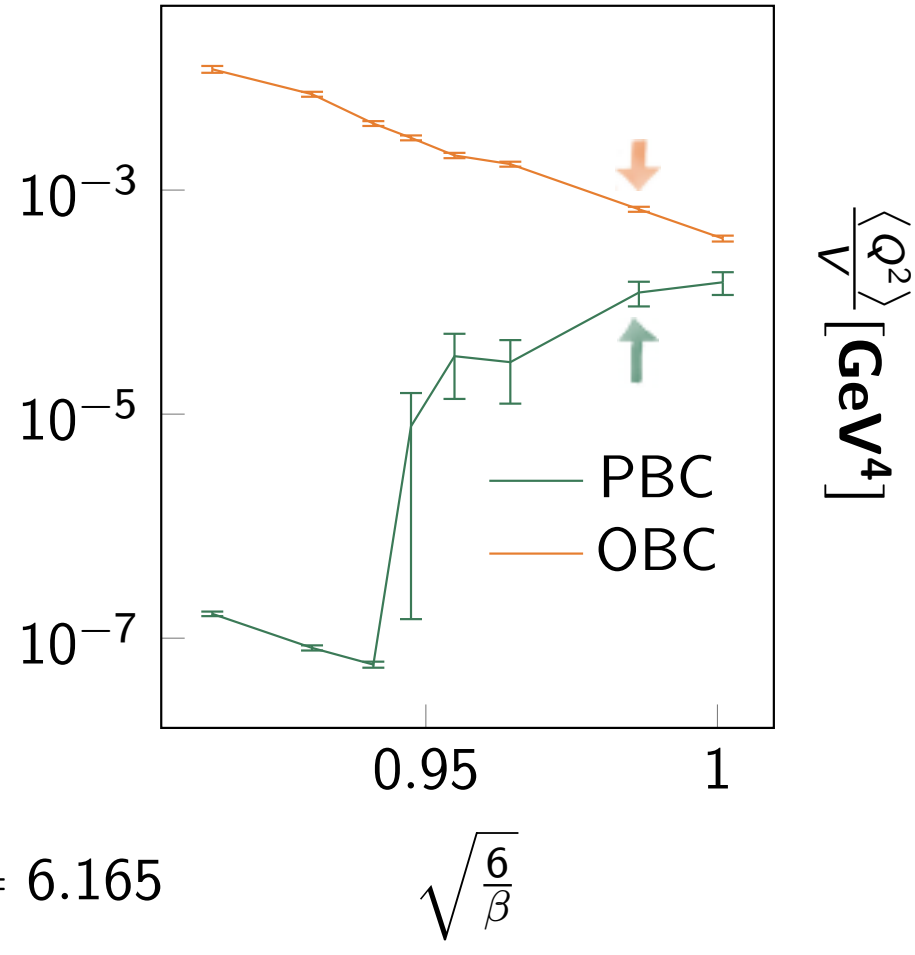

OBC
4
2
0
−2
−4
Q
0
200
400
600
800
N_{conf}


$T \approx 1.28\,T_c$
10^{-3}
10^{-5}
10^{-7}
PBC
OBC
0.95
1
$\sqrt{\frac{6}{\beta}}$
$\frac{\langle Q^2 \rangle}{V}$ [GeV^4]

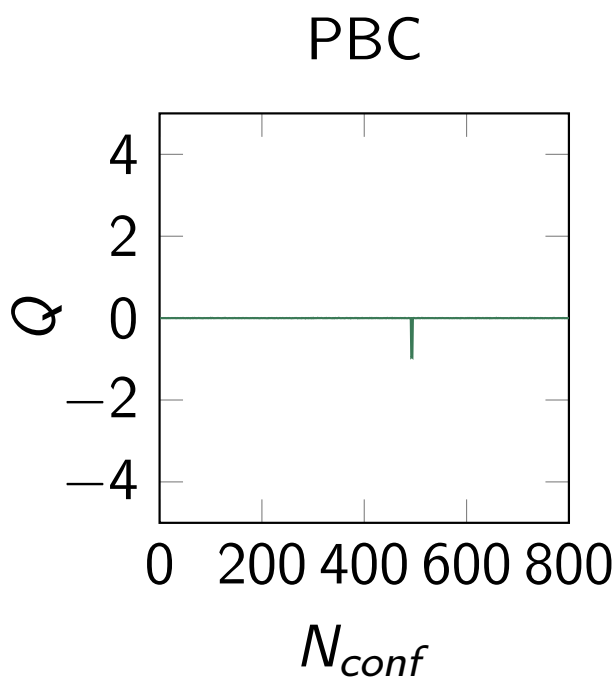


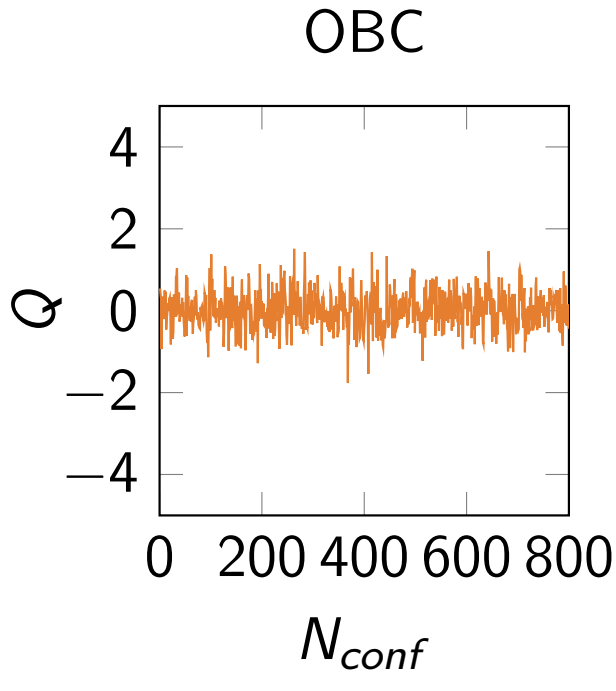


$T \approx 1.28\,T_c$

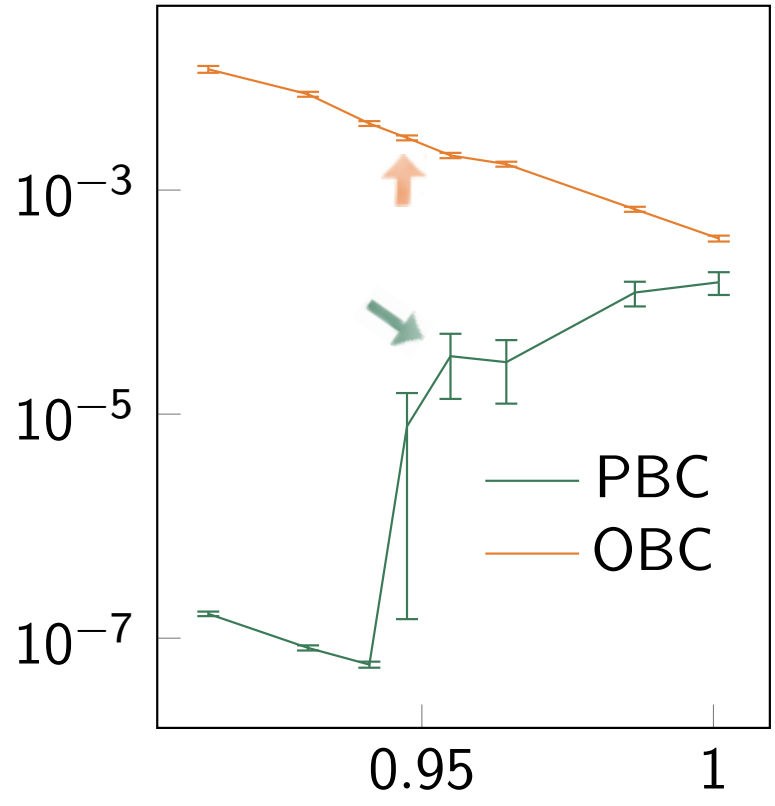


$\beta = 6.165$

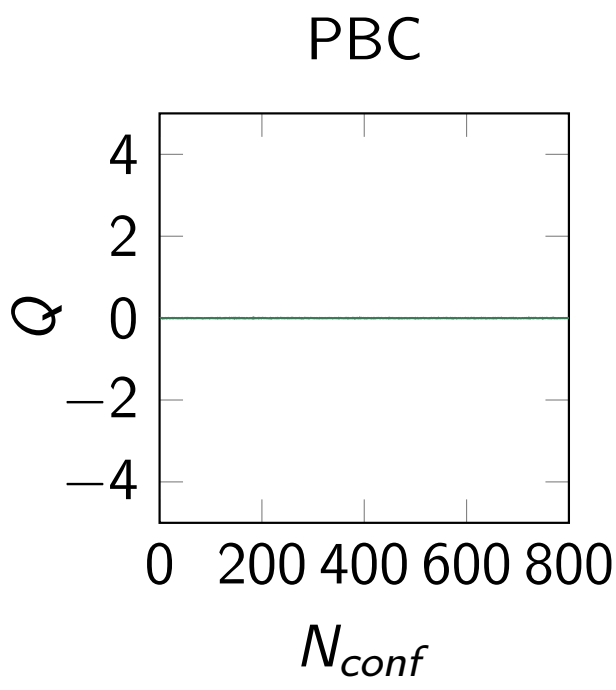


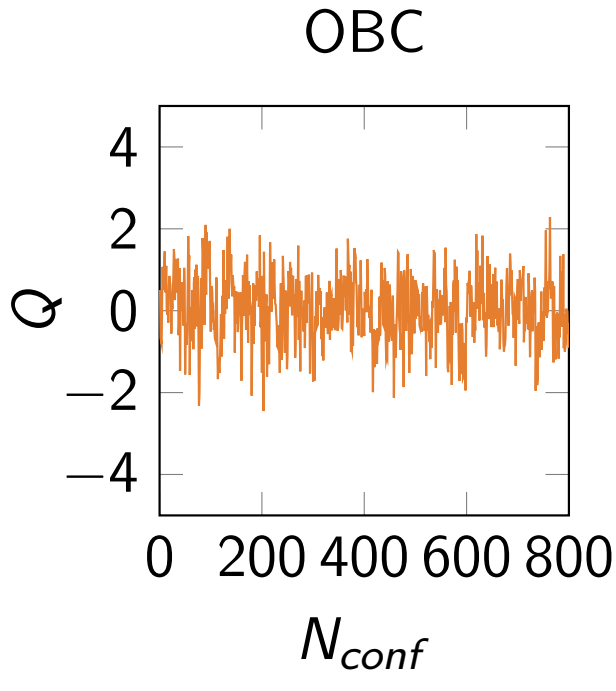


$T \approx 1.28\,T_c$

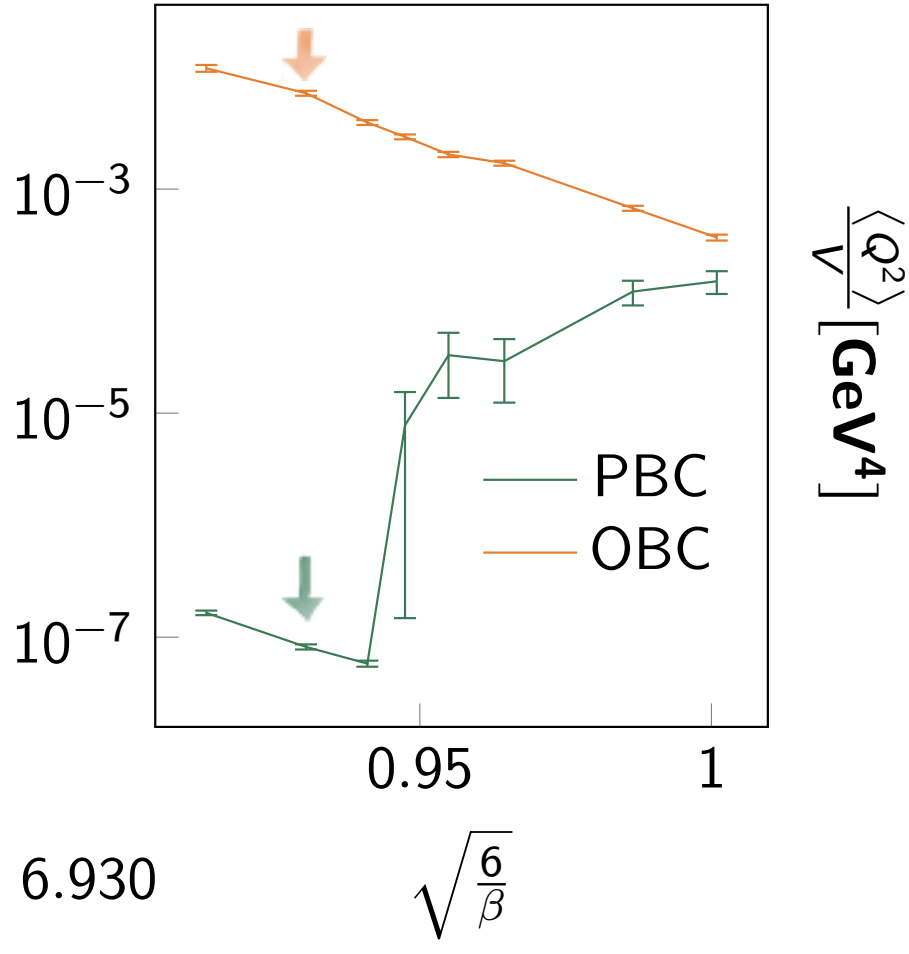


$\beta = 6.580$



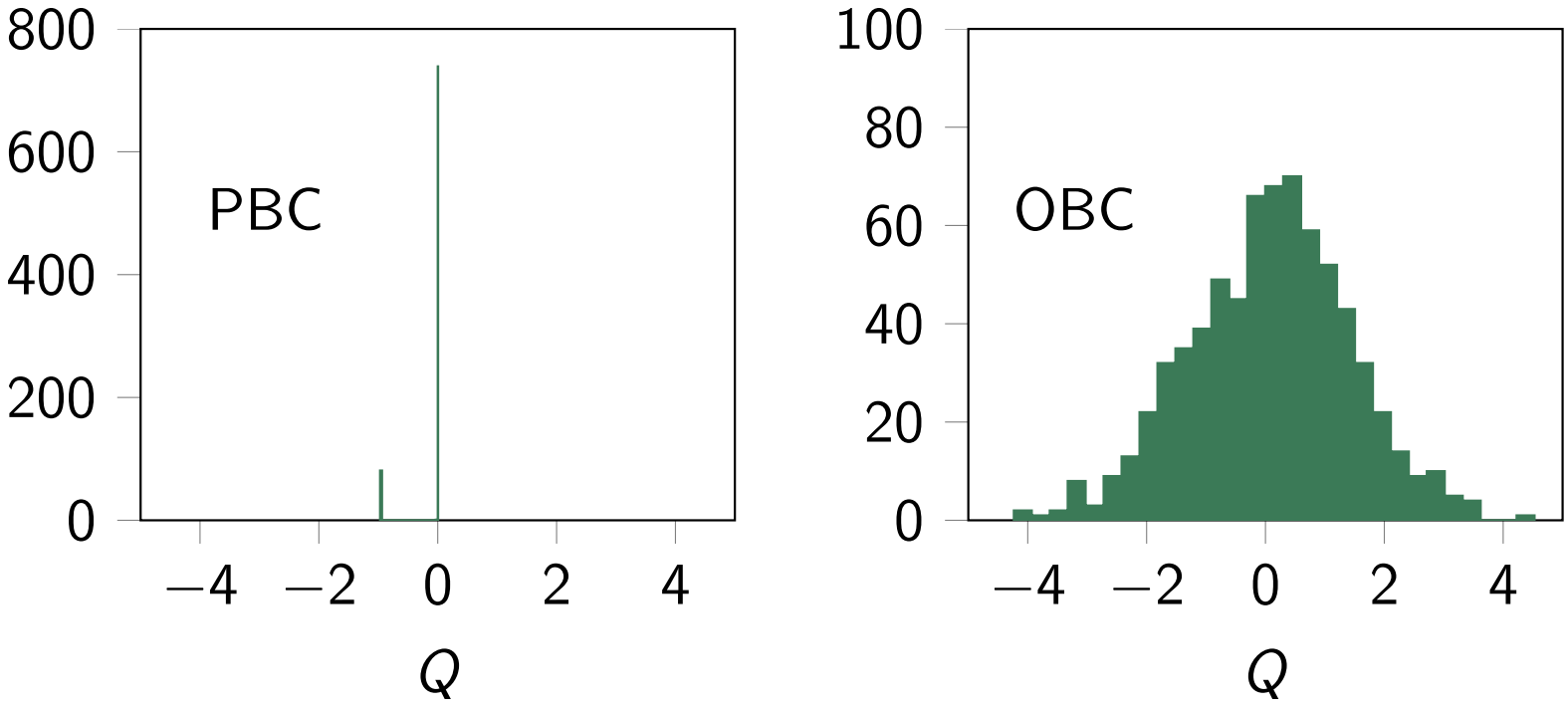


$T \approx 1.28\,T_c$



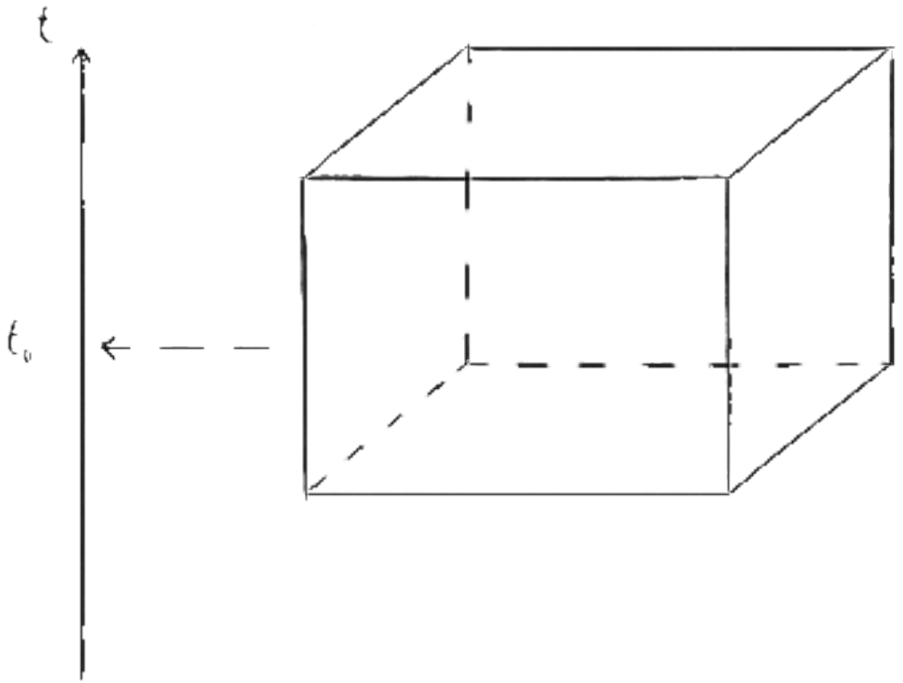
$\beta = 6.930$

$32^4,\ \beta = 6.872,\ T \approx 0$



Finite Size Effects

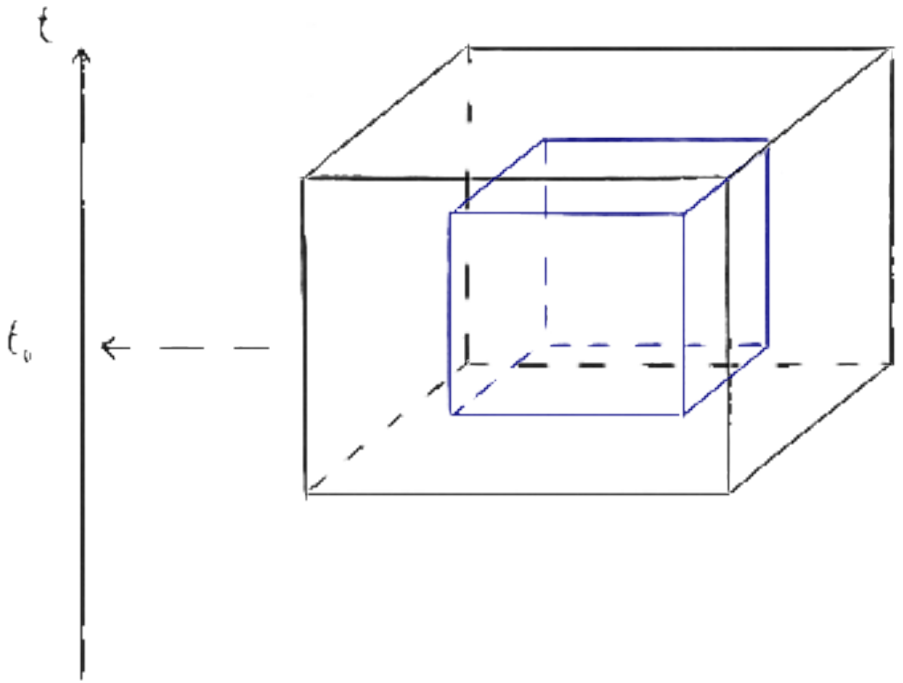
$$V_s = L_s^3$$



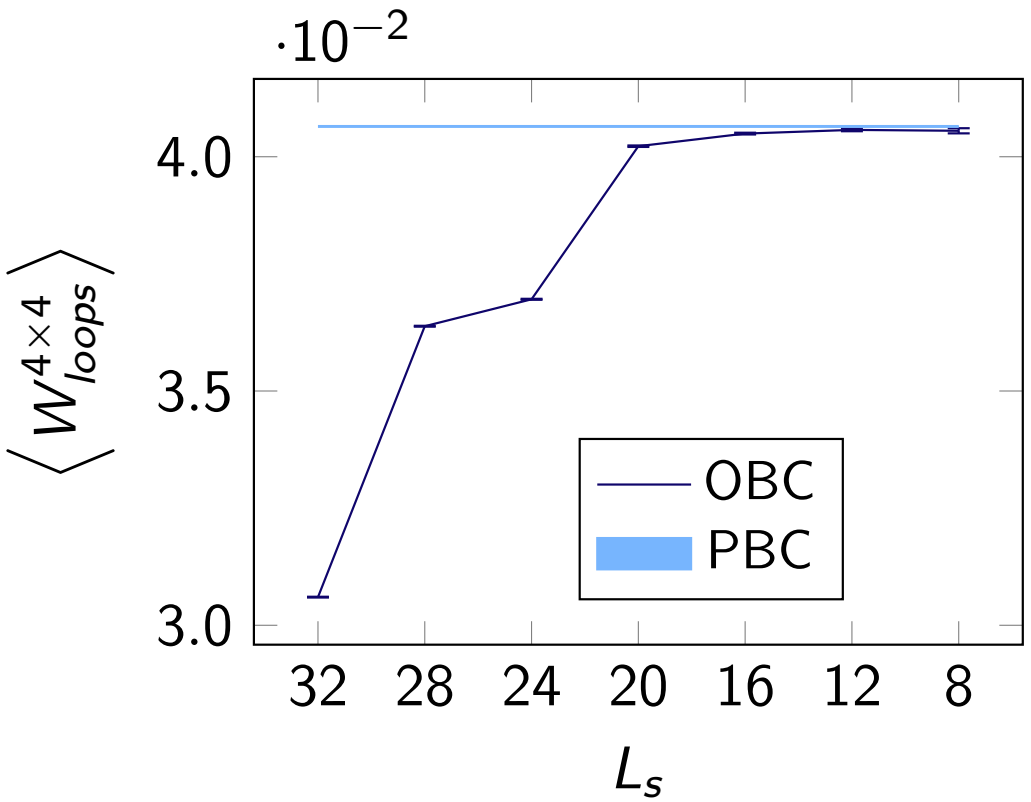
Finite Size Effects

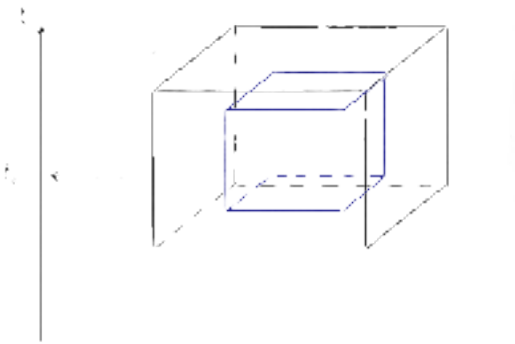
$$V_s = L_s^3$$

$$V_s' = L_s'^3$$



Finite Size Effects





Outlooks: Switching between Boundary Conditions

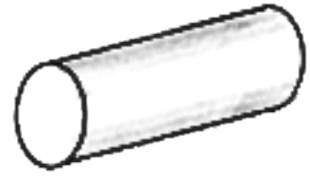
Do n_{PBC} sweeps with PBC

Outlooks: Switching between Boundary Conditions

Do n_{PBC} sweeps with PBC

↓

Switch PBC to OBC
in some direction(s)

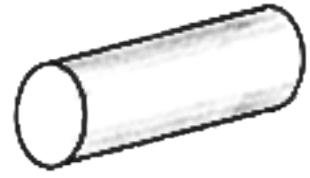


Outlooks: Switching between Boundary Conditions

Do n_{PBC} sweeps with PBC

Switch PBC to OBC
in some direction(s)

Do n_{OBC} sweeps



Outlooks: Switching between Boundary Conditions

Do n_{PBC} sweeps with PBC

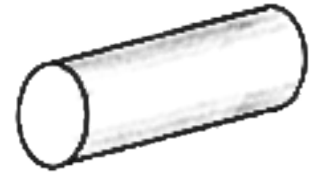
↓

Switch PBC to OBC
in some direction(s)

Do n_{OBC} sweeps

↓

Switch back



Outlooks: Switching between Boundary Conditions

Do n_{PBC} sweeps with PBC

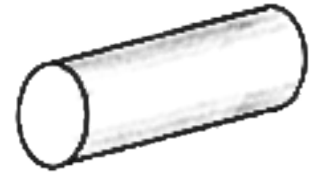
↓

Switch PBC to OBC
in some direction(s)

Do n_{OBC} sweeps

↓

Switch back



Do n_{PBC} sweeps

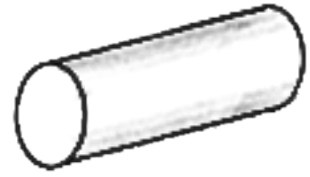
Outlooks: Switching between Boundary Conditions

Do n_{PBC} sweeps with PBC

↓ **Switch PBC to OBC** in some direction(s)

Do n_{OBC} sweeps

↓ **Switch back**



Do n_{PBC} sweeps

↓

...

Outlooks: Switching between Boundary Conditions

Do n_{PBC} sweeps with PBC

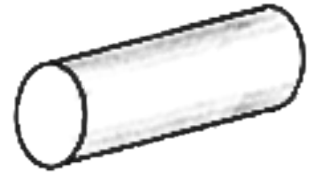
↓

Switch PBC to OBC
in some direction(s)

Do n_{OBC} sweeps

↓

Switch back



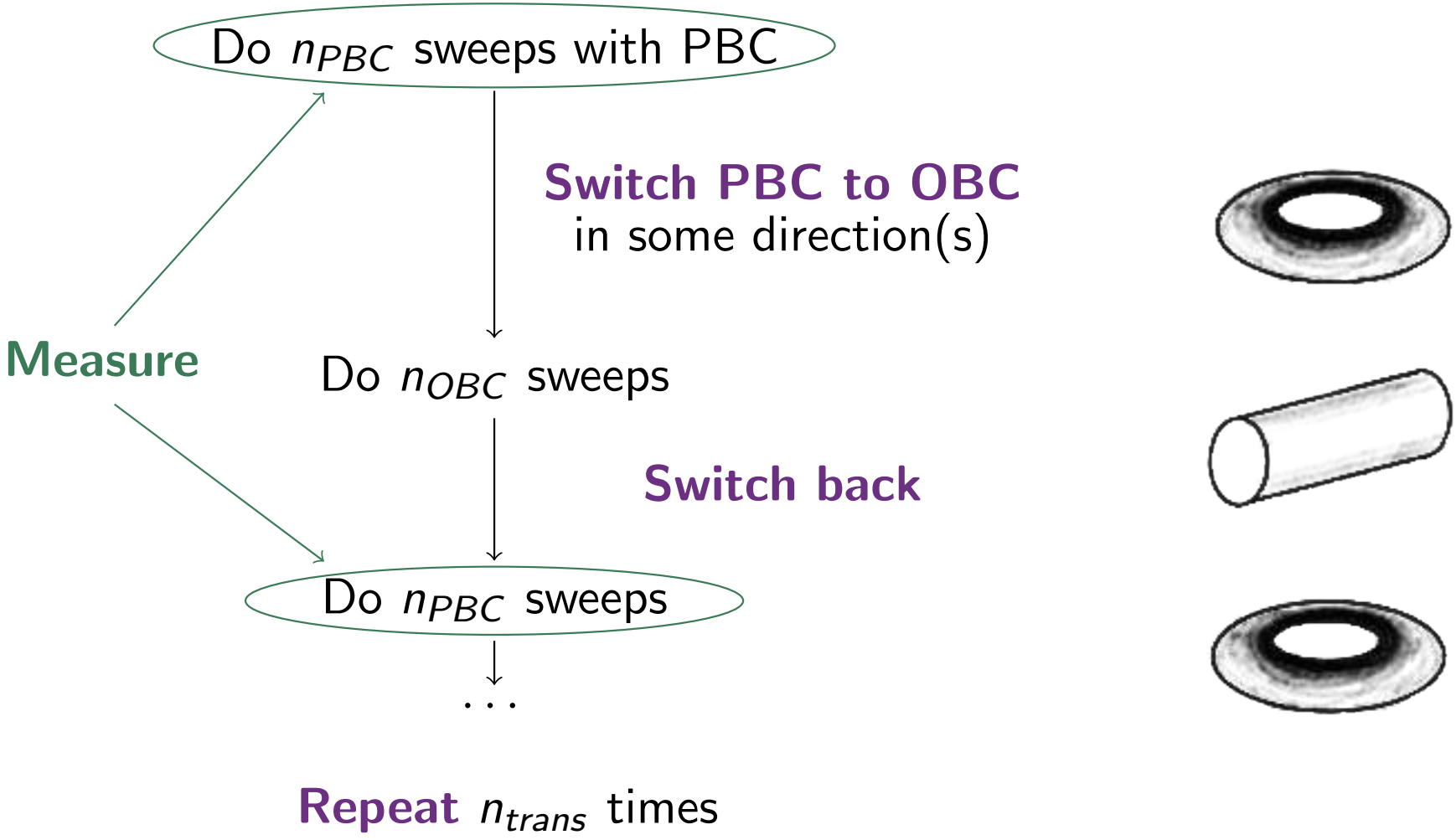
Do n_{PBC} sweeps

↓

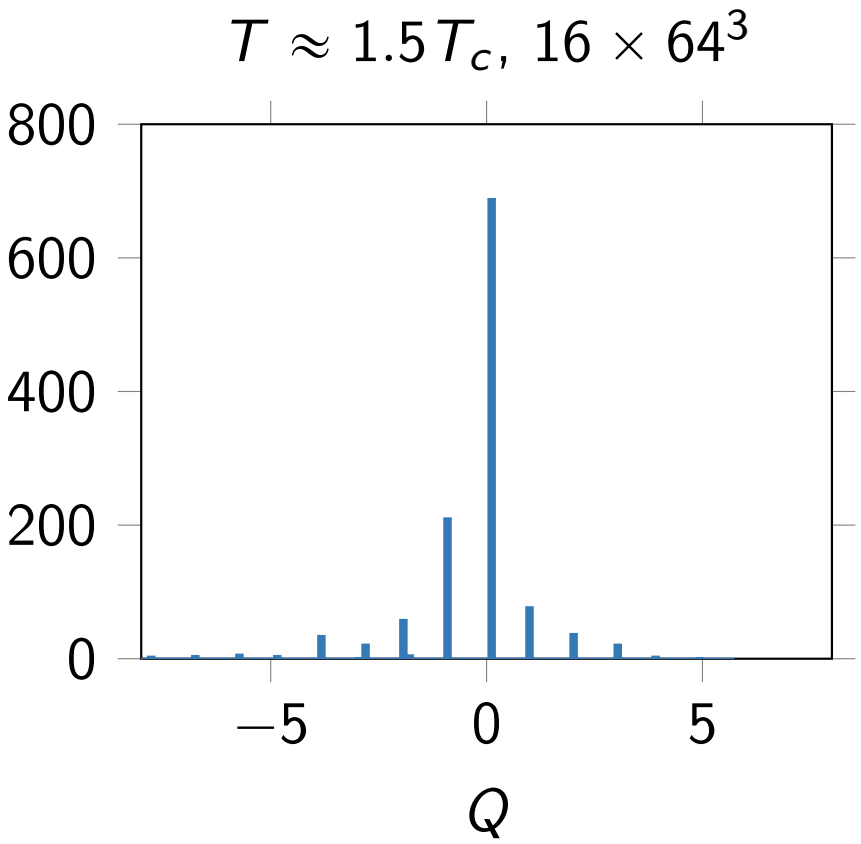
...

Repeat n_{trans} times

Outlooks: Switching between Boundary Conditions

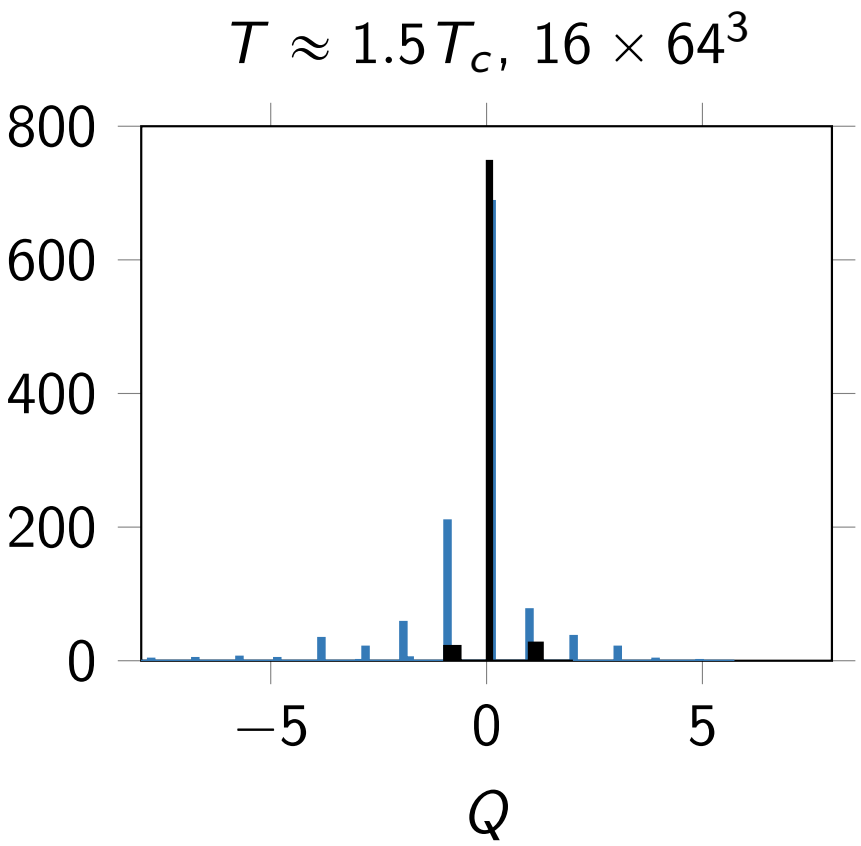


First Results



Generates higher Q's

First Results



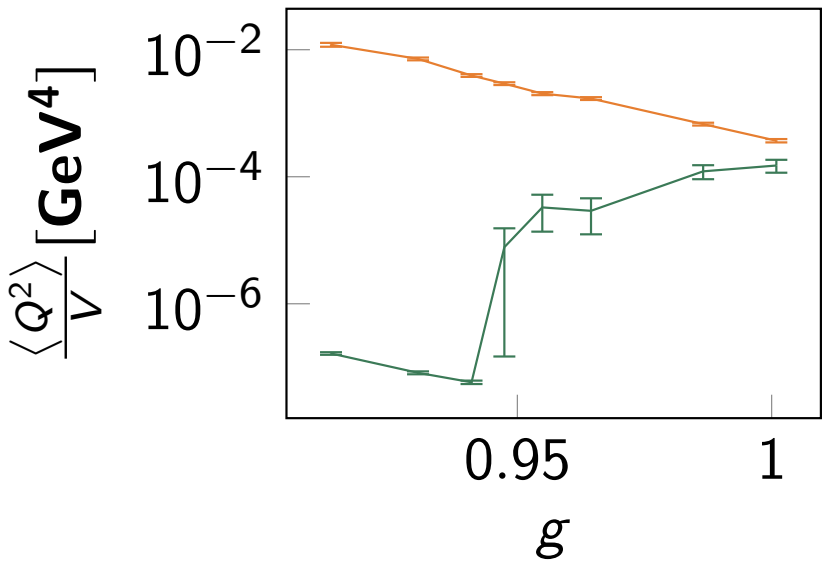
Generates higher Q's

but

oversamples

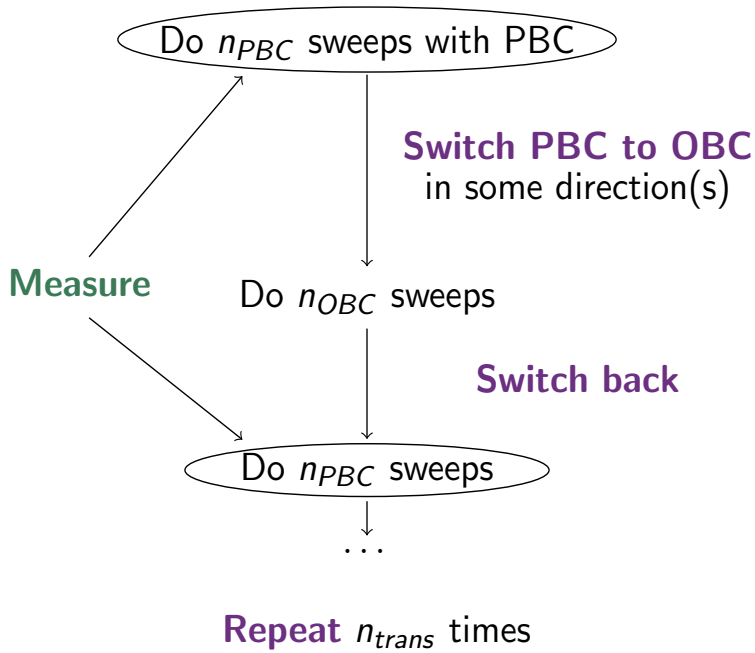
To Sum Up

- **OBC also solve topological freezing at finite temperature**
- May use them algorithmically



To Sum Up

- OBC also solve topological freezing at finite temperature
- **May use them algorithmically**



Thank you!

(... and https://www.pinterest.com/pin/571746115169525297/ for the Moebius strip)