Fermion Bag Approach
to Hamiltonian Lattice Field Theories

Shailesh Chandrasekharan
(Duke University)

work done in collaboration with Emilie Huffman

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Develop non-perturbative approaches to study them!

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So new models have become accessible
and some old models can now be solved more efficiently!

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Debbio, Hands, Kogut, Kocic,Kim, Strouthos, Sinclair,…(1990's, 2000's)

Drut and Lahde, 2009, (Staggered fermions, Coulomb Interactions)

Typical lattice sizes used less than 2500 spatial sites, but non-zero mass!

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Determination of critical exponents have remained unsatisfactory.
Room for improvement.

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Biggest spatial lattices studied:

Otsuka, Yunoki, Sorella, (2016)

- 2600 sites (honeycomb lattice)
- 1600 sites (square lattice)

Are there examples of unsolved problems, where progress would be useful?

Classic Example

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"Repulsive Hubbard (t-U) Model" for graphene

$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma} + U \sum_{i} \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right)$$

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massless fermions

massive fermions,
anti-ferromagnetic order

U_c

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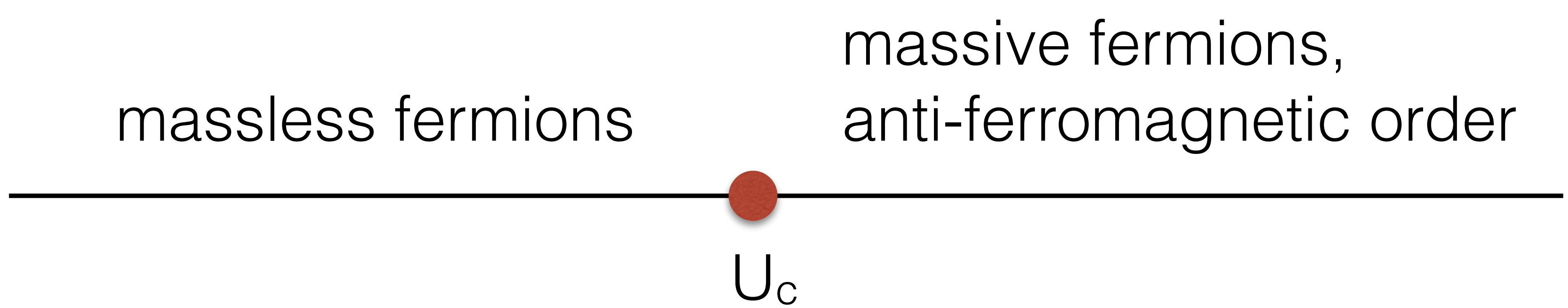

Can we reproduce the physics close to U_c with staggered fermions?

Staggered fermion approach:
(N_f = 2, 4 component massless Dirac fermions)

Hands et. al, 2009

$$S = \frac{1}{2} \sum_{x,y,i=1,2} \psi_{x,i} M_{x,y} \psi_{y,i} - U \sum_{\langle xy \rangle} \psi_{x,1}\psi_{x,2}\psi_{y,1}\psi_{x,2}$$

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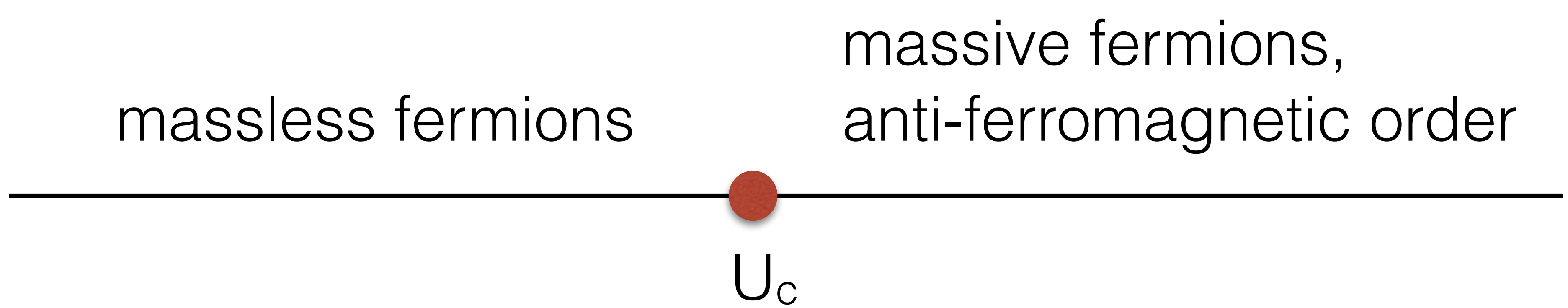

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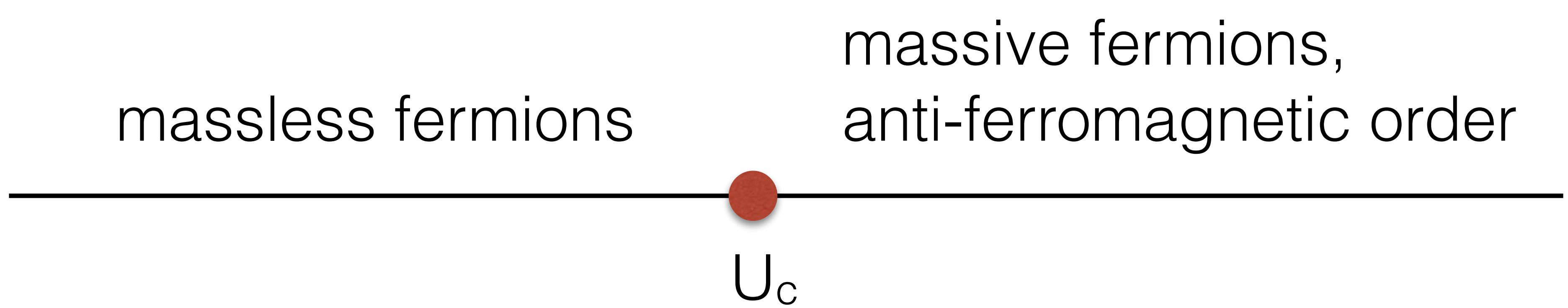

No lattice field theory results with staggered fermions due to sign problems.

Wipf et. al., Lattice (2017)

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Majorana fermions $\xi_i = (c_i + c_i^\dagger), \quad \bar{\xi}_i = i(c_i^\dagger - c_i)$

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commute

$$\mathrm{Tr}(\exp(-\beta H)) = \sum_{[\phi]} \Big(\mathrm{Pf}(G[\phi])\Big)^2$$

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This structure is not obvious in the Lagrangian approach

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Large scale calculations should help resolve such disputes!

The lattice QCD community could bring its expertise to the field!

- Use HMC algorithms to go to large lattices ?

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Our motivation is to bring the idea of fermion bags to solve lattice Hamiltonian problems.

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Can we extend the idea to Hamiltonian systems?

Continuous Time (CT) Approach

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In Hamiltonian fermion systems the partition function
can be expanded in powers of the interaction in continuous time

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \int dt_1 dt_2 \ldots dt_k \ \mathrm{Tr}\left(e^{-\beta H_0} \ H_{\mathrm{int}}(t_1) H_{\mathrm{int}}(t_2) \ldots H_{\mathrm{int}}(t_k)\right)$$

CT INT method, Rubtsov, Lichtenstein,…

Diagrammatic Determinantal MC, Prokof'ev, Svistunov

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Fermion Bag Idea: $H_0 = 0 \qquad H_{\mathrm{int}} = \sum_{\langle ij\rangle} H_{ij}$

$$H_{ij} \;=\; -\delta\ \mathrm{e}^{\alpha(i\bar{\xi}_i \xi_j + i\bar{\xi}_j \xi_i)/2} \;=\; -\delta\ \mathrm{e}^{\alpha(c_i^\dagger c_j + c_j^\dagger c_i)}$$

$$Z \;=\; \sum_{[b]} \int dt_1 dt_2 \ldots dt_k\ \mathrm{Tr}\Big(H_{i_1 j_1}(t_1) H_{i_2, j_2}(t_2) \ldots H_{i_k j_k}(t_k)\Big)$$

Illustration of the “bond” configuration

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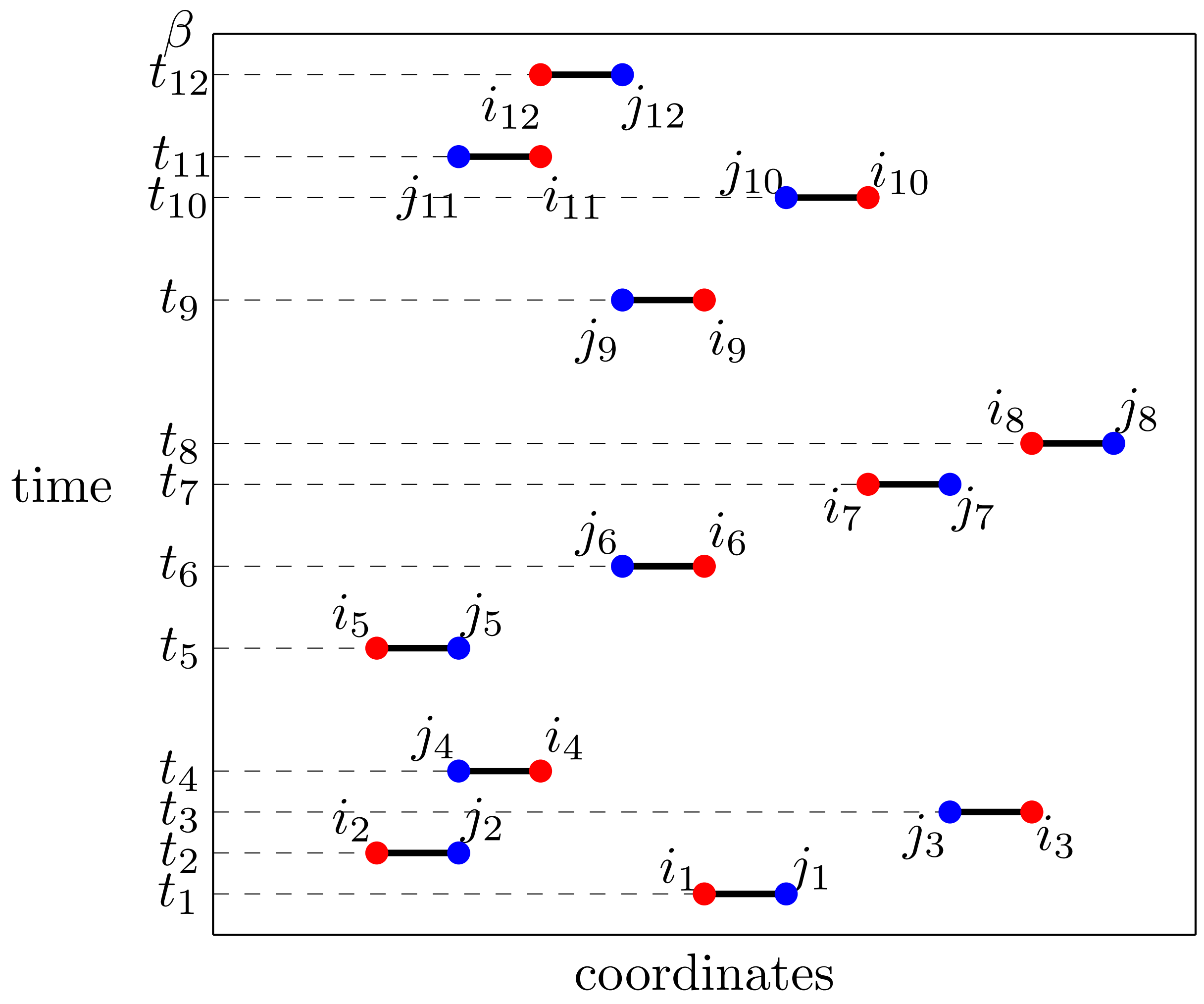

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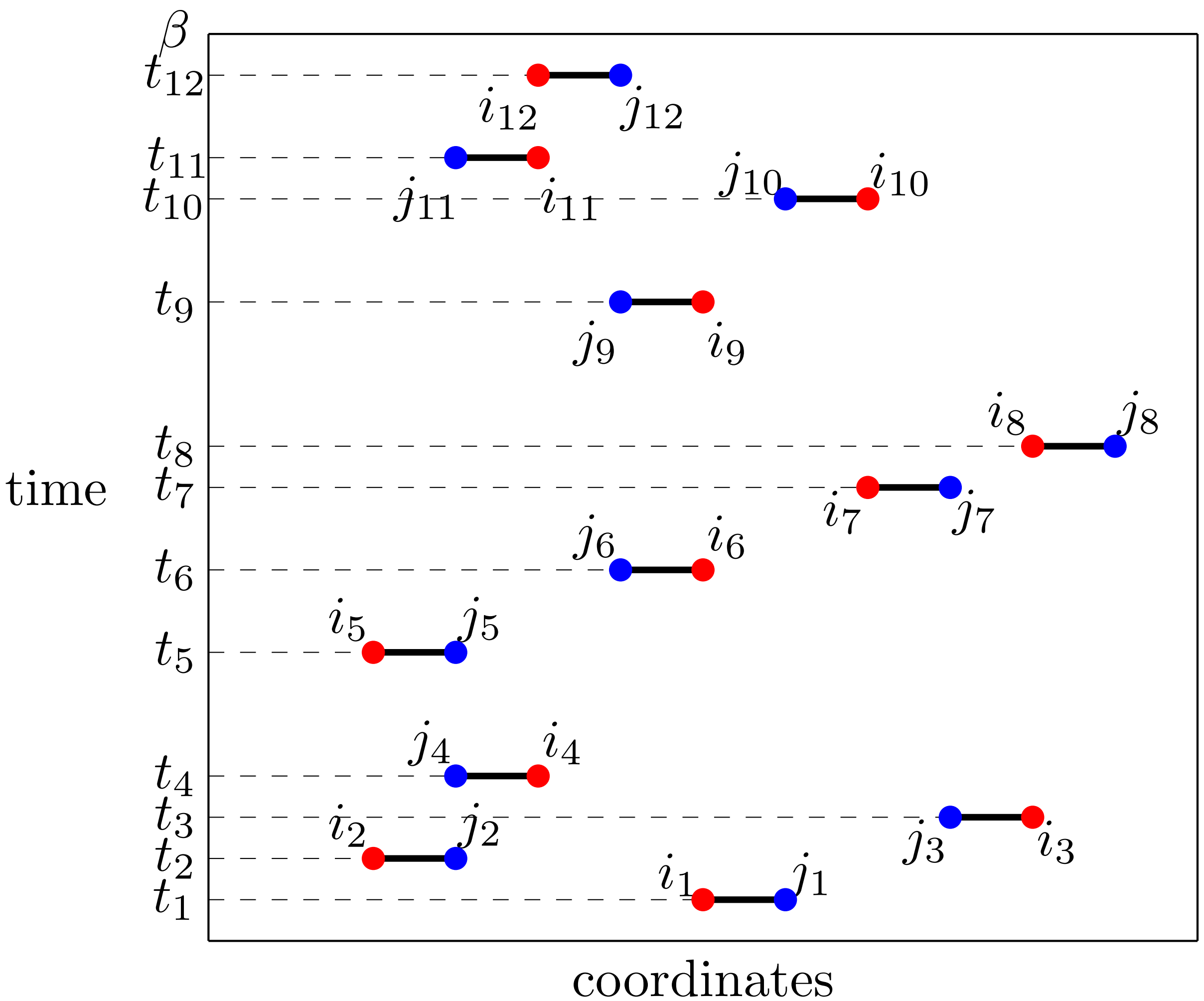

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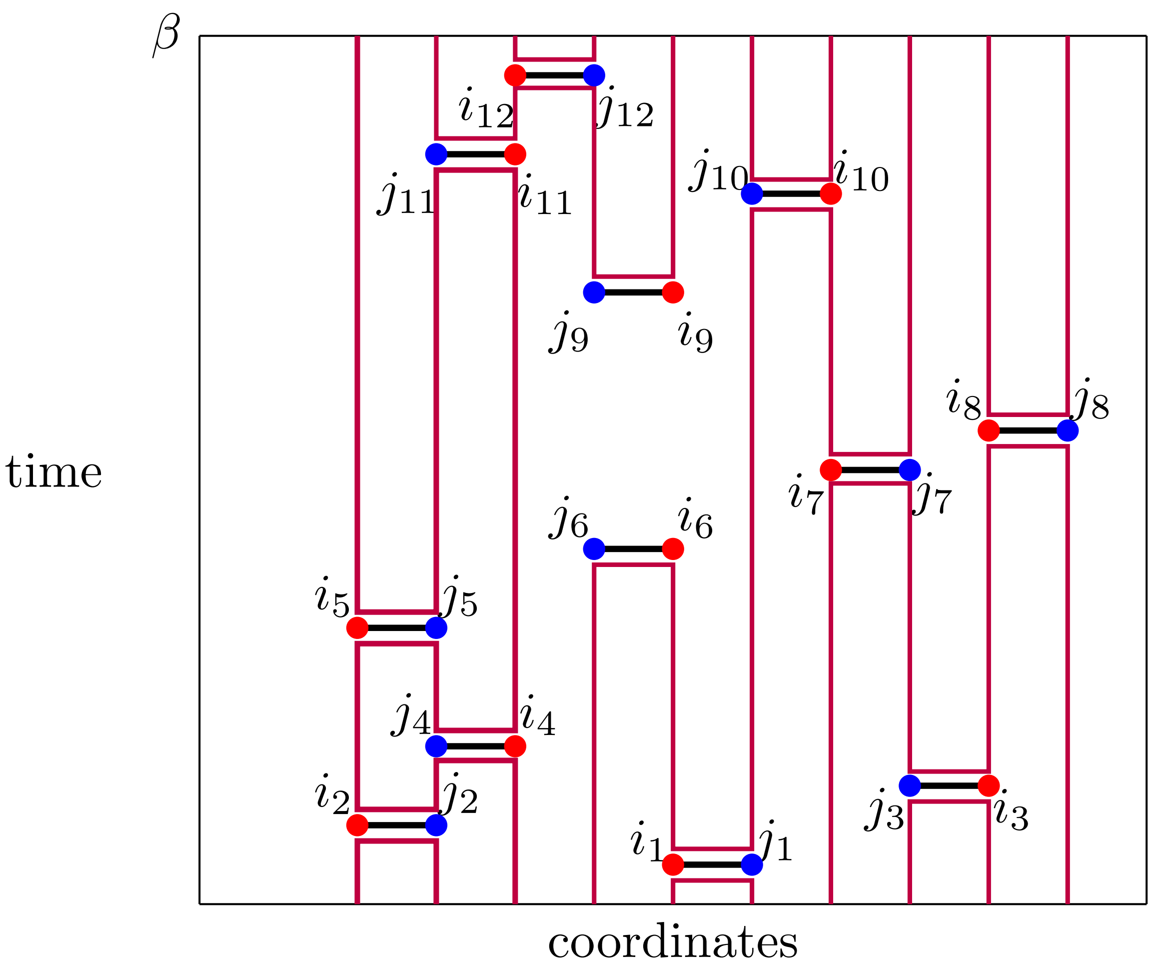

Naive fermion bag configuration

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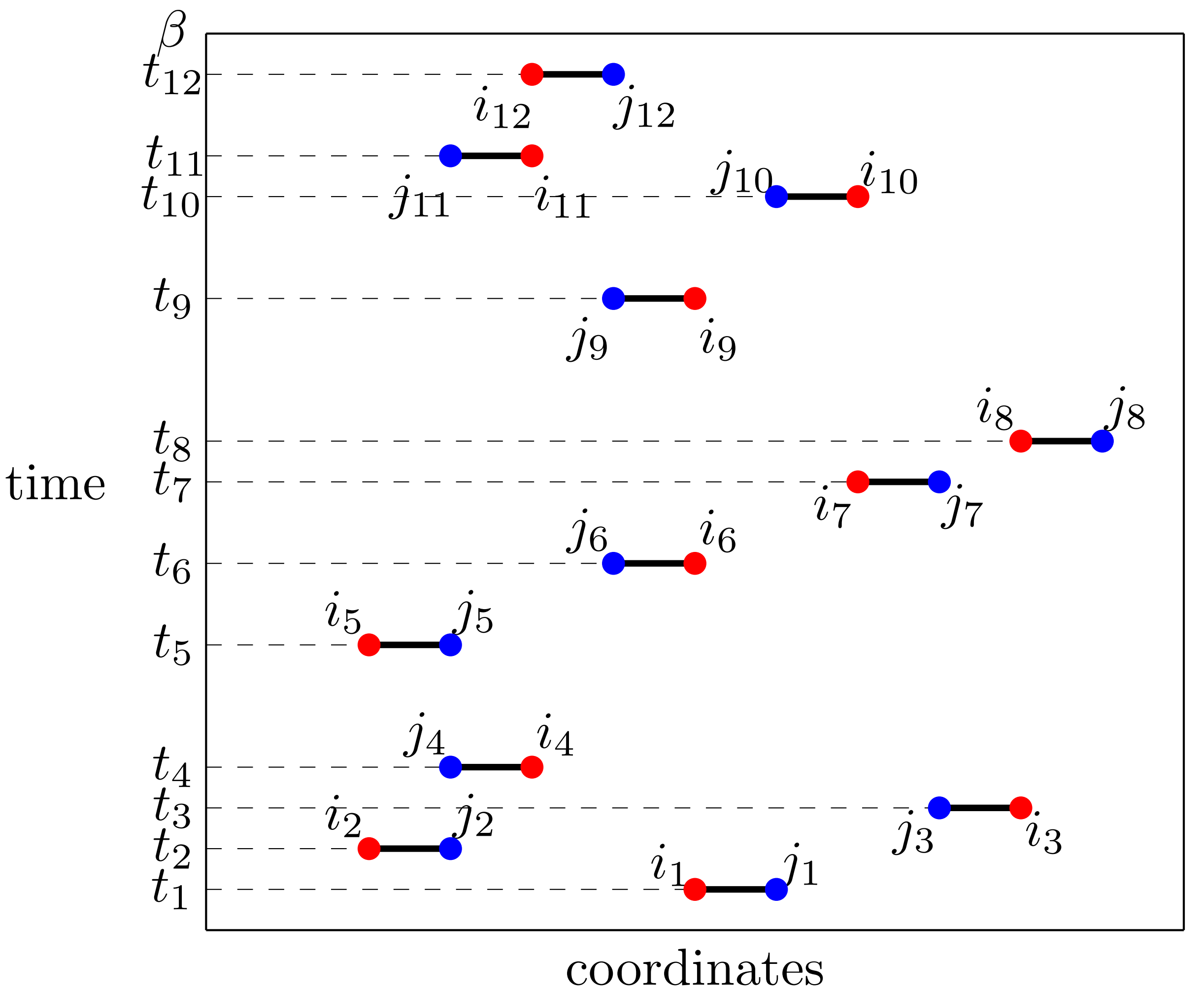

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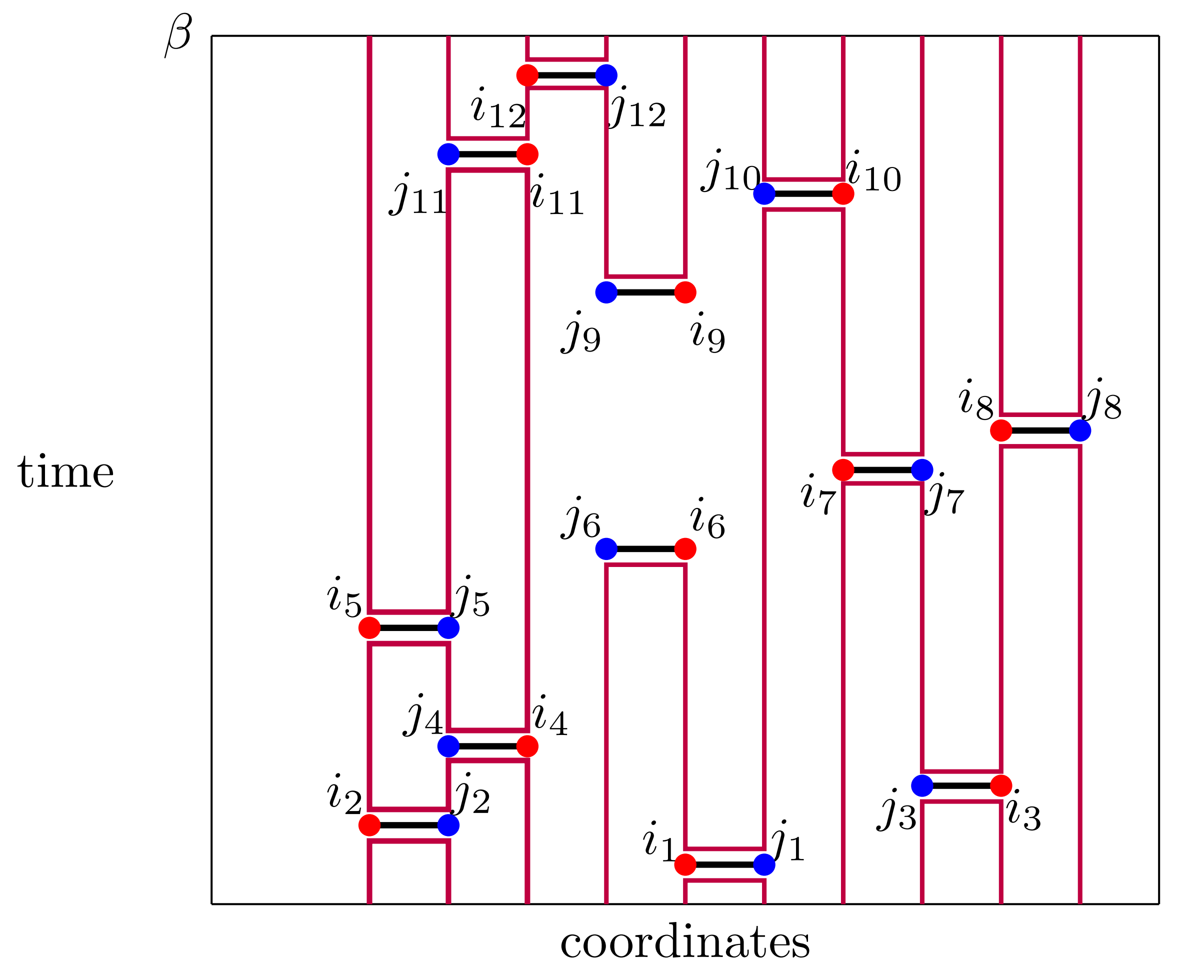

Naive fermion bag configuration

Naive fermion bag approach is equivalent to
Diagrammatic Determinantal MC, which is very inefficient

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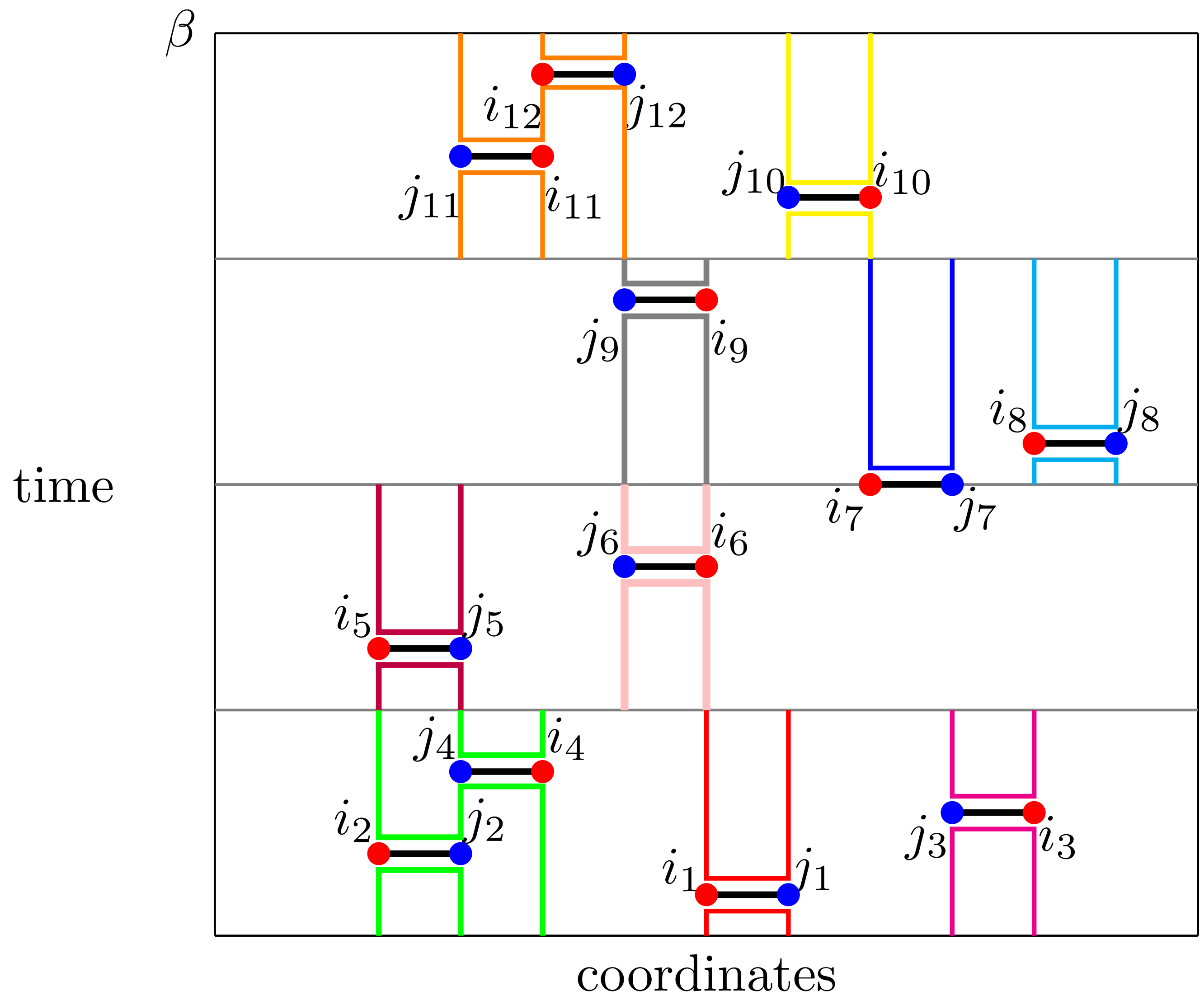

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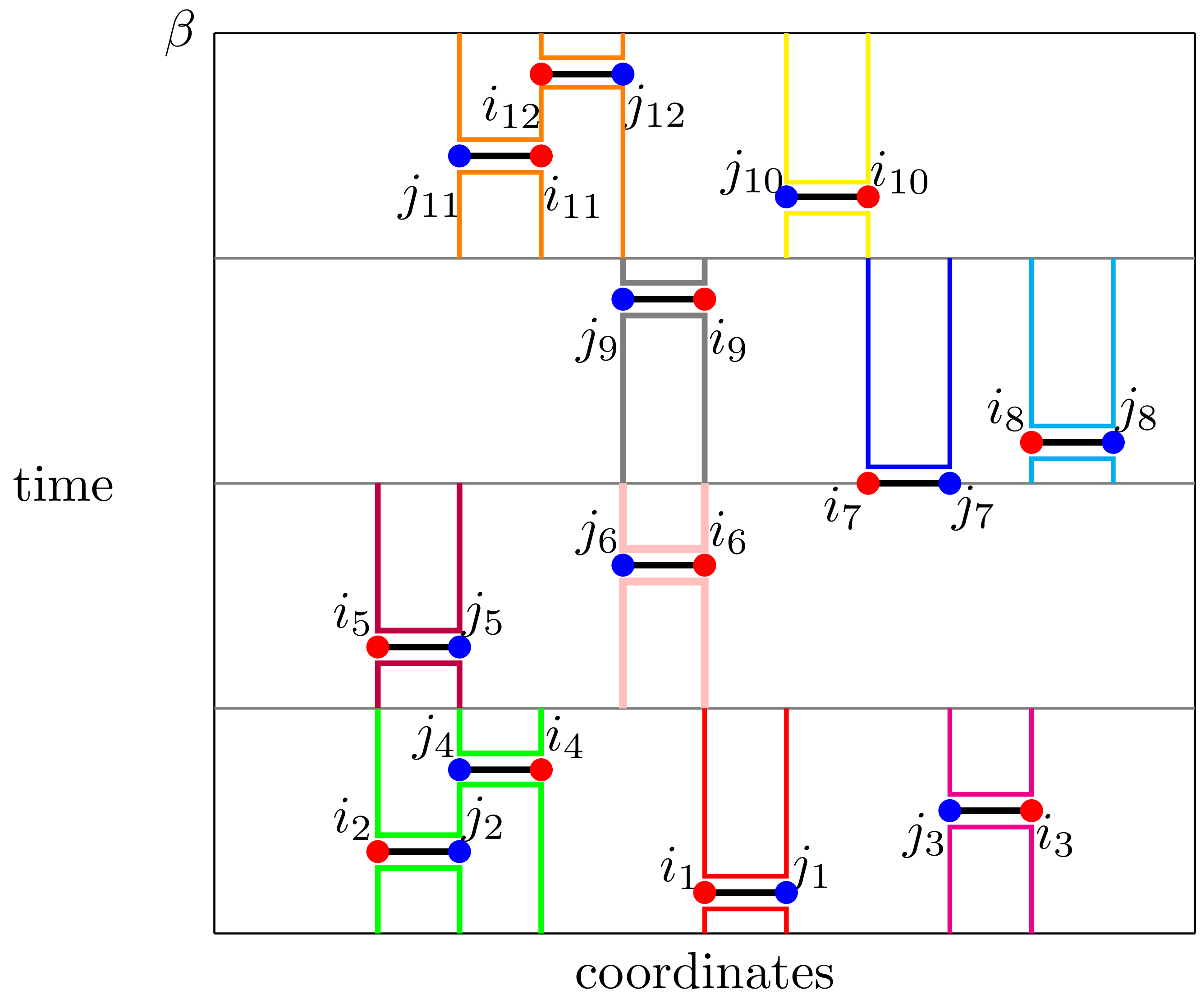
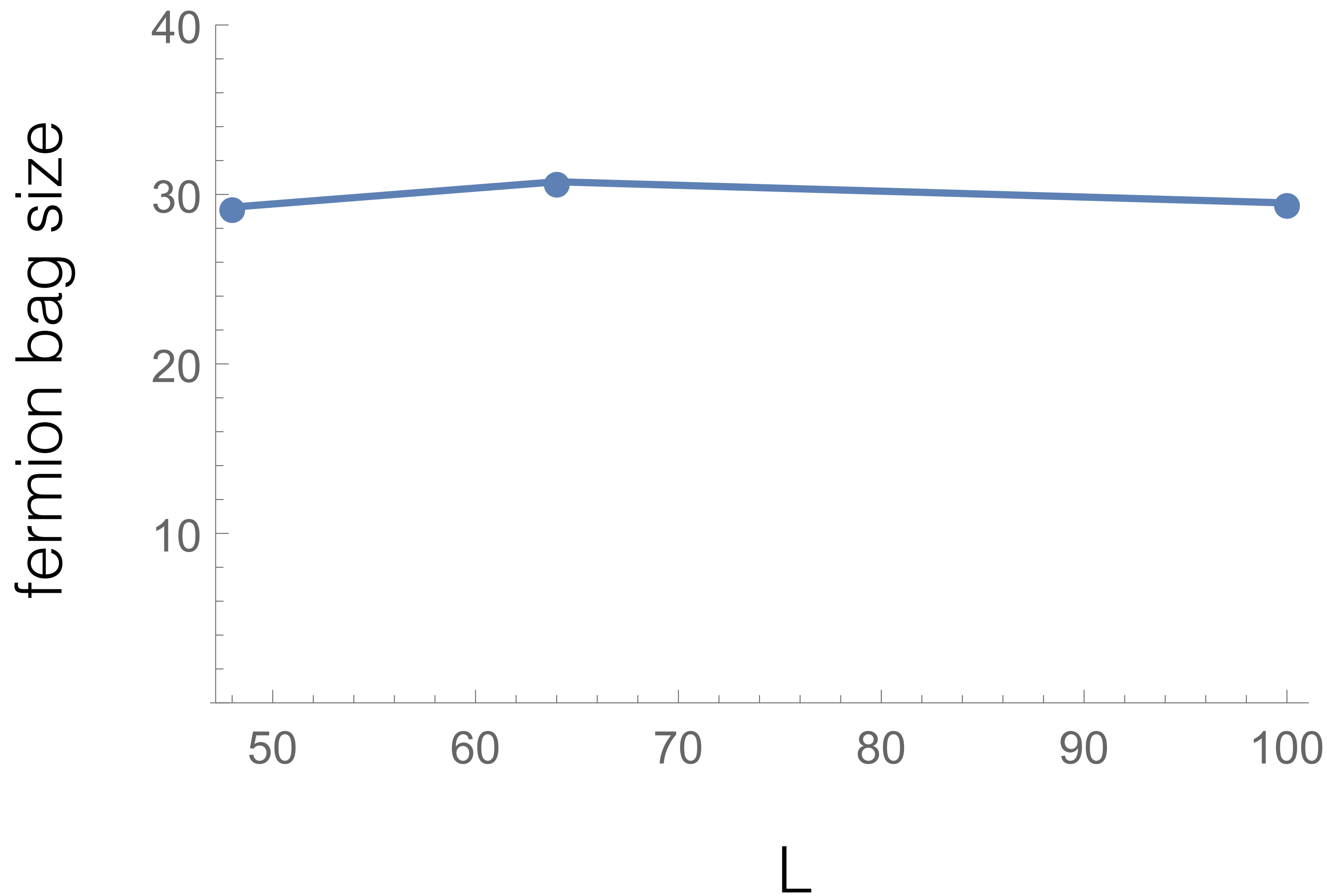


Similar to the local factorization algorithm:

Ce, Giusti and Schaefer, 2016

Fermion bag size as a function of spatial volume



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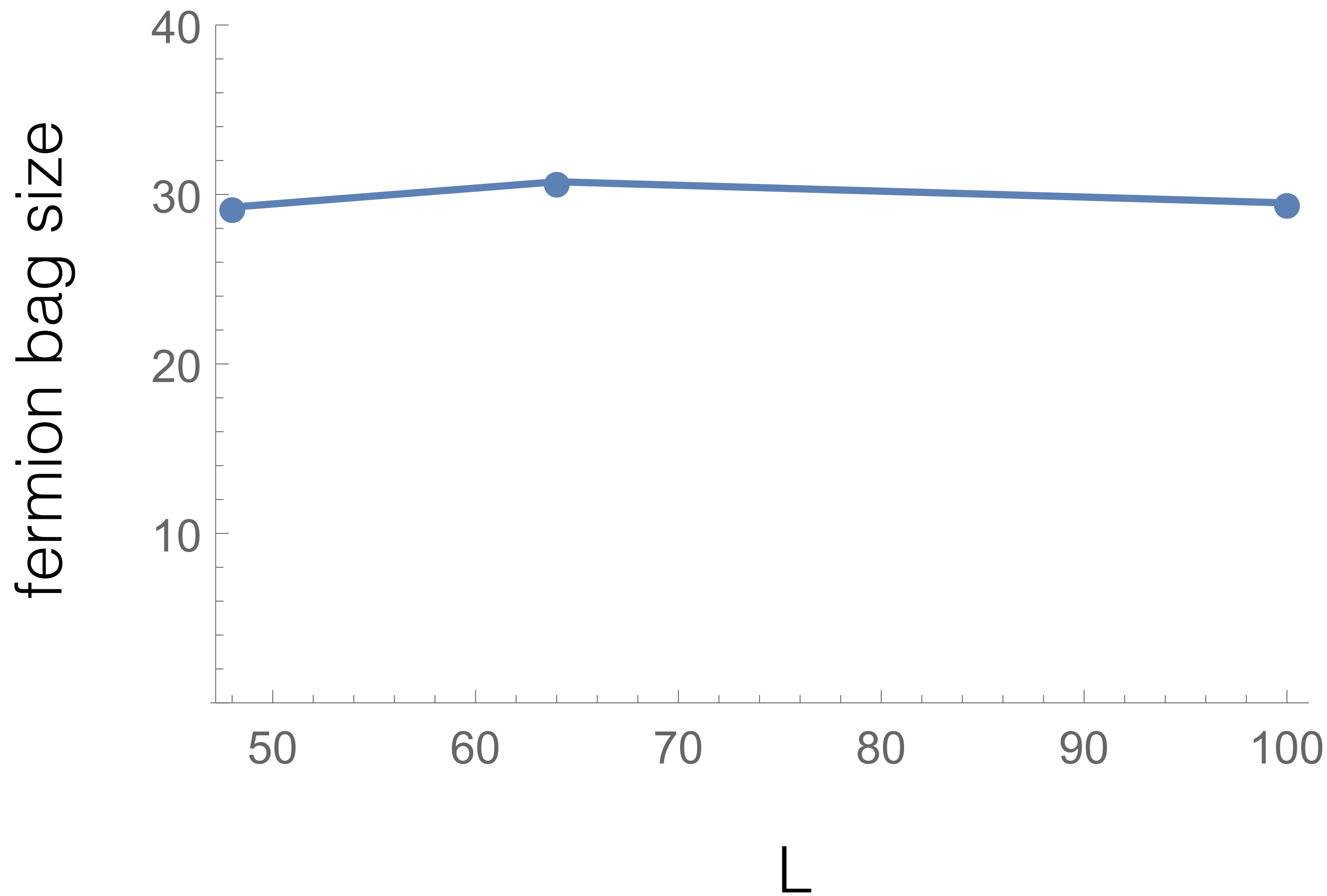
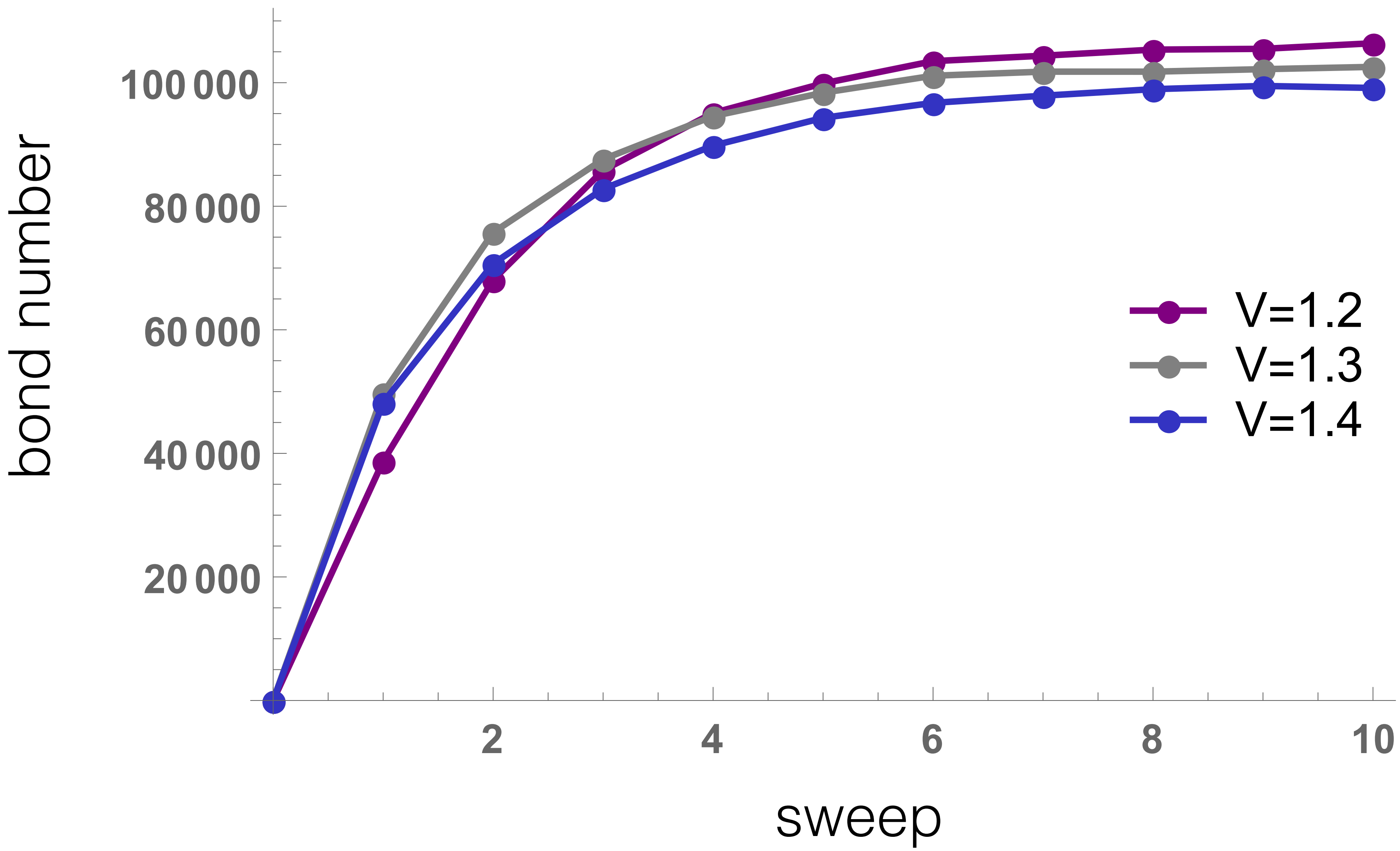


Fast updates possible within time slices!
A similar update is used in auxiliary field MC,
but here there is a bigger gain.

Equilibration on 100 x 100 lattice, β = 4



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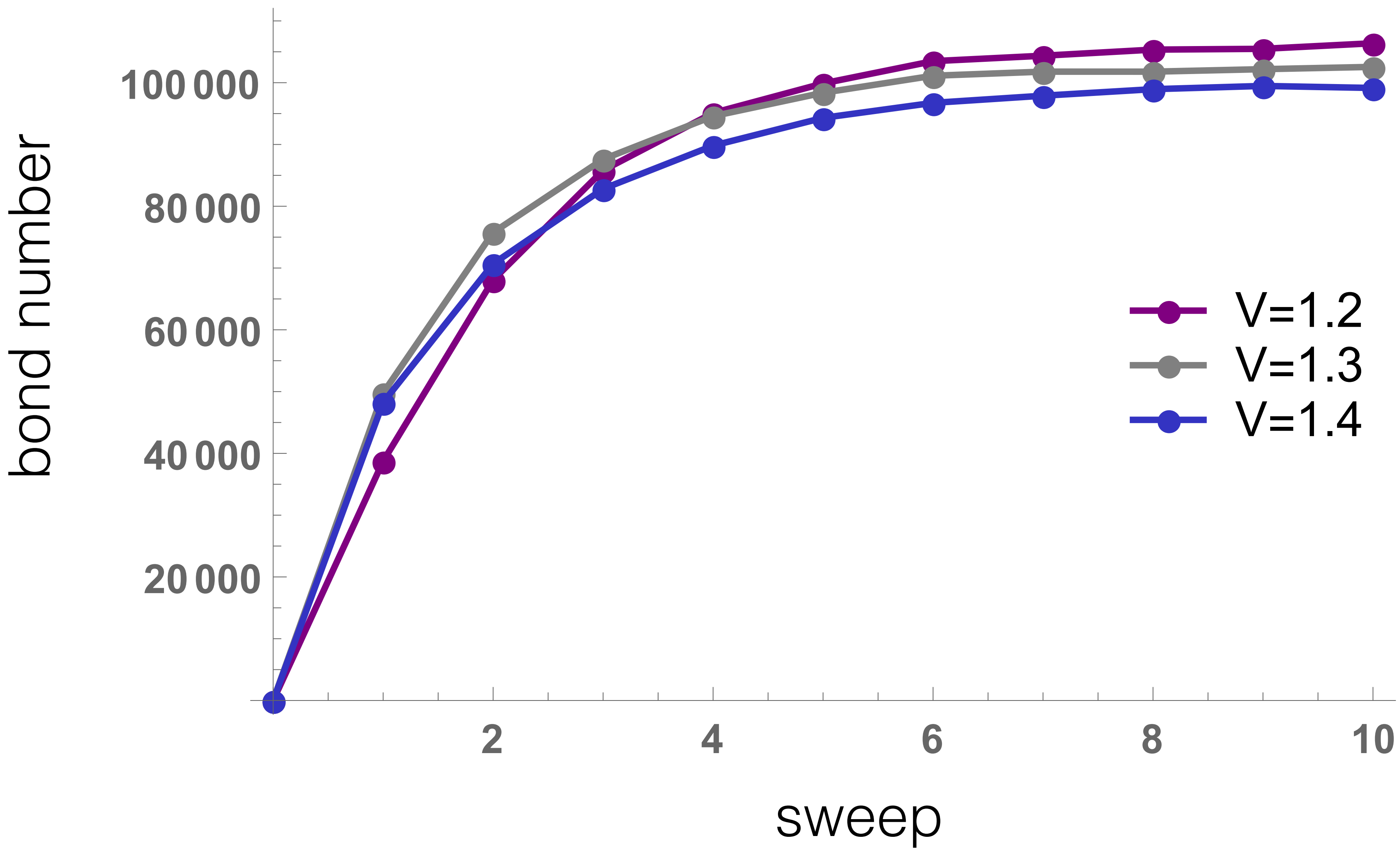
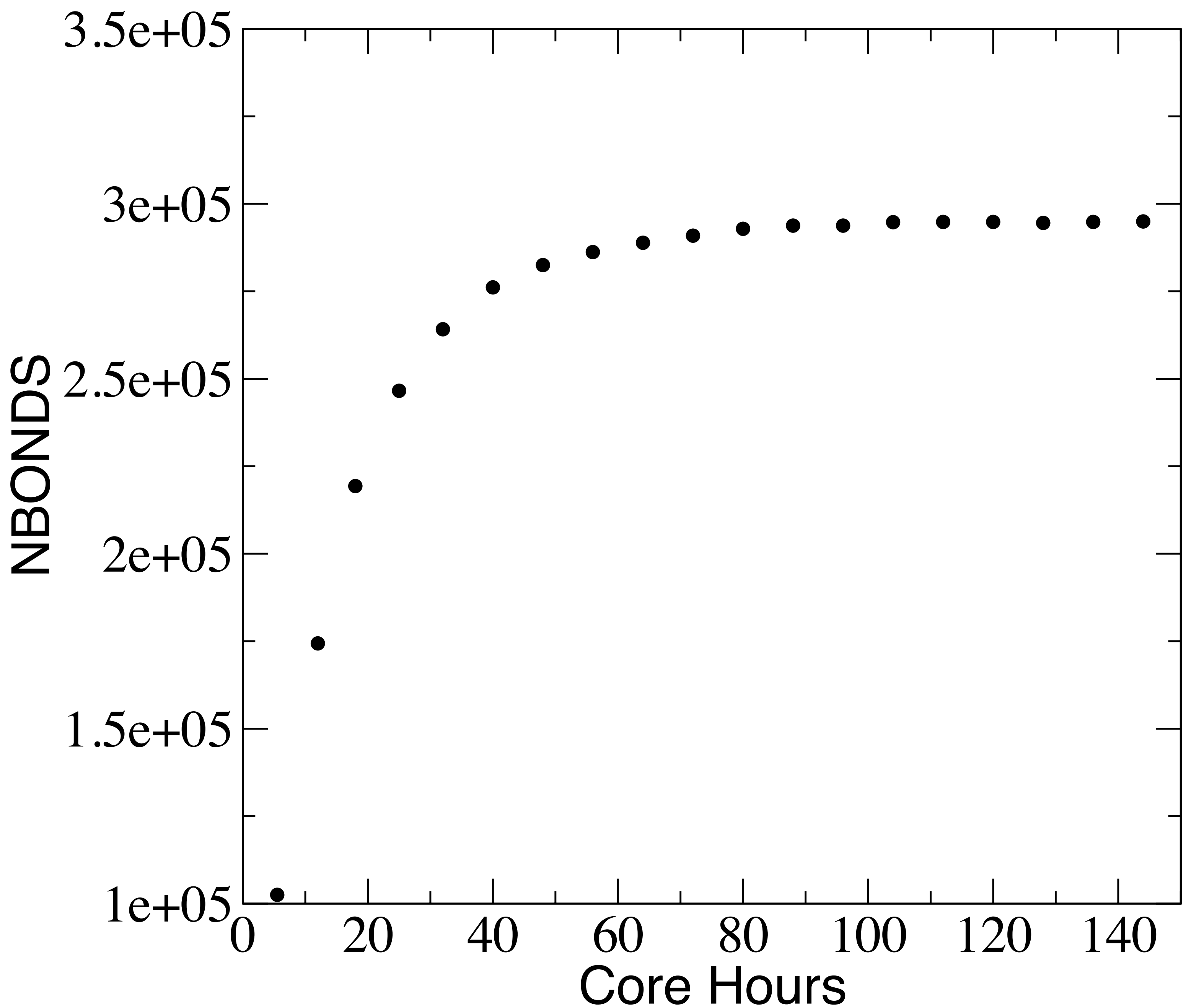
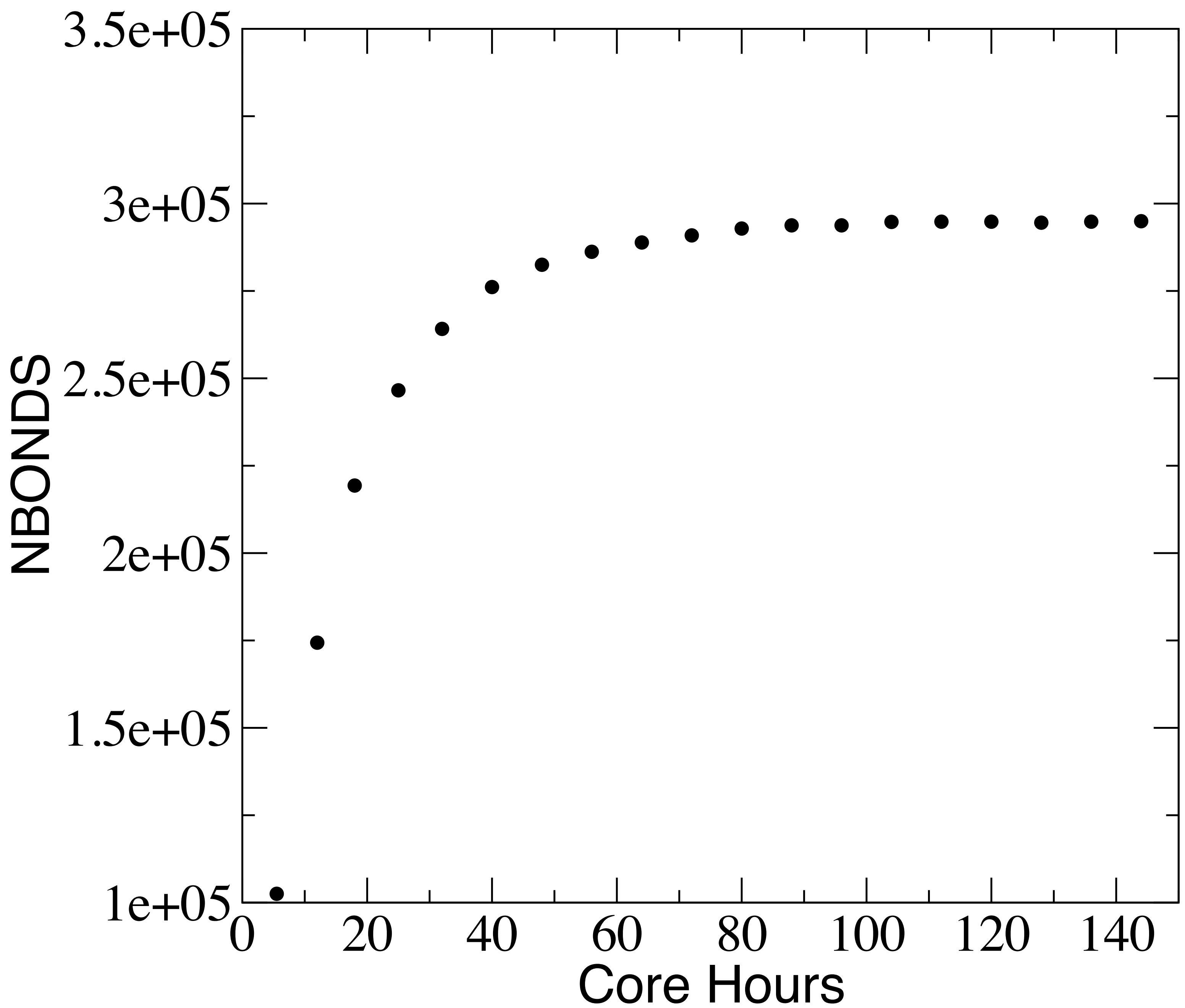


Fakher Assaad (Sign 2017): This may be impossible with auxiliary field MC, due to stabilization issues!

Equilibration on 48 x 48 lattices with β = 48

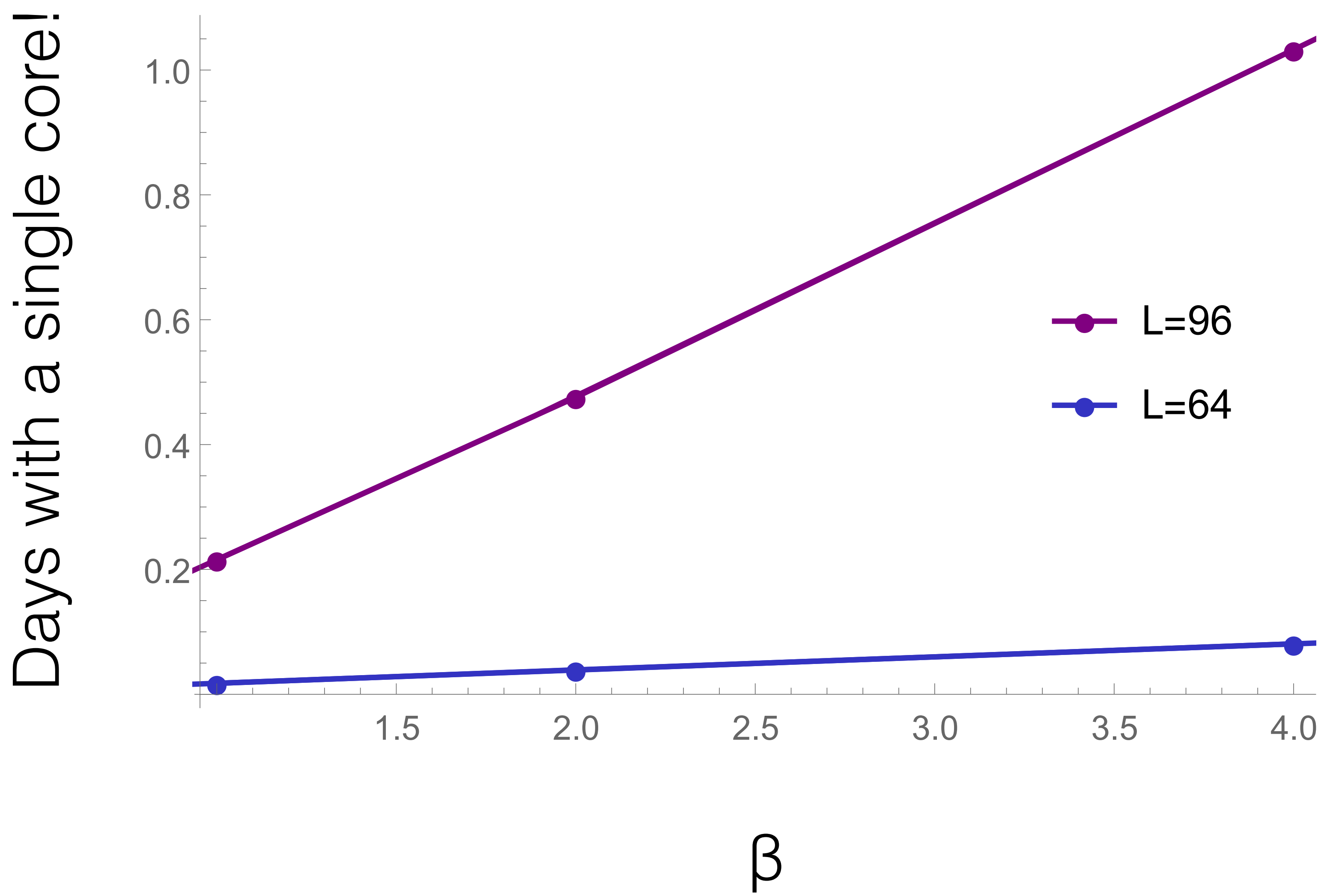


Equilibration on 48 x 48 lattices with β = 48



Almost the biggest lattices
ever simulated in the current context!

Scaling of the algorithm: $L^6 \beta$



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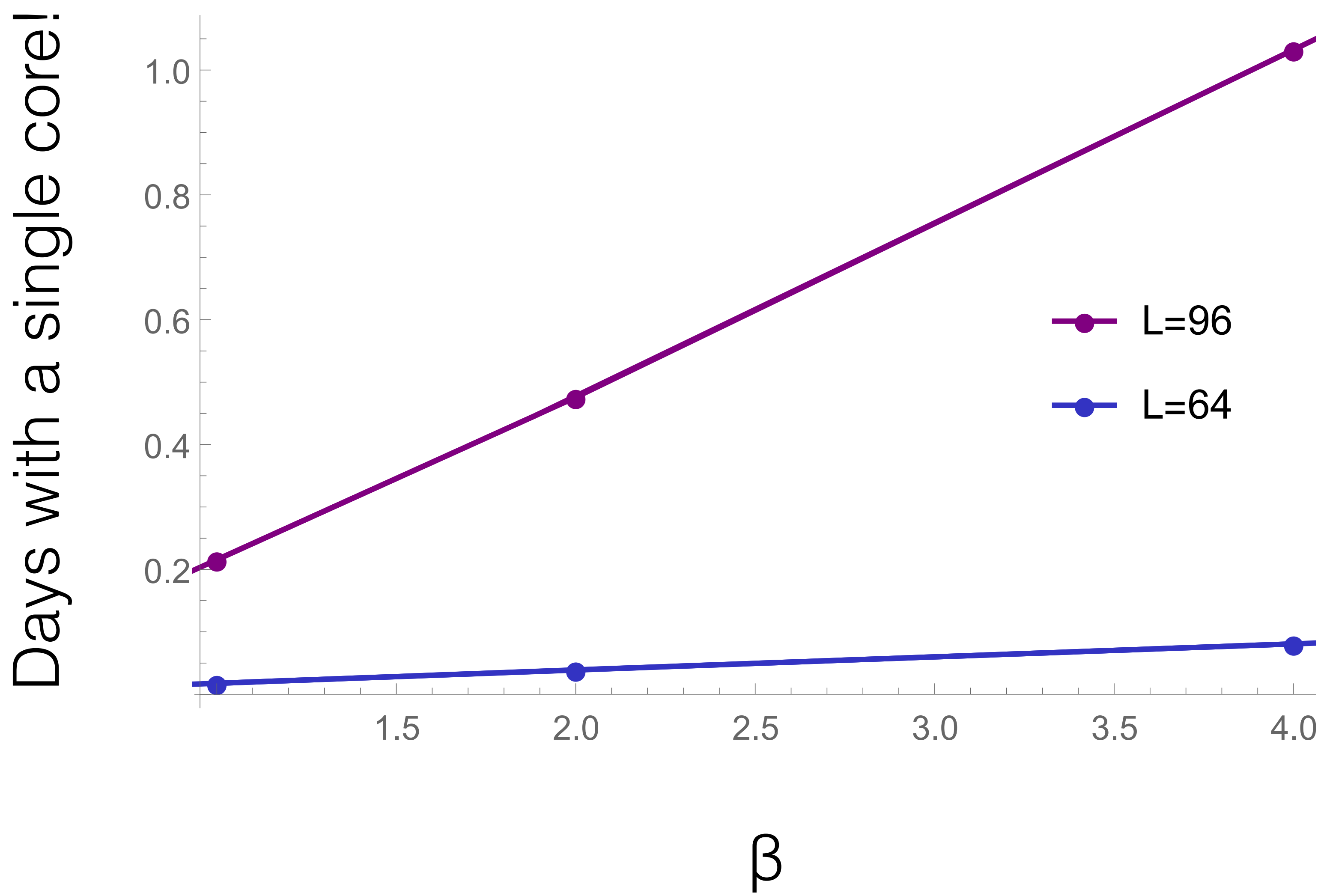

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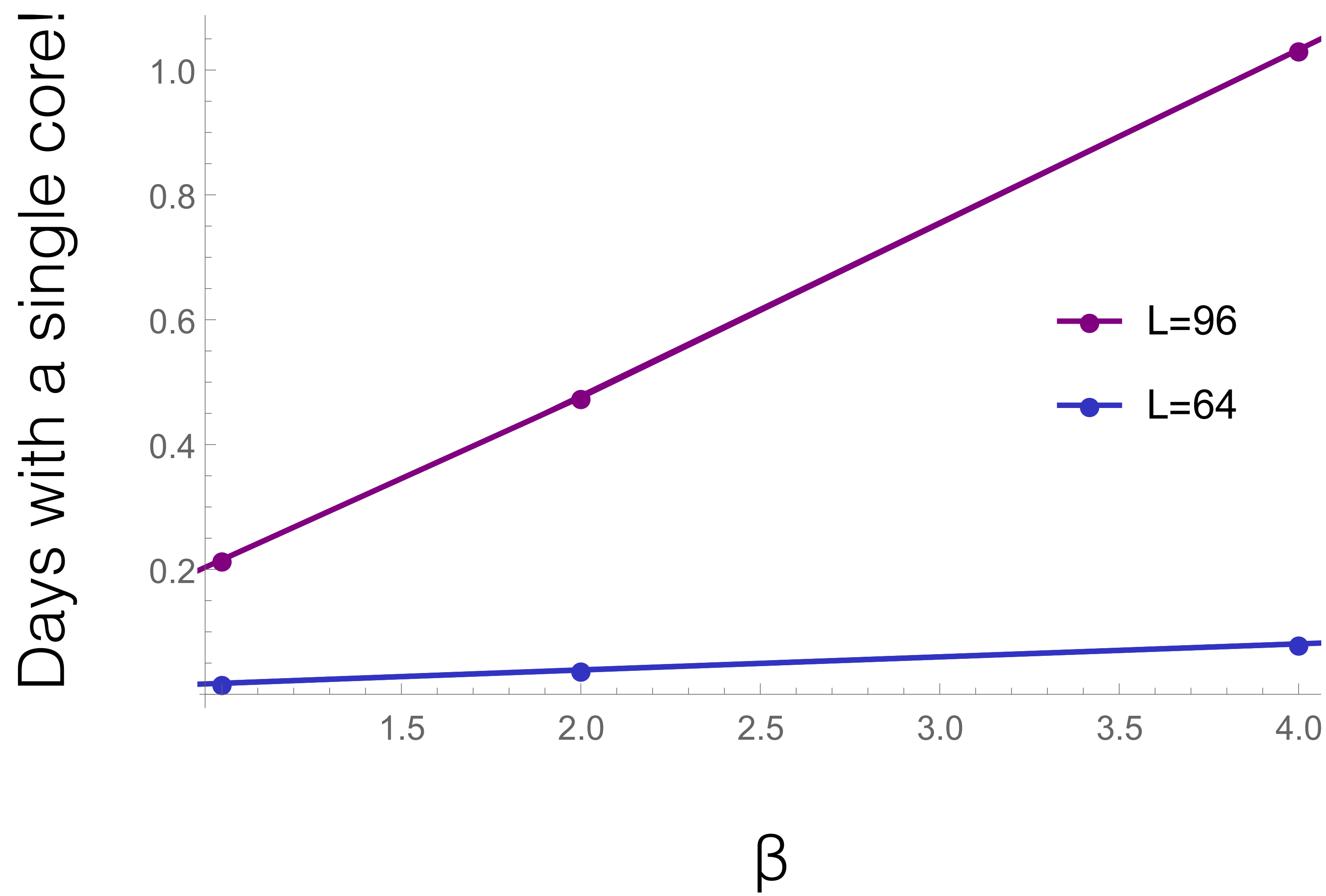

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Explore ways to accelerate to do even L=100 (10,000 sites) at low T.

Results $\beta = L$

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density-density correlation ratio

$$R = \left\langle \left(n_0 - \frac{1}{2}\right)\left(n_{L/2} - \frac{1}{2}\right) \right\rangle$$

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symmetric phase: (semi-metal) $R \sim \frac{1}{L^4}$

broken phase: (charge density wave) $R \sim \text{Const.}$

critical point: $R \sim \frac{1}{L^{1+\eta}}$

Correlation Ratio: $R \approx A/L^{1+\eta}$ at $V = V_c$

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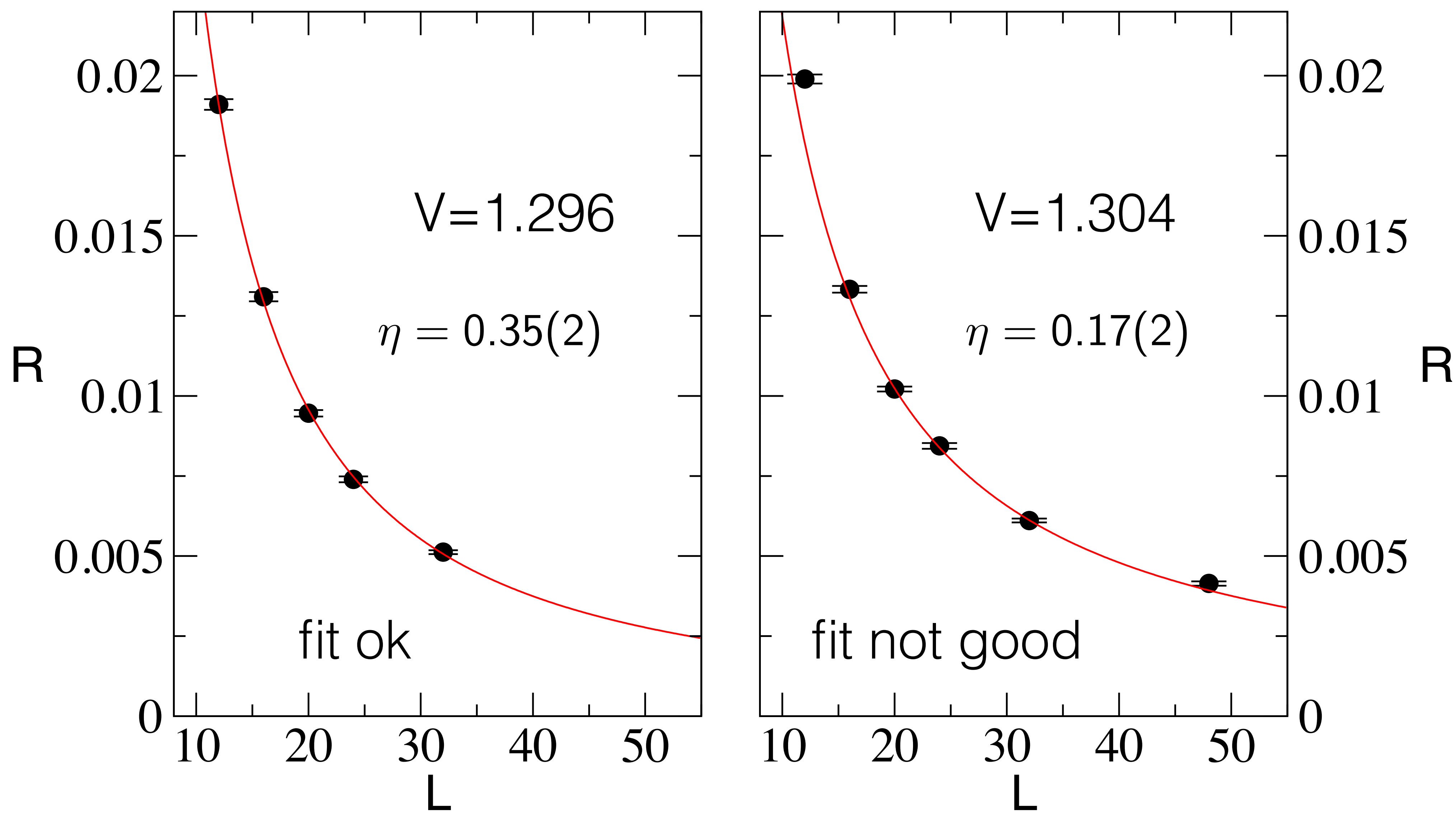

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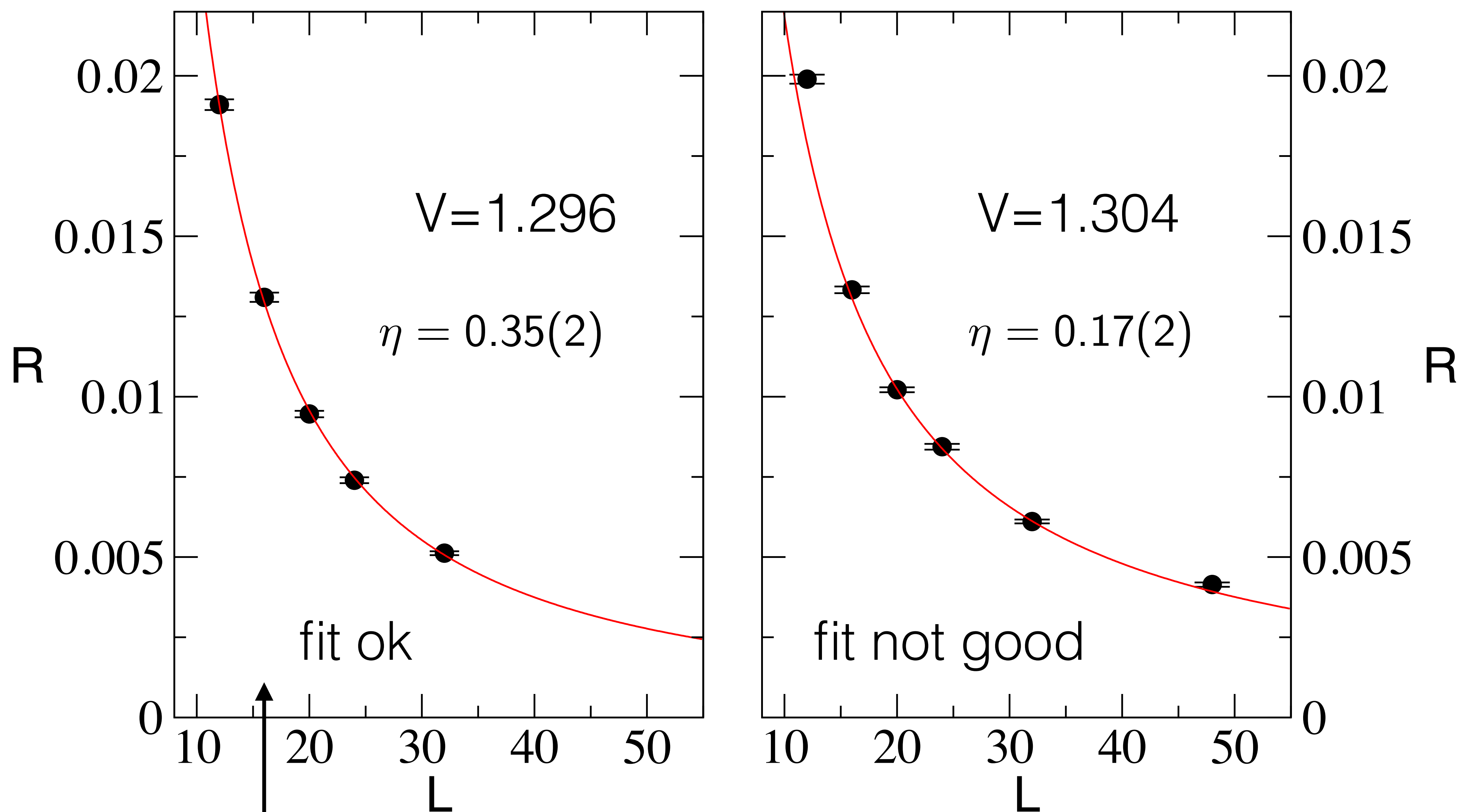

Li, Jiang and Yao, 2014
(484 sites)

$\nu = 0.77(3), \eta = 0.45(2)$

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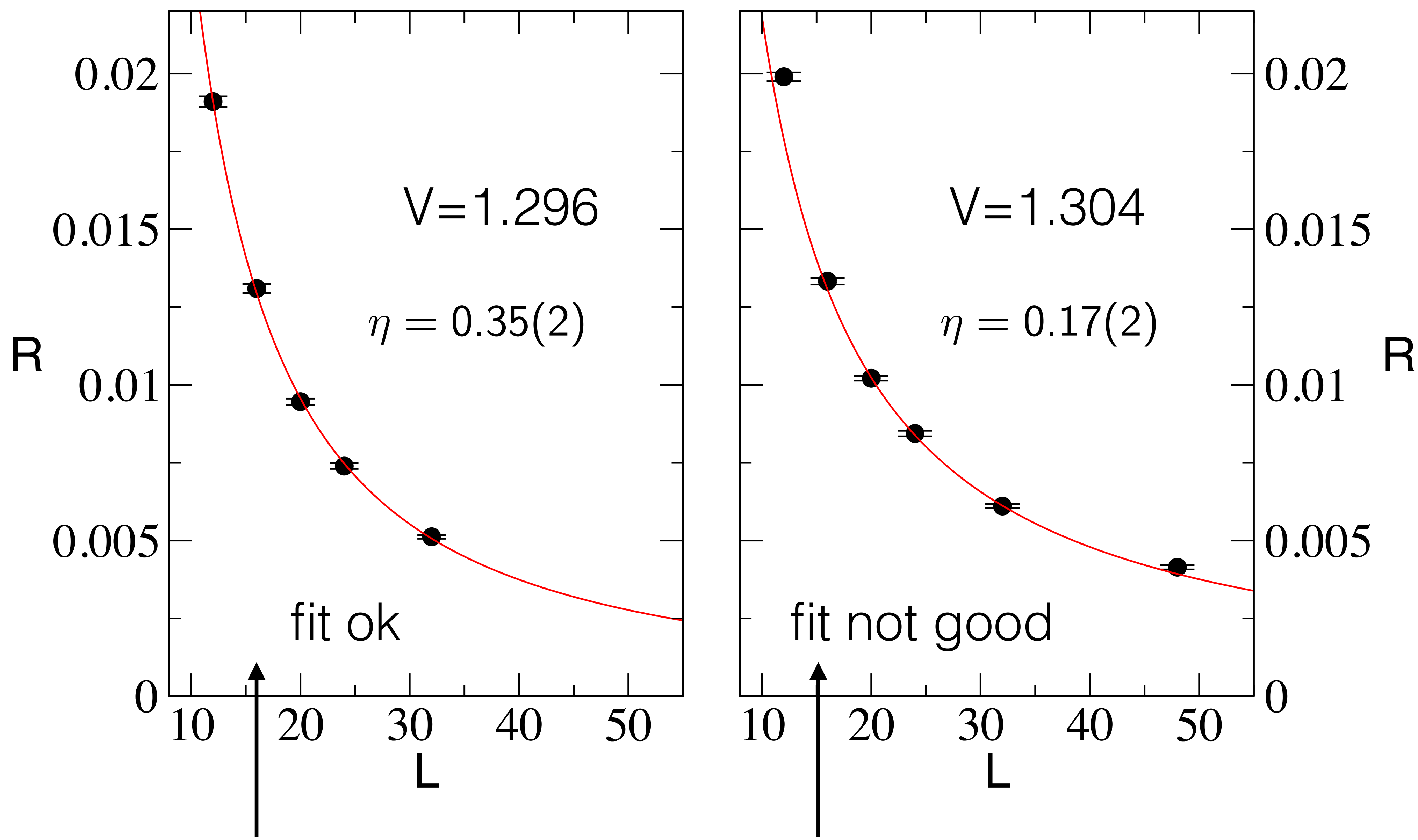

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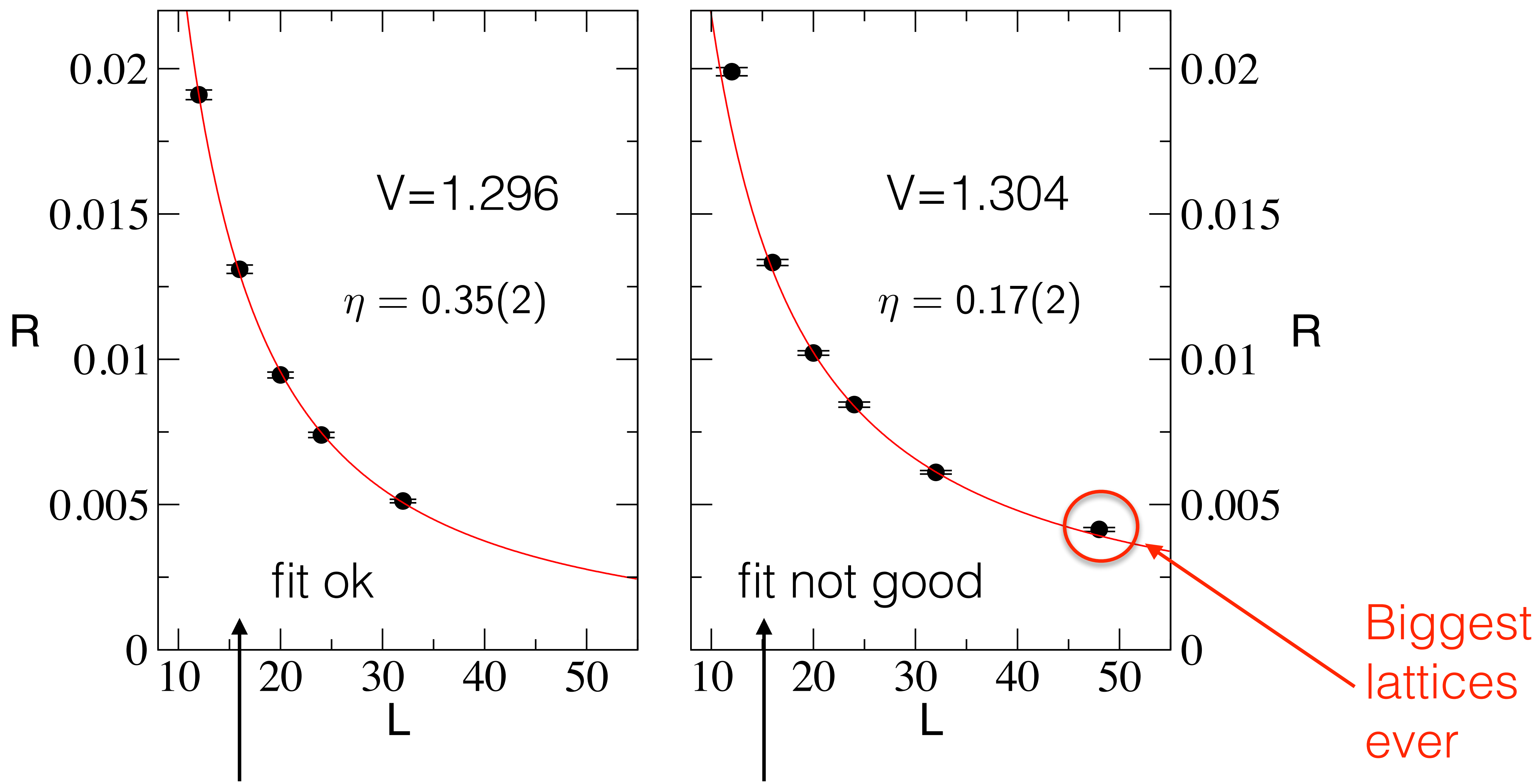

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Stay Tuned for more results
on large lattices!

Conclusions

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Opportunities exist to explore the HMC approach to study large lattices. But it is important to study the massless limit.

Ideas based on fermion bags offer an alternate method. In some cases they seem to allow us to study large lattices that seemed difficult earlier.