Fermion Bag Approach to Hamiltonian Lattice Field Theories

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Motivation

Strongly interacting massless Dirac fermions with four-fermion interactions in (2+1)D are known to contain many interesting quantum critical points.

Park, Rosenstein and Warr, 1990

A. Gross-Neveu models have quantum critical points separating massless and massive phases.

B. Thirring models behave differently depending on flavor numbers.

Welleneghausen, Schmidt, Wipf 2017

C. Novel critical points also seem to emerge where fermions become massive but without any spontaneous symmetry breaking.

Ayyar and S.C, 2014
Catterall, 2015

Can we compute the properties of these critical points accurately?

Review: Gross Neveu Models

Many types of models can be written down

4 x 4 Dirac space

$$S = S_0 + S_{\text{int}} \qquad S_0 = \int d^3x\, \overline{\psi}(\gamma_\mu \otimes I)\partial_\mu \psi$$

N x N flavor matrix

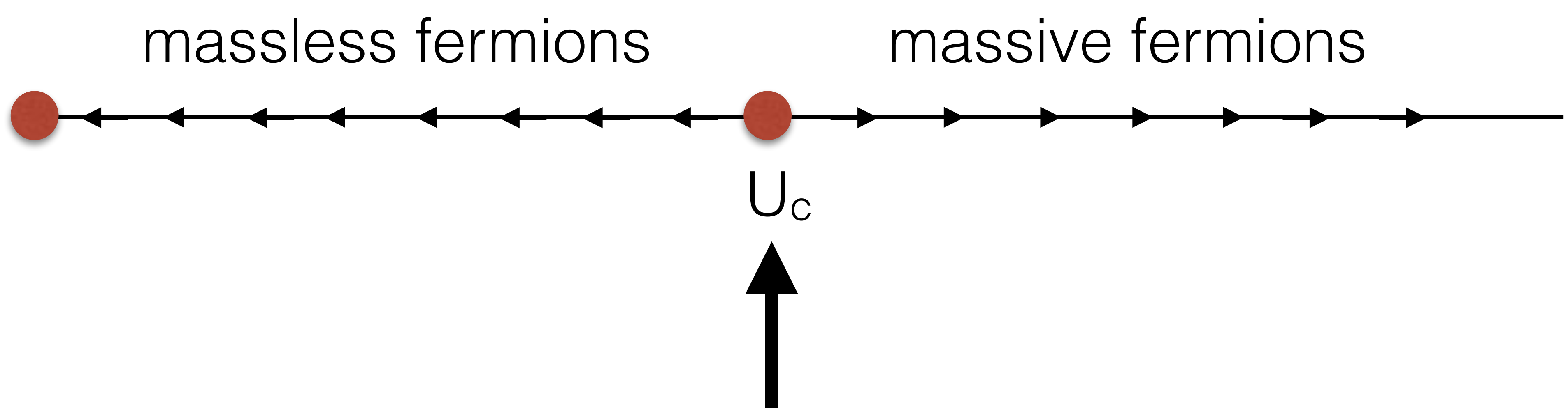
Chiral Ising $\quad S_{\text{int}} = \frac{U}{2}\int d^3x \left[\overline{\psi}(I \otimes I)\psi\right]^2$

Chiral XY $\quad S_{\text{int}} = \frac{U}{2}\int d^3x \left\{ \left[\overline{\psi}(I \otimes I)\psi\right]^2 - \left[\overline{\psi}(\gamma_5 \otimes I)\psi\right]^2 \right\}$

Chiral Heisenberg $\quad S_{\text{int}} = \frac{U}{2}\int d^3x \left[\overline{\psi}(I \otimes \vec{\sigma})\psi\right]^2$

In these models the four-fermion interaction becomes "relevant" non-perturbatively.

Park, Rosenstein and Warr, 1990



Goal is to find the properties of this critical point

There are different universality class for each Ising, XY, Heisenberg type interactions that also depend on the value of N!

Focus on the simplest Gross Neveu models: N = 1

Difficult in the action formulation on the lattice

a. N=1 staggered fermion models suffer from sign problems.

b. Overlap/Domain wall fermions will be computationally difficult.

c. SLAC fermions are non-local, but …. (talk to Andreas Wipf)

Hamiltonian Staggered Fermions do produce N=1 Dirac fermion.

Sign problems can be solved!

Huffman and S.C, 2013; Li, Jiang and Yao, 2014; Wei, Wu, Li, Zhang and Xiang, 2016

MC calculations have recently emerged.

Summary of Recent results

N=1 (Ising)	η	ν	Largest 2D Lattice size	Fermion Formulation
ε-expansion (1)	0.49	0.91	-	-
FRG (1)	0.55	0.93	-	-
Bootstrap (2)	0.54	1.32	-	-
MC (3)	0.30(1)	0.80(3)	256	staggered
MC (4)	0.45(2)	0.77(3)	484	staggered
MC (5)	0.63(3)	0.91(3)	576	SLAC

(1) Zerf, et. al., PRD 96, (2017)
(2) ILiesiu, et. al., JEHP 04 (2016)
(3) Wang,Corboz,Troyer, New J. of Phys. 16 (2014).
(4) Li, Jiang and Yao, New J. of Phys. 17 (2015).
(5) D. Schmidt, PhD Thesis (2015)

Can we do better with staggered fermions?

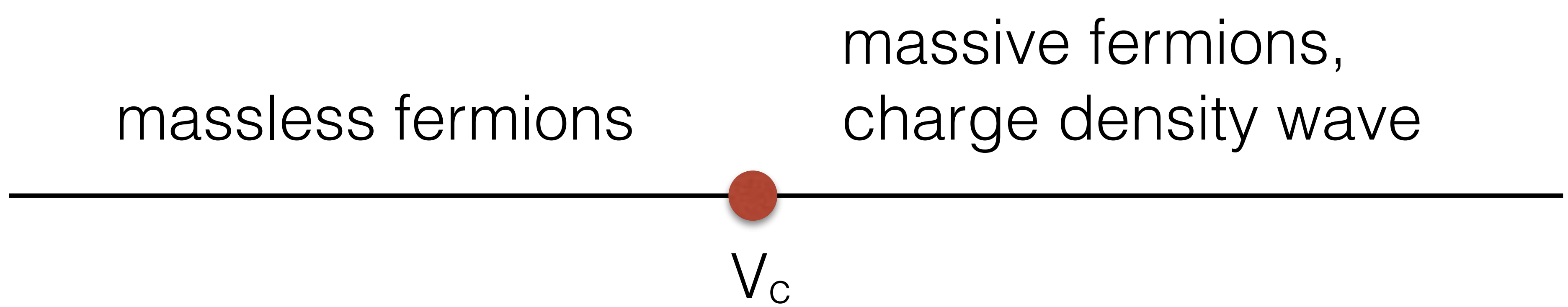
The Repulsive t-V model

Hamiltonian on a square lattice:

$$H = -t \sum_{\langle ij \rangle} \eta_{ij} \, (c_i^\dagger c_j + c_j^\dagger c_i) \; + \; V \sum_{\langle ij \rangle} \left(n_i - \frac{1}{2}\right) \left(n_j - \frac{1}{2}\right)$$

staggered phases = π-flux

At small couplings describes N = 1, 4-component massless Dirac fermions. Chiral Symmetry is Z_2.



Continuous Time Approach

Rombouts, Heyde and Jachowicz, 1999

Rubtsov and Lichtenstein, 2001

Monte Carlo algorithms can be constructed using the expansion:

$$Z = \int_0^{\beta} dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{k-1}} dt_k \,\mathrm{Tr}\Big(\mathrm{e}^{-H_0(\beta - t_1)} \left(-H_{\mathrm{int}}\right) \mathrm{e}^{-H_0(t_1 - t_2)} \left(-H_{\mathrm{int}}\right) \ldots \mathrm{e}^{-H_0 t_k} \Big)$$

where $H = H_0 + H_{\mathrm{int}}$

But, what should we choose for H_0 and H_{int} ?

In the case of the t-V model we showed that if we choose

Huffman and SC, 2013

$$H_0 = \sum_{\langle ij \rangle} t_{ij} \left(c_i^{\dagger} c_j + c_j^{\dagger} c_i \right) \qquad H_{\mathrm{int}} = V \sum_{\langle ij \rangle} \left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right)$$

the sign problem is solved!

So if we assume that $H_{b=\langle ij \rangle} = V(n_i - \frac{1}{2})(n_j - \frac{1}{2})$ then

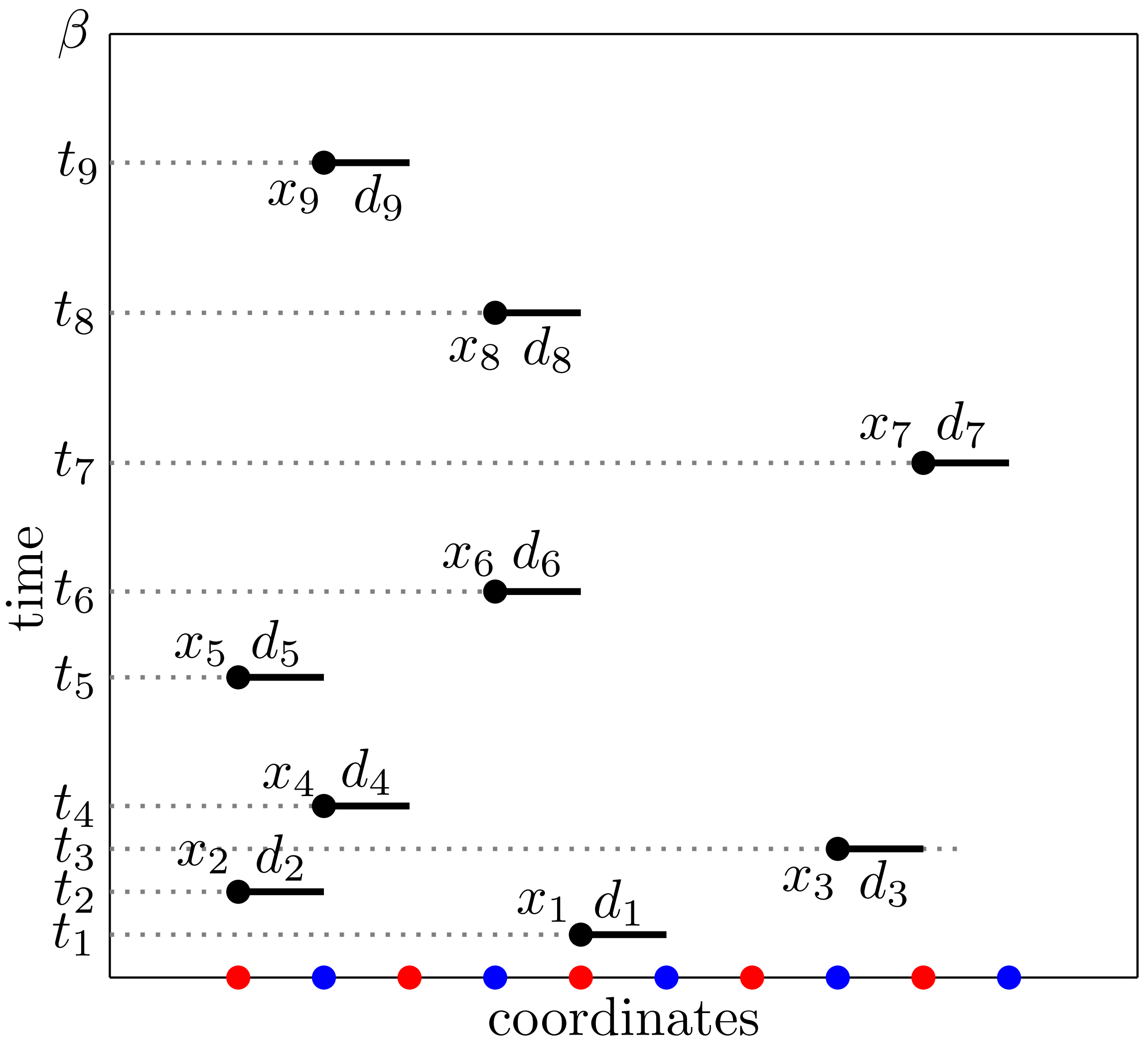
$H_{\text{int}} = \sum_b H_b$ and we can write

$$Z = \int [dt] \sum_{[b]} \mathrm{Tr}\left(e^{-H_0(\beta - t_1)} (-H_{b_1}) \, e^{-H_0(t_1 - t_2)} (-H_{b_2}) \, \ldots \, H_{b_k} e^{-H_0 t_k} \right)$$

Here [b] represents a configuration of nearest neighbor bonds and

[b] configuration

b = (x,d)



We then showed that

Huffman and SC, 2014

$$\mathrm{Tr}\left(e^{-H_0(\beta-t_1)}\,(-H_{b_1})\,e^{-H_0(t_1-t_2)}\,(-H_{b_2})\,\ldots\,(-H_{b_k})\,e^{-H_0 t_k}\right) = \Big(\mathrm{Pf}(A[b])\Big)^2$$

$$Z = \int [dt] \sum_{[b]} \Big(\mathrm{Pf}(A([b]))\Big)^2$$

2k x 2k
matrix!

Thus, the sign Problem was solved!

But k in the interesting region can be very large on large lattices

$$k \sim 10^5 - 10^6$$

Need more ideas to develop an efficient algorithm!

Insight from Auxiliary Field Approach

Blancenbecler, Scalapino, Sugar, 1981

Partition function: $Z = \mathrm{Tr}\left(e^{-H\beta}\right)$

Traditional auxiliary field approach: $H = H_0 + H_{int}$

$$Z = \mathrm{Tr}\left(e^{-\varepsilon H_0} e^{-\varepsilon H_{int}} \ldots e^{-\varepsilon H_0} e^{-\varepsilon H_{int}}\right)$$

$$= \sum_{[\phi]} \mathrm{Tr}\left(e^{-c^\dagger M(\phi_1) c}\; e^{-c^\dagger M(\phi_2) c} \;\ldots\; e^{-c^\dagger M(\phi_{L_t}) c}\right)$$

$$= \sum_{[\phi]} \mathrm{Det}\left(1 + e^{-M(\phi_1)}\; e^{-M(\phi_2)} \;\ldots\; e^{-M(\phi_{L_t})}\right)$$

V x V matrices

$$= \sum_{[\phi]} \mathrm{Det}\left(1 + B_1\, B_2 \ldots B_{L_t}\right)$$

BSS formula

Solution to the sign problem requires special properties for the B's

In the spin-full Hubbard model at half filling the sign problem was solved early because of the following relations:

$$e^{\,-\;c^\dagger M(\phi) c} \;\longrightarrow\; e^{\,-\;c_\uparrow^\dagger M(\phi) c_\uparrow \;-\; c_\downarrow^\dagger M(\phi) c_\downarrow}$$

$$B \;\rightarrow\; B_\uparrow \;\otimes\; B_\downarrow \quad \text{where} \quad B_\uparrow \;=\; B_\downarrow$$

$$\mathrm{Det}\left(1 \;+\; B_1\; B_2\; \ldots\; B_{L_t}\right) \;\rightarrow\; \mathrm{Det}\left(1 \;+\; B_1 \otimes B_1\;\; B_2 \otimes B_2\; \ldots\; B_{L_t} \otimes B_{L_t}\right)$$

$$= \;\left\{\mathrm{Det}\left(1 \;+\; B_1\; B_2\; \ldots\; B_{L_t}\right)\right\}^2$$

It was not clear how to extend this to the spin-less case in the t-V model

The idea remained hidden in our work

$(\mathrm{Pf}(A[b]))^2$ = two commuting spaces?

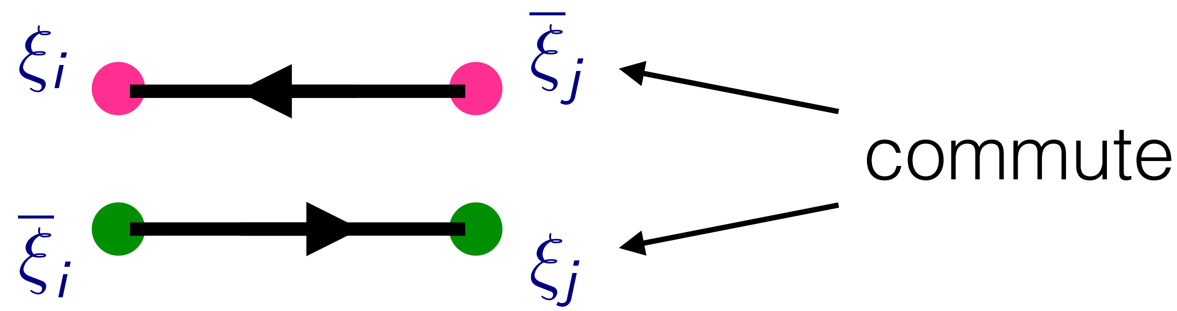
It was discovered a few months later!

Li, Jiang and Yao, 2014;

Trick: Majorana Representation:

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

$$H \ = \ \sum_{\langle ij \rangle} \ \Big\{ - \frac{it_{ij}}{2}(\bar{\xi}_i\xi_j + \bar{\xi}_j\xi_i) \ + \ V\bar{\xi}_i\xi_j\bar{\xi}_j\xi_i \Big\}$$



We can now identify two commuting spaces (like the spin degree of freedom) and so we can again use an auxiliary field approach:

$$Z \ = \ \sum_{[\phi]} \ \Big(\mathrm{Pf}(1 + B_1 B_2 \ldots B_{L_t})\Big)^2$$

AF Approach or CT Approach?

Auxiliary field approach

$$Z = \sum_{[\phi]} \Big(\mathrm{Pf}(1 + B_1 B_2 \ldots B_{L_t})\Big)^2$$

V x V matrix

But, multiplying many V x V matrices leads to singularities!

Continuous Time approach

$$Z = \int [dt] \sum_{[b]} \Big(\mathrm{Pf}(A([b]))\Big)^2$$

k x k matrix

k turns out to be much larger than V!

Can we combine the two ideas along with ideas of fermion bags to obtain an efficient approach?

Fermion Bag Approach

Huffman, SC (2017)

The idea is to choose H_0 and H_{int} carefully so that one can identify fermion bags, while keeping the sign problem solved!

We should also be able to use the BSS type formula to be able to work with small matrices if possible.

Idea: Write

Wang, Liu, Troyer 2016

$$H = -\sum_{\langle ij \rangle} \delta \, \mathrm{e}^{2\alpha \, (c_i^\dagger c_j \, + \, c_j^\dagger c_i)}$$

$$\delta = \frac{V^2}{t} \left(1 - (V/2t)^2\right)$$

$$\cosh(2\alpha) = \frac{1 + (V/2t)^2}{1 - (V/2t)^2}, \quad \sinh(2\alpha) = \frac{V}{t} \, \frac{1}{1 - (V/2t)^2}$$

Remember the partition function

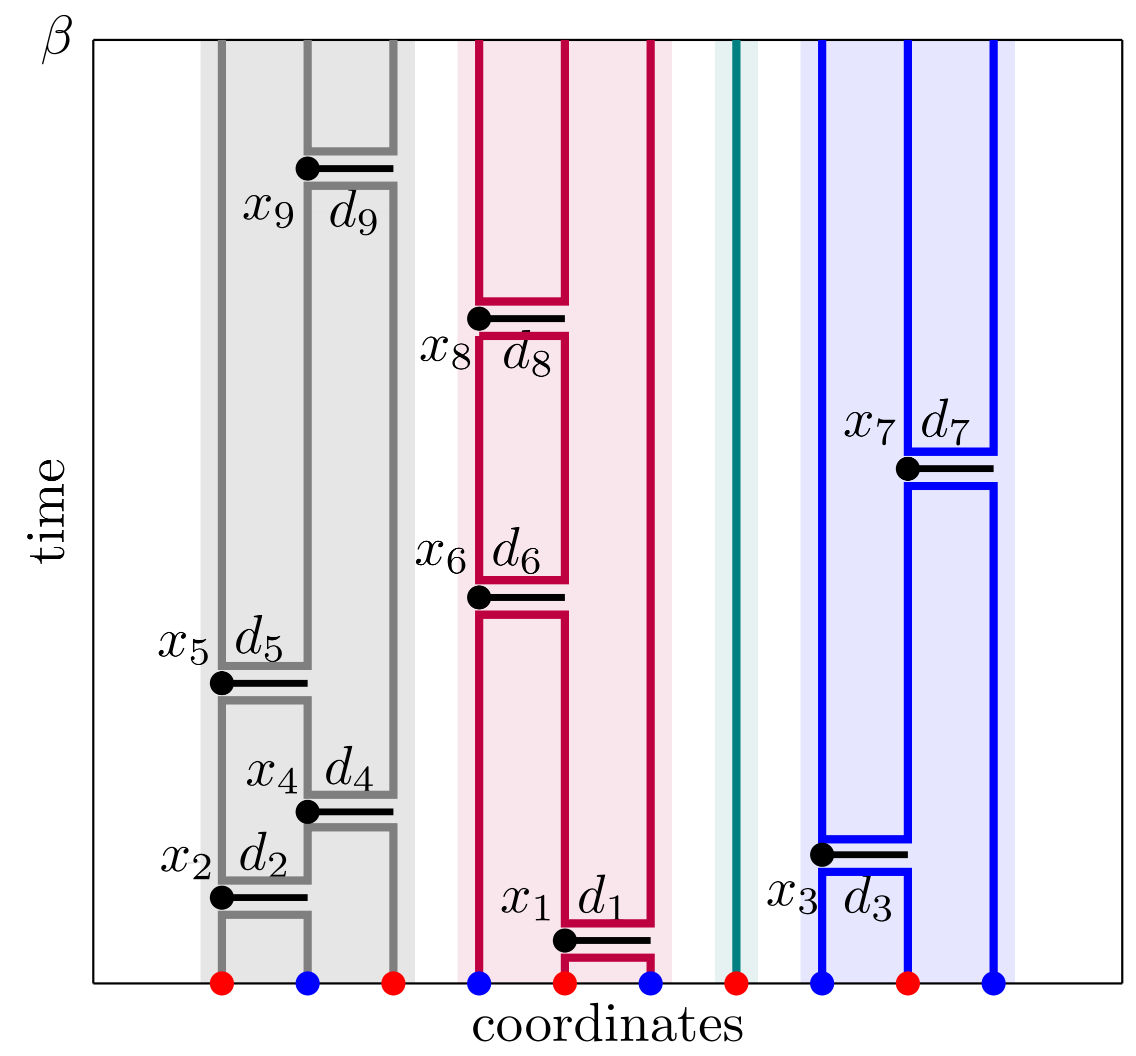
$$Z \;=\; \int [dt] \sum_{[b]} \mathrm{Tr}\Big(\mathrm{e}^{-H_0(\beta - t_1)} \; (-H_{b_1}) \; \mathrm{e}^{-H_0(t_1 - t_2)} \; (-H_{b_2}) \; \ldots \; H_{b_k} \mathrm{e}^{-H_0 t_k} \Big)$$

Let us now choose

$$H_0 \;=\; 0$$

$$H_b \;=\; -\delta \; \mathrm{e}^{2\alpha \; (c_i^\dagger c_j \;+\; c_j^\dagger c_i)}$$

The [b] configuration
now splits the lattice into fermion bags



Fermion Bags

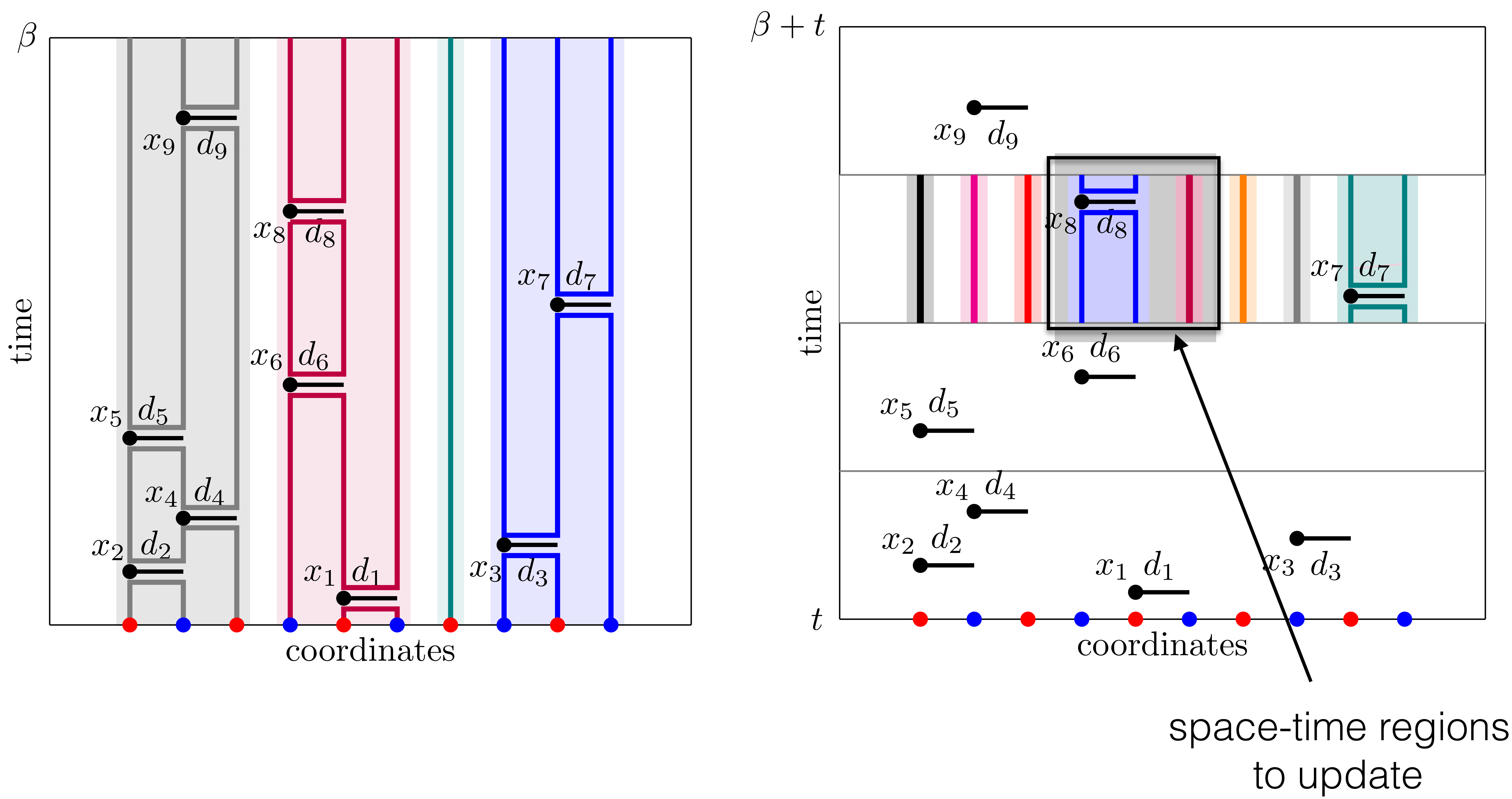
The partition function can be written using the BSS-type formula

$$Z = \int [dt] \sum_{[b]} \delta^k \, \mathrm{Det}\left(1 + B_1 \, B_2 \, ... \, B_k\right)$$

Every "B" matrix is associated with a bond and is a V x V unit matrix except for a 2 x 2 block that correspond to two nearest neighbor sites of a bond.

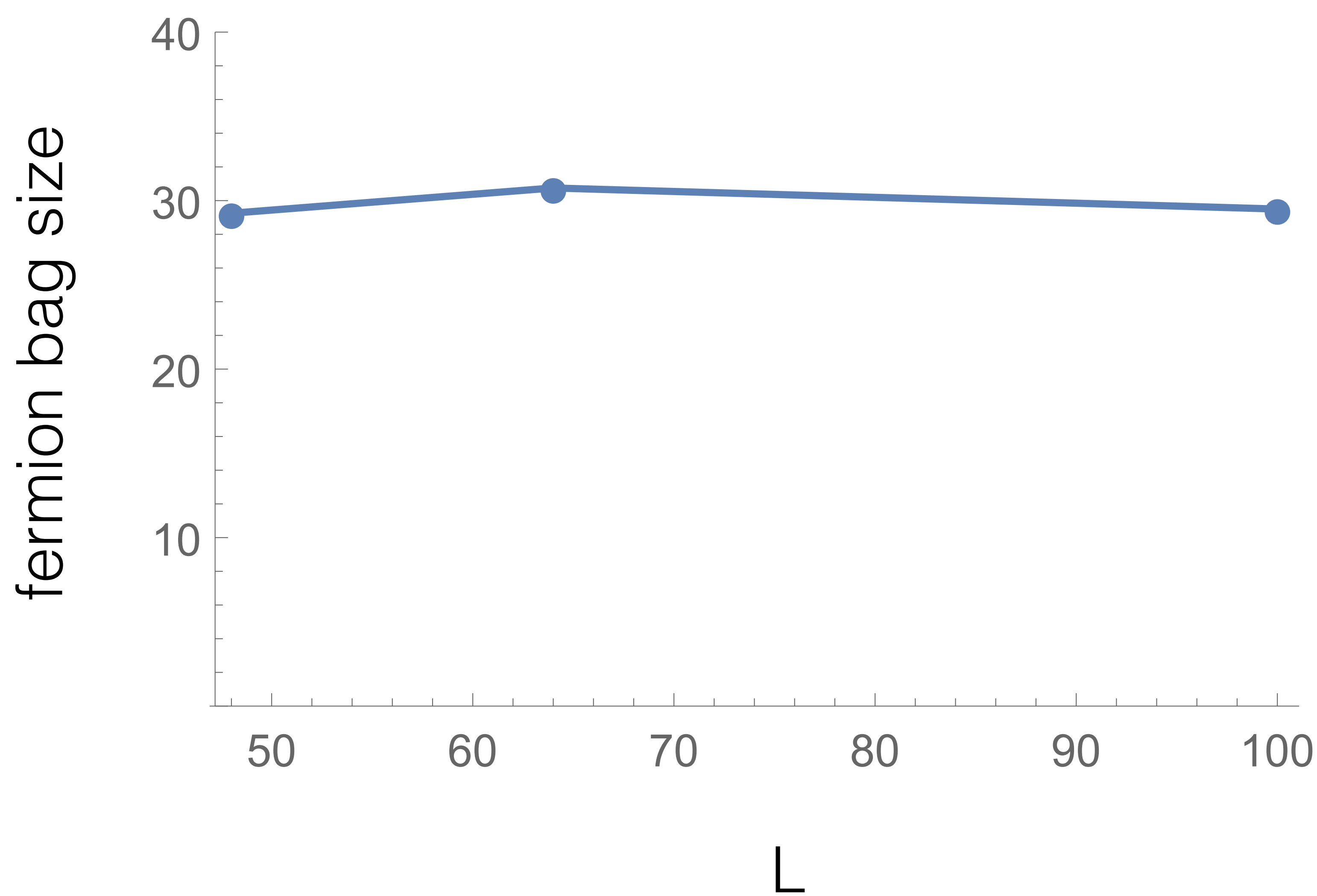
$$B = \begin{pmatrix} 1 & 0 & ... & 0 & ... & 0 & ... & 0 \\ 0 & 1 & ... & 0 & ... & 0 & ... & 0 \\ . & . & ... & . & ... & . & ... & . \\ . & . & ... & . & ... & . & ... & . \\ . & . & ... & . & ... & . & ... & . \\ 0 & 0 & ... & \cosh(2\alpha) & ... & \sinh(2\alpha) & ... & 0 \\ . & . & ... & . & ... & . & ... & . \\ . & . & ... & . & ... & . & ... & . \\ . & . & ... & . & ... & . & ... & . \\ 0 & 0 & ... & \sinh(2\alpha) & ... & \cosh(2\alpha) & ... & 0 \\ . & . & ... & . & ... & . & ... & . \\ . & . & ... & . & ... & . & ... & . \\ . & . & ... & . & ... & . & ... & . \\ 0 & 0 & ... & 0 & ... & 0 & ... & 1 \end{pmatrix}$$

At small T fermion bags will merge!
but at high T we will get many fermion bags



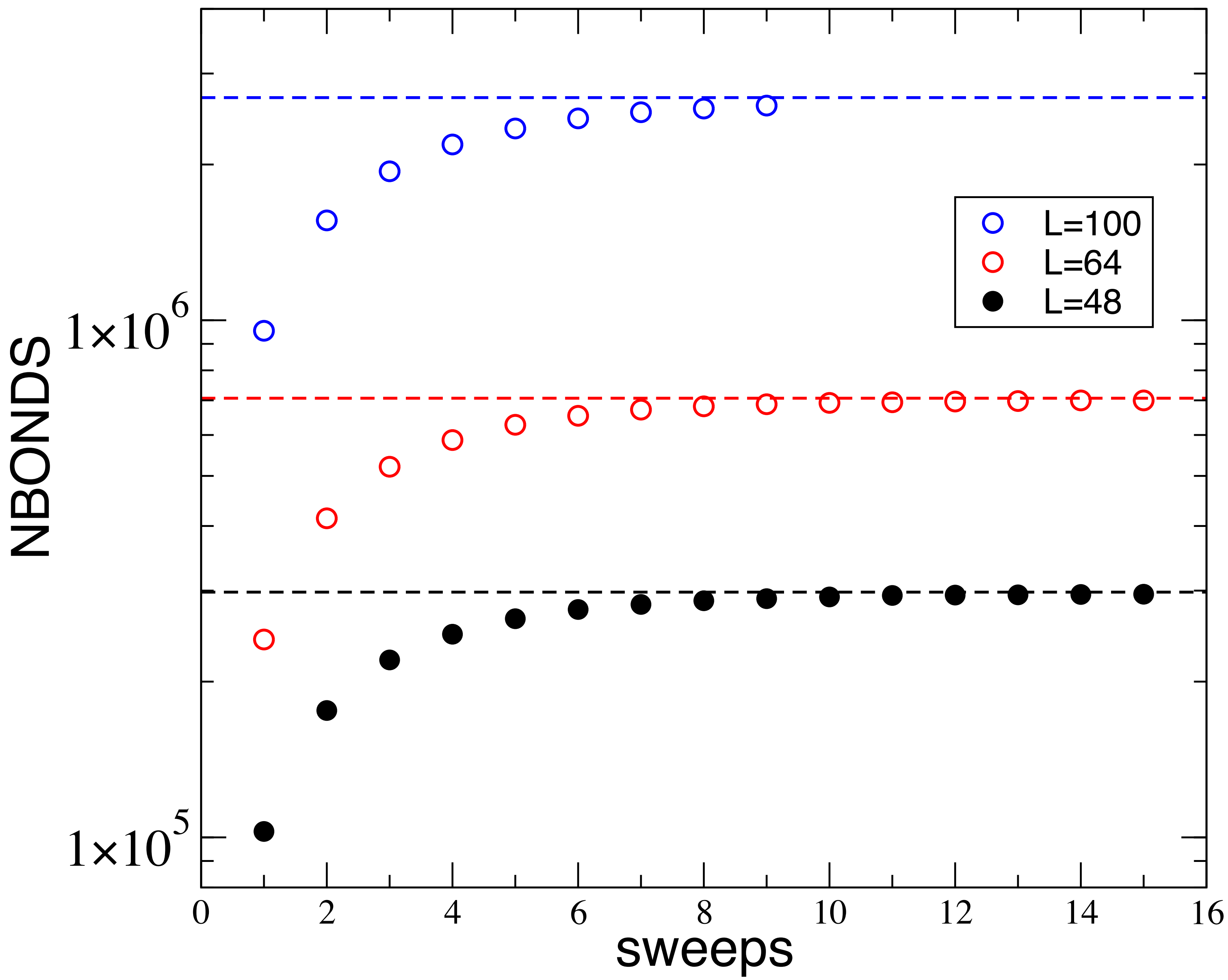
Fermion bag size as a function of spatial volume

$\Delta\tau$ = 1/4 seems like a sweet spot near the critical coupling.



Fast updates possible within space-time slices Δt = 1/4!
A similar update is used in traditional auxiliary field approach, but there every single time slice is used. A big gain in the fermion bag approach.

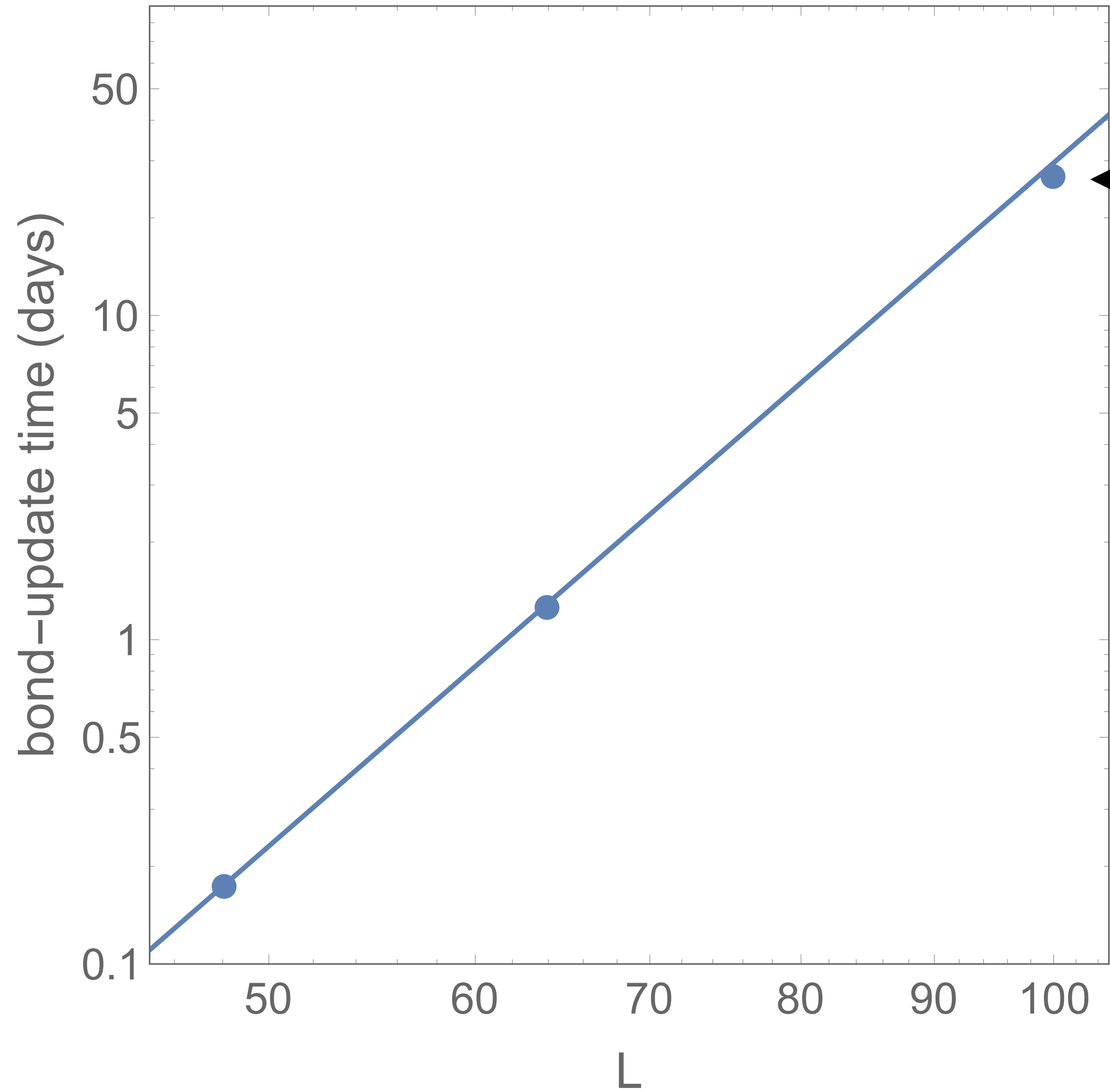
Equilibration (L=β)



The biggest lattices ever studied in the field of strongly coupled fermionic quantum criticality are around L=48!

Scaling of the algorithm: $V^3 \beta = L^7$

timings on a single core!



L=100
30 days

We can accelerate the algorithm further if we abandon the continuous time approach, in line with “Lattice Field Theory” paradigm!

Results

We choose $\beta = L$ and compute the equal time density-density correlation function

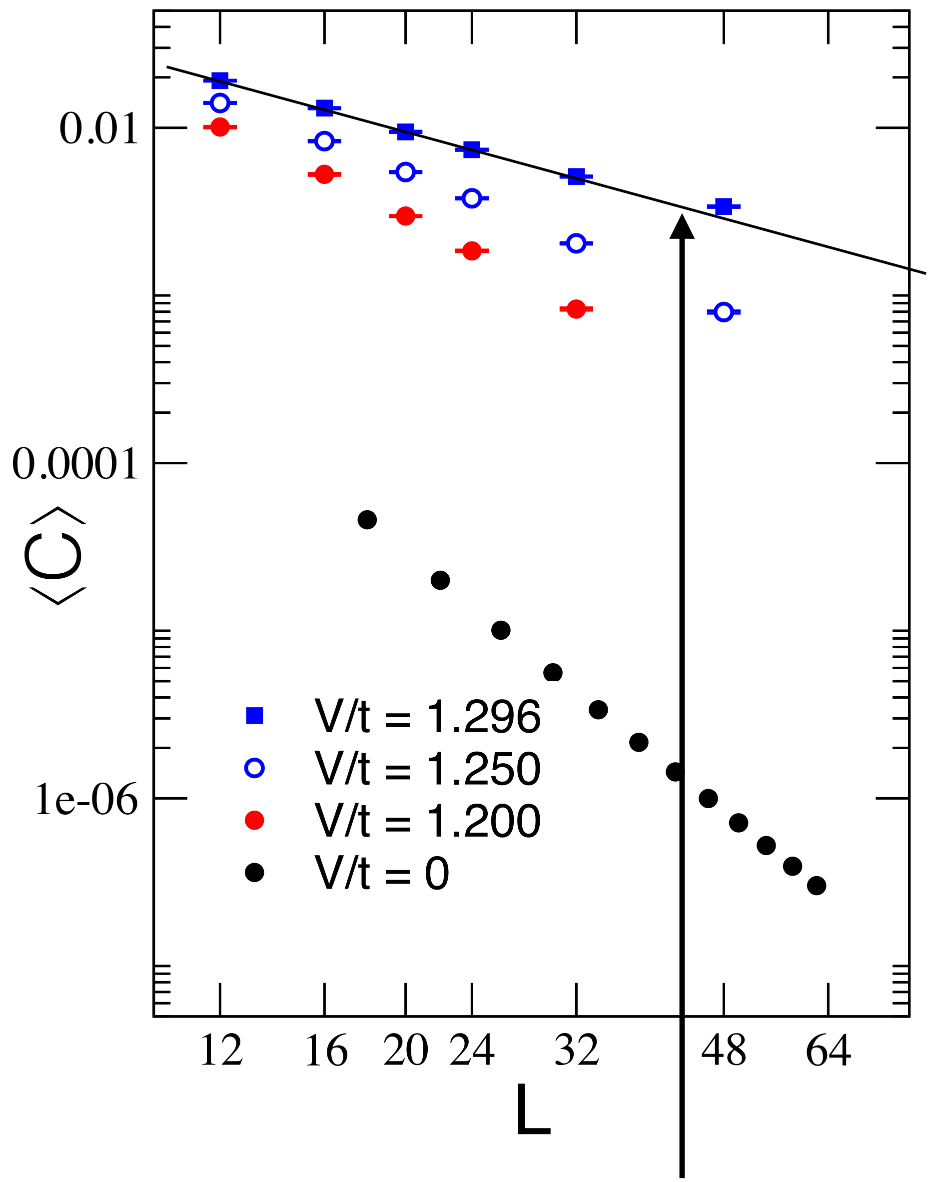
$$\langle C \rangle = \left\langle \left(n_0 - \frac{1}{2}\right)\left(n_{L/2} - \frac{1}{2}\right) \right\rangle$$

symmetric massless fermion phase: $\langle C \rangle \sim \dfrac{1}{L^4}$

broken massive fermion phase: $\langle C \rangle \sim \mathrm{Constant.}$

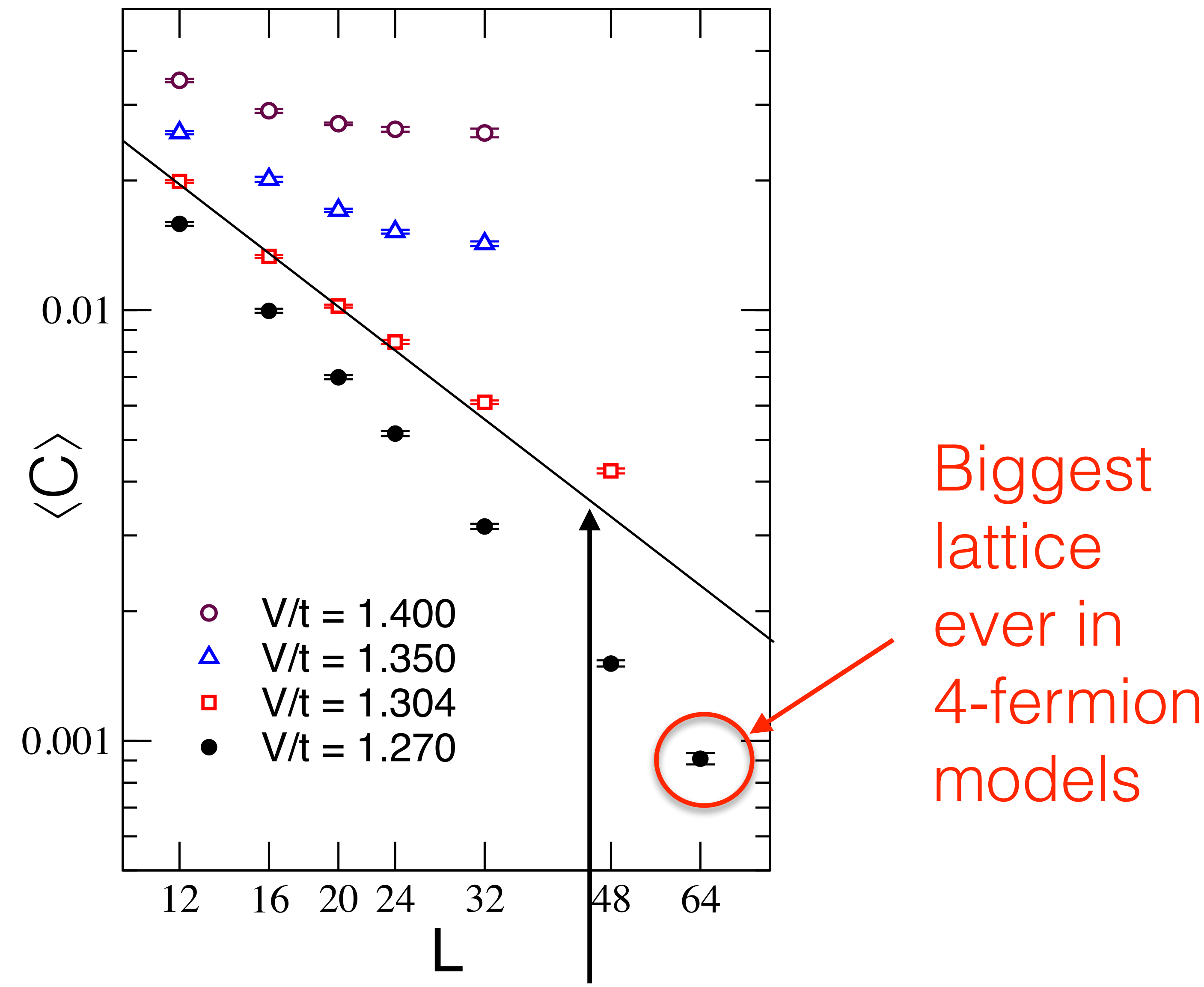
at the critical point: $\langle C \rangle \sim \dfrac{1}{L^{1+\eta}}$

Our results



Li, Jiang and Yao, 2014
(968 sites)

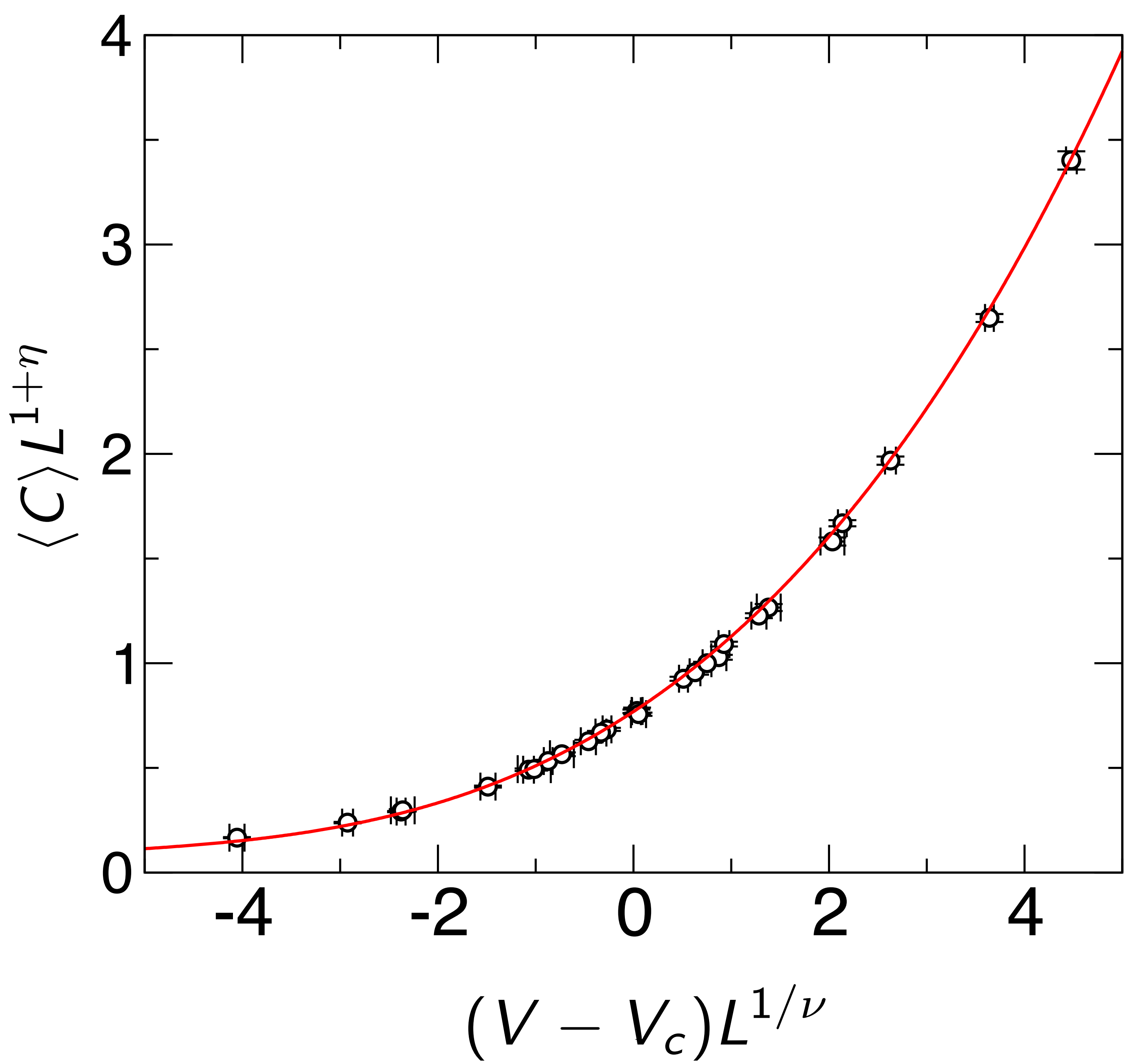
$\nu = 0.77(3), \eta = 0.45(2)$



Wang, Carboz and Troyer, 2014
(225 sites)

$\nu = 0.80(2), \eta = 0.30(1)$

Critical Scaling: $\langle C \rangle = \frac{1}{L^{1+\eta}} f((V - V_c)L^{1/\nu}/t)$



$V_c = 1.2793(15)$ $\eta = 0.53(4)$, $\nu = 0.88(1)$ $\chi^2/DOF \sim 0.8$

Summary of results for N=1 Ising Universality

N=1 (Ising)	η	ν	Largest 2D Lattice size	Fermion Formulation
ε-expansion (1)	0.49	0.91	-	-
FRG (1)	0.55	0.93	-	-
Bootstrap (2)	0.54	1.32	-	-
MC (3)	0.30(1)	0.80(3)	256	staggered
MC (4)	0.45(2)	0.77(3)	484	staggered
MC (5)	0.63(3)	0.91(3)	576	SLAC
MC This Work	0.53(3)	0.88(2)	4096	staggered

(1) Zerf, et. al., PRD 96, (2017)
(2) ILiesiu, et. al., JEHP 04 (2016)
(3) Wang,Corboz,Troyer, New J. of Phys. 16 (2014).
(4) Li, Jiang and Yao, New J. of Phys. 17 (2015).
(5) D. Schmidt, PhD Thesis (2015)
(6) Huffman, SC PRD 96 (2017) + recent results

Conclusions

Hamiltonian methods offer a new approach to study four-fermion field theories, especially to uncover 2+1d physics.

New solutions to sign problems have emerged recently, hence many more models (of interest in CM physics) have now become tractable.

Check out a paper about emergent SUSY, Li et.al., : 1711.04772

Ideas based on fermion bags may be applicable to many of these models and may help us explore large lattices.

Calculations of the critical exponents with up to 64^2 lattices now available for the N=1 chiral Ising universality class. Agreement with ε-expansion and FRG methods is observed.