Hamming distance and the onset of quantum criticality

September 13th, 2022

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Funding:

CSRC

NSFC
National Natural Science Foundation of China

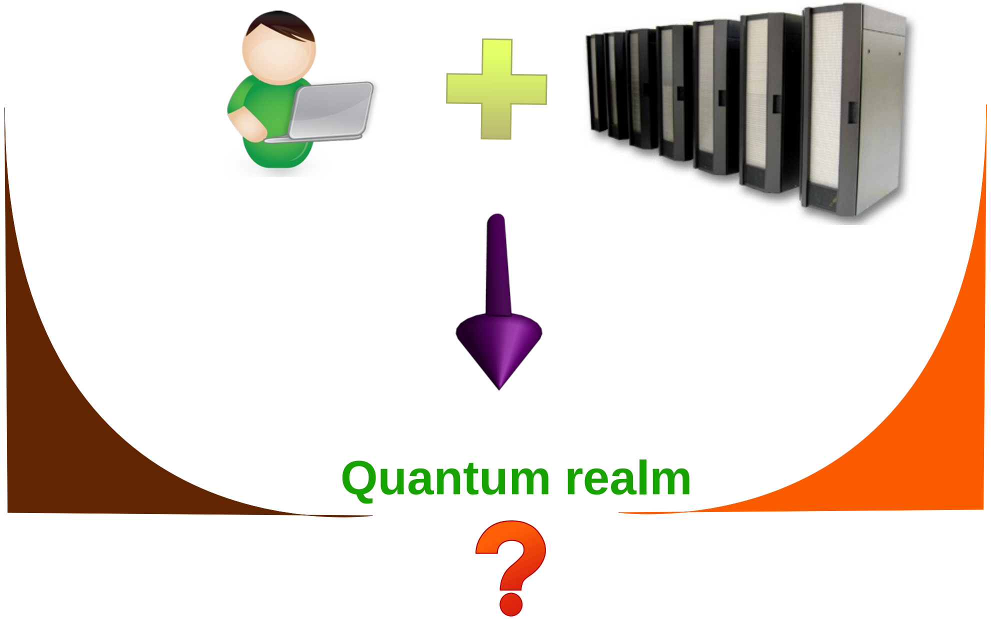
Quantum many-body systems: exponential walls within classical computations

1) Obtaining quantum states: exponentially large (Hilbert) space

2) Directly obtaining estimations for observables: the "sign problem"

Hilbert space wall:

The number of states
in the computation grows
exponentially with the
physical system size



Sign problem:

Importance sampling
leads to "negative probabilities"

Who's afraid of the ~~big bad wolf~~ sign problem?

- Well, a lot of us, it is widespread in many fields

Generally: Importance sampling leads to negative weights or unphysical solutions

Quantum chemistry: Diffusion Monte Carlo

J. Chem. Phys. **131**, 054106 (2009)

Nuclear and high energy: Green's function Monte Carlo
Variational quantum Monte Carlo
Lattice QCD methods

Rev. Mod. Phys. **87**, 1067 (2015)
Lattice methods for QCD, WS (2006)

Condensed matter physics: World-line quantum Monte Carlo
Stochastic Series Expansion
Auxiliary field quantum Monte Carlo

Hirsch et al. Phys. Rev. B **26** 5033 (1982)
Sandvik, Kurkijarvi, Phys. Rev. B **43**, 5950 (1991)
BSS, Phys. Rev. D **24**, 2278 (1981)

Main problem: There is no easy solution to it…. It is conjectured to be NP-hard!

Troyer Wiese, PRL 94, 170201 (2005)

The origin of the sign problem (via examples)

1) Trotter decomposition $\mathcal{Z} = \mathrm{Tr}\, e^{-\beta \hat{H}} = \mathrm{Tr}\, [e^{-\Delta\tau \hat{H}}]^{L_\tau} \sim \mathrm{Tr}\, [e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}]^{L_\tau}$

2) Hubbard Stratonovich transformation $e^{-\Delta\tau U (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})} = \frac{1}{2} e^{-U\Delta\tau/4} \sum_{s_i = \pm 1} e^{\lambda s_i (n_{i\uparrow} - n_{i\downarrow})}$

→ Fermions are now quadratic + bosonic field $s_i \to s_{i,\tau}$ D+1 dimensions

3) Fermionic integration in D+1 dimensions

$$\mathcal{Z} = \sum_{\{s_{i\tau}\}} \mathrm{Tr}_\uparrow \, [e^{\vec{c}_\uparrow^\dagger K \vec{c}_\uparrow} e^{\vec{c}_\uparrow^\dagger V^1 \vec{c}_\uparrow} \cdots e^{\vec{c}_\uparrow^\dagger K \vec{c}_\uparrow} e^{\vec{c}_\uparrow^\dagger V_\tau^L \vec{c}_\uparrow}] \; \mathrm{Tr}_\downarrow \, [e^{\vec{c}_\downarrow^\dagger K \vec{c}_\downarrow} e^{-\vec{c}_\downarrow^\dagger V^1 \vec{c}_\downarrow} \cdots e^{\vec{c}_\downarrow^\dagger K \vec{c}_\downarrow} e^{-\vec{c}_\downarrow^\dagger V_\tau^L \vec{c}_\downarrow}]$$

$$\mathcal{Z} = \sum_{\{s_{i\tau}\}} \det[I + e^K e^{V^1} \cdots e^K e^{V^{L_\tau}}] \, \det[I + e^K e^{-V^1} \cdots e^K e^{-V^{L_\tau}}]$$

$$\mathcal{Z} \equiv \sum_{\{s_{i\tau}\}} \det \mathrm{M}^\uparrow_{\{s_{i,\tau}\}} \cdot \det \mathrm{M}^\downarrow_{\{s_{i,\tau}\}}$$

Sign problem: determinants are not always positive

Sign problem affecting observables

One does not sample according to "negative probabilities":

$$W(x) \equiv \mathrm{det}\mathsf{M}^{\uparrow}_{\{s_{i,\tau}\}} \cdot \mathrm{det}\mathsf{M}^{\downarrow}_{\{s_{i,\tau}\}} \longrightarrow |W(x)| = |\mathrm{det}\mathsf{M}^{\uparrow}_{\{s_{i,\tau}\}} \cdot \mathrm{det}\mathsf{M}^{\downarrow}_{\{s_{i,\tau}\}}|$$

Consequence: shifts the sign from the weight onto the observable

Defining: $W(x) \equiv s(x)|W(x)|$ $\qquad s(x) = \pm 1$

Average of observable:

$$\langle \hat{O} \rangle = \frac{\sum_x O(x)s(x)|W(x)|}{\sum_x s(x)|W(x)|} = \frac{\left[\sum_x O(x)s(x)|W(x)|\right] / \sum_x |W(x)|}{\left[\sum_x s(x)|W(x)|\right] / \sum_x |W(x)|} \equiv \frac{\langle sO \rangle_{|W|}}{\langle s \rangle_{|W|}}$$

The problem becomes apparent when $\langle s \rangle_{|W|}$ systematically decreases over the sampling

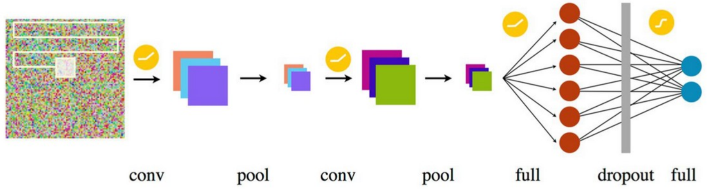
New ideas have emerged to circumvent it

Machine learning quantum phases of matter beyond the fermion sign problem

Peter Broecker[1], Juan Carrasquilla[2], Roger G. Melko[2,3] & Simon Trebst[1]

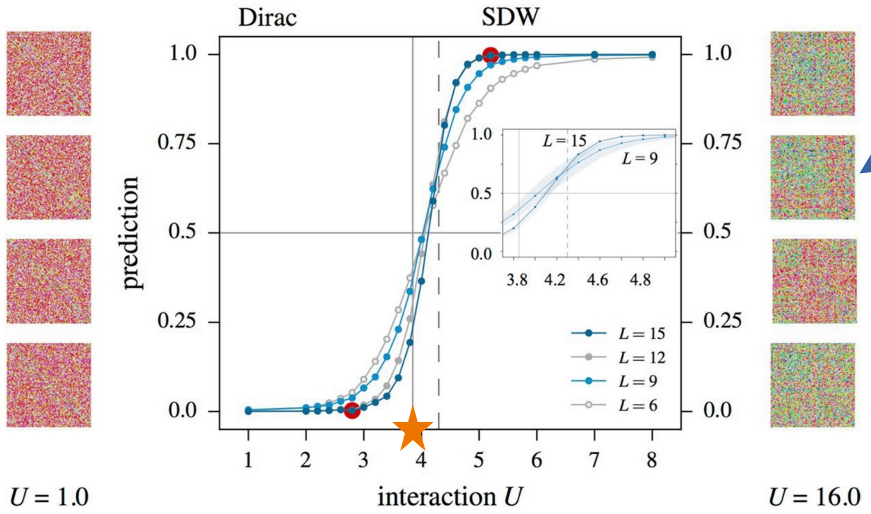
[Scientific Reports 7: 8823 (2017)]

Using convolutional neural networks for pattern recognition →
goal: identify quantum critical points



Application:
SU(2) honeycomb Hubbard model

★ : QCP



Green's functions matrix

$$[G_\sigma] = [M_\sigma^{-1}]$$

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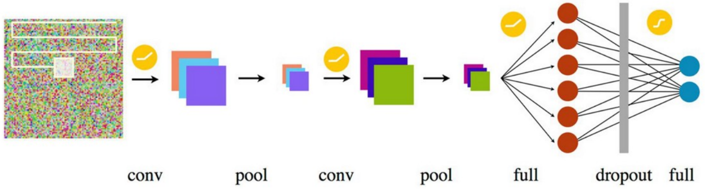

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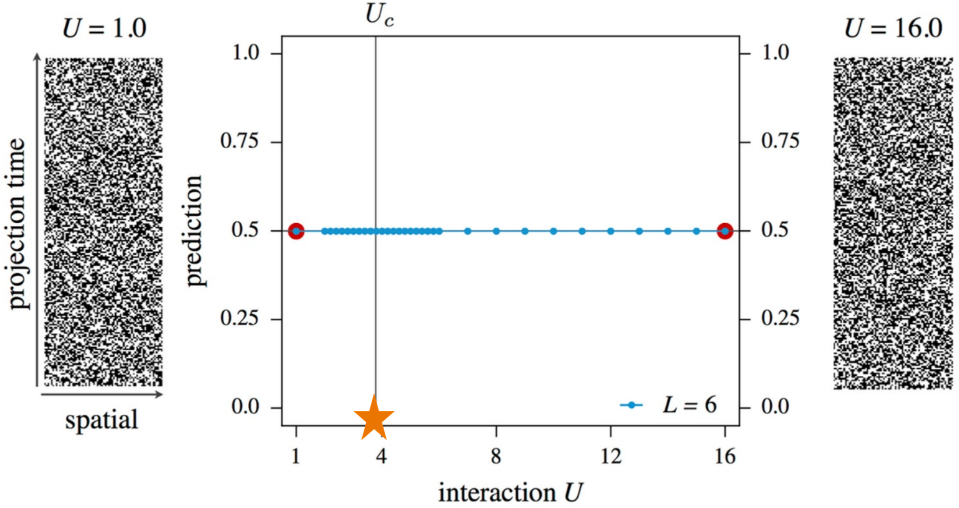


Hubbard-Stratonovich field configuration

No signal...

New ideas have emerged to circumvent it

PHYSICAL REVIEW X **11,** 011040 (2021)

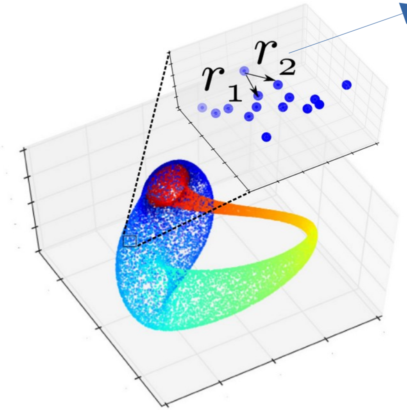
Unsupervised Learning Universal Critical Behavior via the Intrinsic Dimension

T. Mendes-Santos,[1,*] X. Turkeshi,[1,2,3,*] M. Dalmonte,[1,2] and Alex Rodriguez[1]

Intrinsic dimension I_d **:** minimum number of variables needed to describe important features of a data set

Synthetic data

Distances in phase space

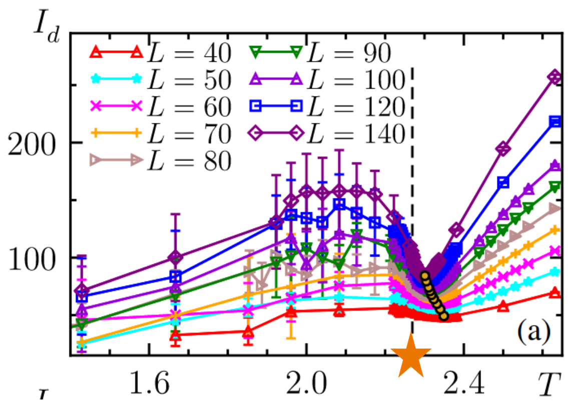


$$r(\vec{X}^i,\vec{X}^j) = \sqrt{2N_c\left(1-\frac{1}{N_c}\sum_{p=1}^{N_c} X_p^i X_p^j\right)}.$$

$$\mu = \frac{\vec{r}_2(x)}{\vec{r}_1(x)}$$: next-nearest : nearest

$$f(\mu) = I_d \mu^{-I_d - 1}$$

2d classical Ising model



$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j$$

$$S_i = \pm 1$$

$$T_c/J = 2/\ln(1+\sqrt{2}) \approx 2.269$$

Facco et al. "Estimating the Intrinsic Dimension of Datasets by a Minimal Neighborhood Information, Sci. Rep. 7, 12140 (2017)]

→ data structures 'simplify' systematically at phase transitions.

New ideas have emerged to circumvent it

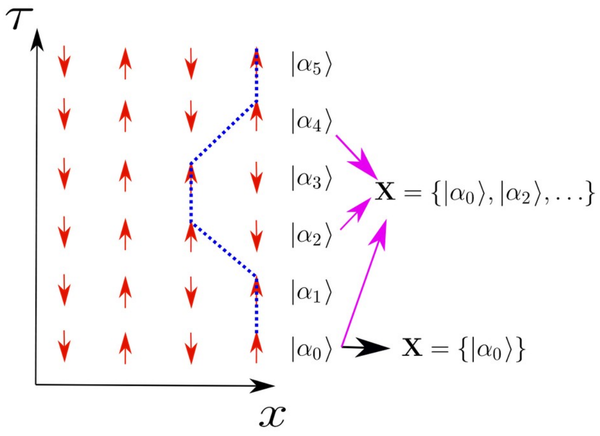
PRX QUANTUM **2**, 030332 (2021)

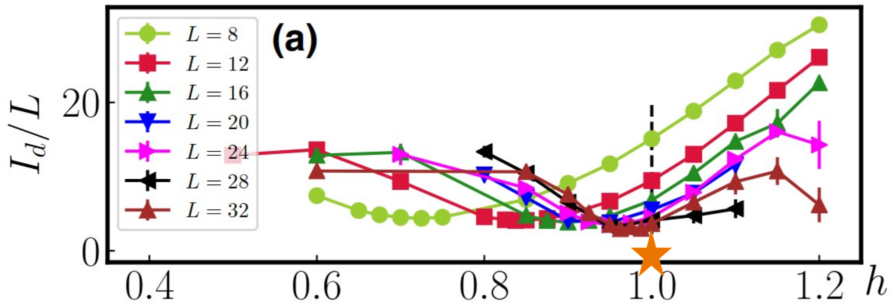
Intrinsic Dimension of Path Integrals: Data-Mining Quantum Criticality and Emergent Simplicity

T. Mendes-Santos,[1,2,*] A. Angelone,[1,3,†] Alex Rodriguez,[1] R. Fazio,[1,4] and M. Dalmonte[1,3]

Intrinsic dimension : minimum number of variables needed to describe important features of a data set

Also applied to quantum systems : Transverse field Ising model $\hat{H} = \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z + h \sum_i \hat{S}_i^x$





★ : QCP

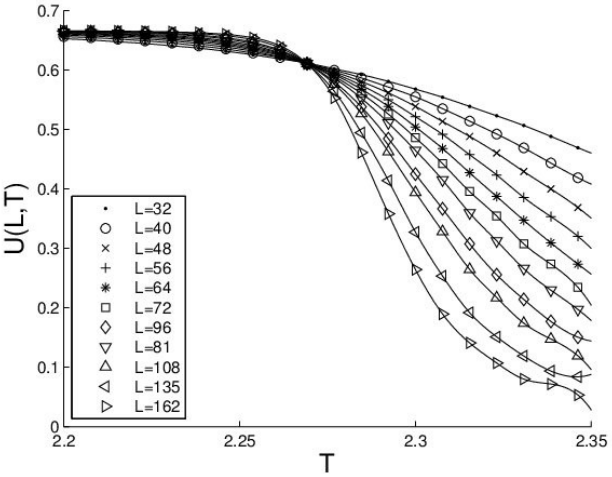
Small drawback: It requires a substantial post-processing [O(N log(N))] related to the NN and NNN quantification of data points in the hyper-dimensional space of configurations

The Ising model

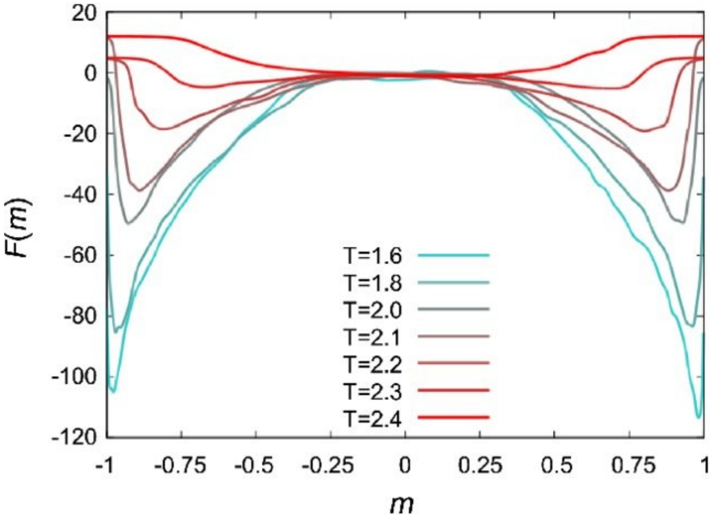
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j \qquad S_i = \pm 1 \qquad T_c/J = 2/\ln(1+\sqrt{2}) \approx 2.269$$

Binder cumulants: $U(L,T) = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$

Free energy:



[Palma, Zambrano, arXiv:0912.0412v1]



Inrok Oh et al.
Bull. Korean Chem. Soc. 2012, 33, No. 3

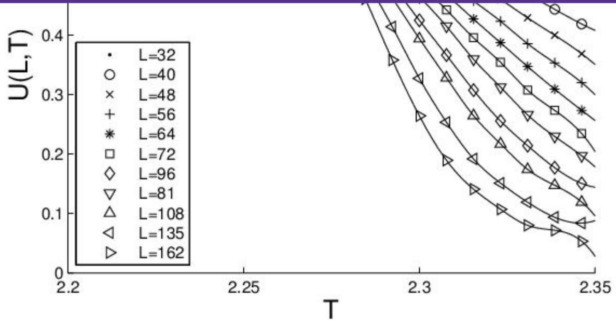
The Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j \qquad S_i = \pm 1 \qquad T_c/J = 2/\ln(1+\sqrt{2}) \approx 2.269$$

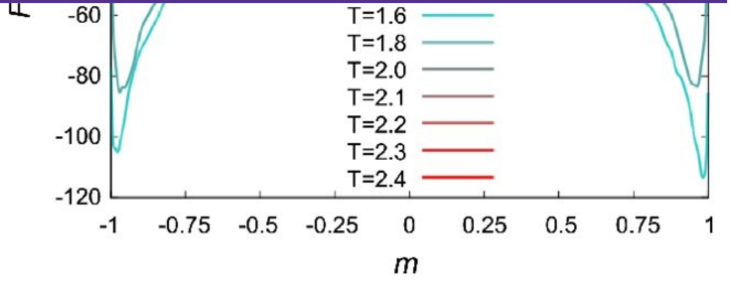
Binder cumulants: $U(L,T) = 1 - \frac{\langle M^4 \rangle}{\cdots}$

Free energy:

The 2^N space of configurations displays highly uneven weights when $T<T_c$

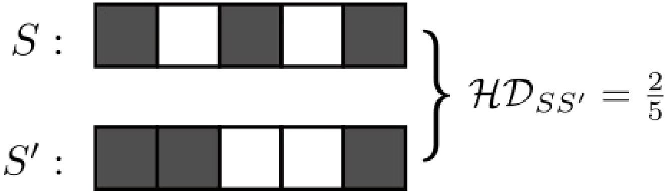


[Palma, Zambrano, arXiv:0912.0412v1]



Inrok Oh et al.
Bull. Korean Chem. Soc. 2012, 33, No. 3

The Hamming distance – quantifying distances traveled within the importance sampling

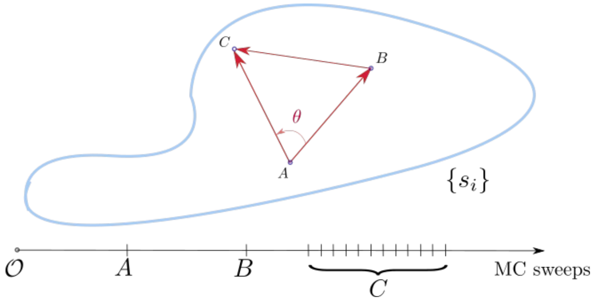


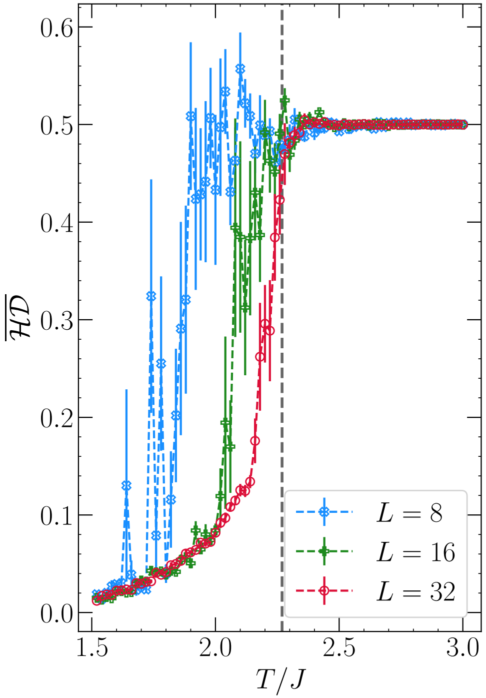
# of unequal elements in two different bitstrings

$\mathcal{HD}_{S,S'} = 0$ Identical strings

$\mathcal{HD}_{S,S'} = 1$ Parity reversed ones

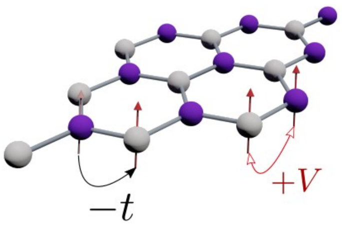
$\mathcal{HD}_{S,S'} = 1/2$ Uncorrelated strings (average)



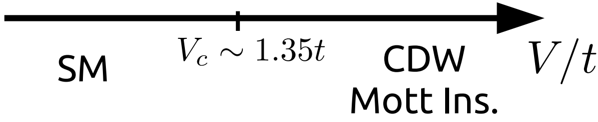


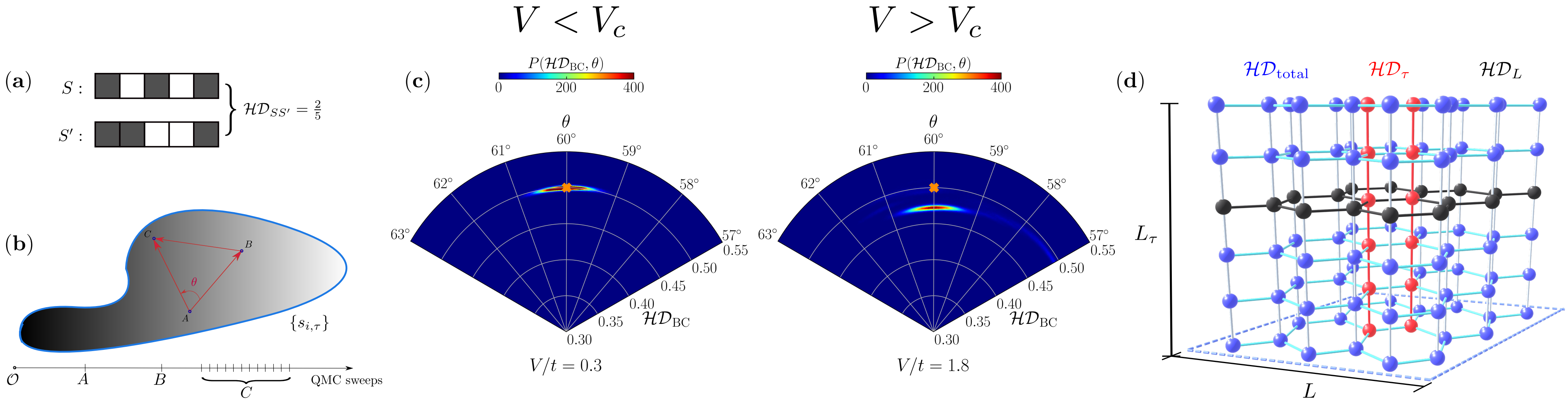
How about quantum systems?

The U(1) honeycomb Hubbard model



$$\hat{H} = -t \sum_{\langle ij \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$





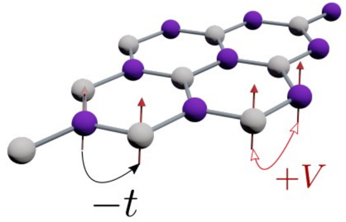
$$\theta = \cos^{-1} \left(\frac{\mathcal{HD}_{AB}^2 + \mathcal{HD}_{AC}^2 - \mathcal{HD}_{BC}^2}{2\mathcal{HD}_{AB}\mathcal{HD}_{AC}} \right)$$: Similarity degree

$\theta = 60^\circ$ → uncorrelated

$\theta \neq 60^\circ$ → some degree of correlation

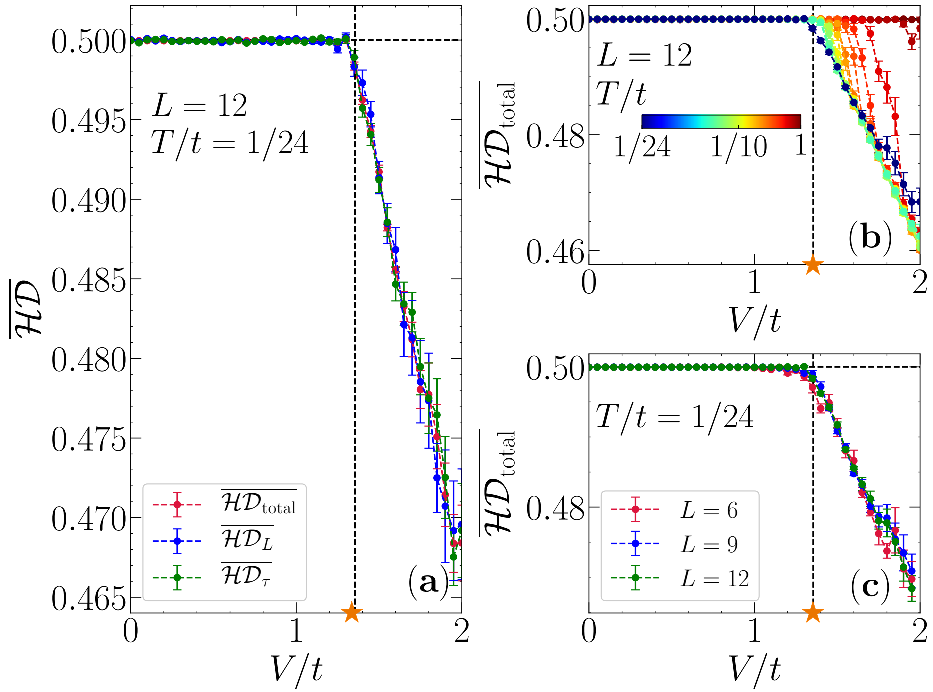
How about quantum systems?

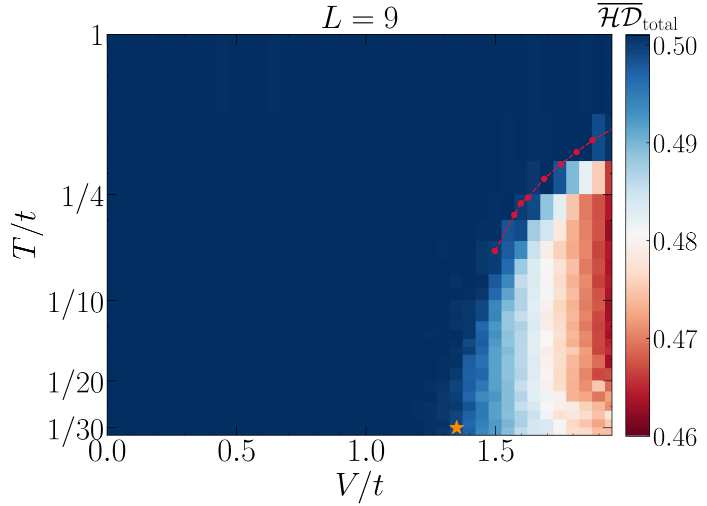
Returning to the U(1) honeycomb Hubbard model



$$\hat{H} = -t \sum_{\langle ij \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

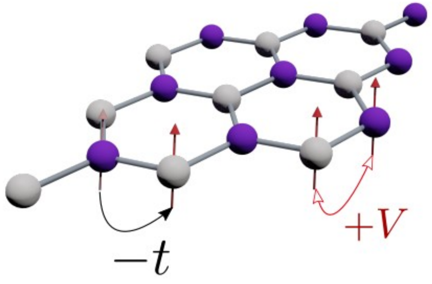
SM $\quad V_c \sim 1.35t \quad$ CDW Mott Ins. $\quad V/t$





Markers from [Hesselmann, Wessel PRB 93, 155157 (2016)]

This occurs despite the existence of a sign problem



$$\hat{H} = -t\sum_{\langle ij\rangle}\left(\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i\right) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j$$

SM — $V_c \sim 1.35t$ — CDW Mott Ins. — V/t

One spin species, the weight is given by a single determinant

$$\mathcal{Z} = \sum_{\{s_{ij,\tau}\}} \det[I + e^K e^{P^1}\cdots e^K e^{P^{L_\tau}}]$$

Sign problem can be dramatic

Continuous time QMC or changing of the basis preclude the sign problem manifestation

Li, Jiang, Yao, Phys. Rev. B 91, 24117 (2015)
Huffman, Chandrasekharan, Phys. Rev. B 89, 111101 (2014)
Wang, Corboz, Troyer, New J. Phys. 16, 103008 (2014)

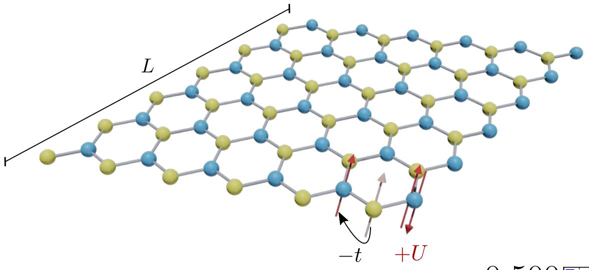
$$\begin{cases} c_i = \frac{1}{2}(\gamma_i^1 + \mathrm{i}\gamma_i^2) \\ c_i^\dagger = \frac{1}{2}(\gamma_i^1 - \mathrm{i}\gamma_i^2) \end{cases} \Rightarrow W(\{s_{ij,\tau}\}) = W_1(\{s_{ij,\tau}\})W_2(\{s_{ij,\tau}\}) \text{ such that } W_1(\{s_{ij,\tau}\}) = W_2^*(\{s_{ij,\tau}\})$$

→ No sign problem!

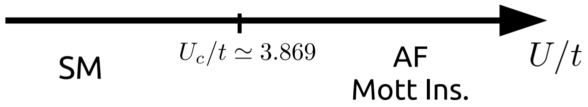
But our results are not in this basis!!

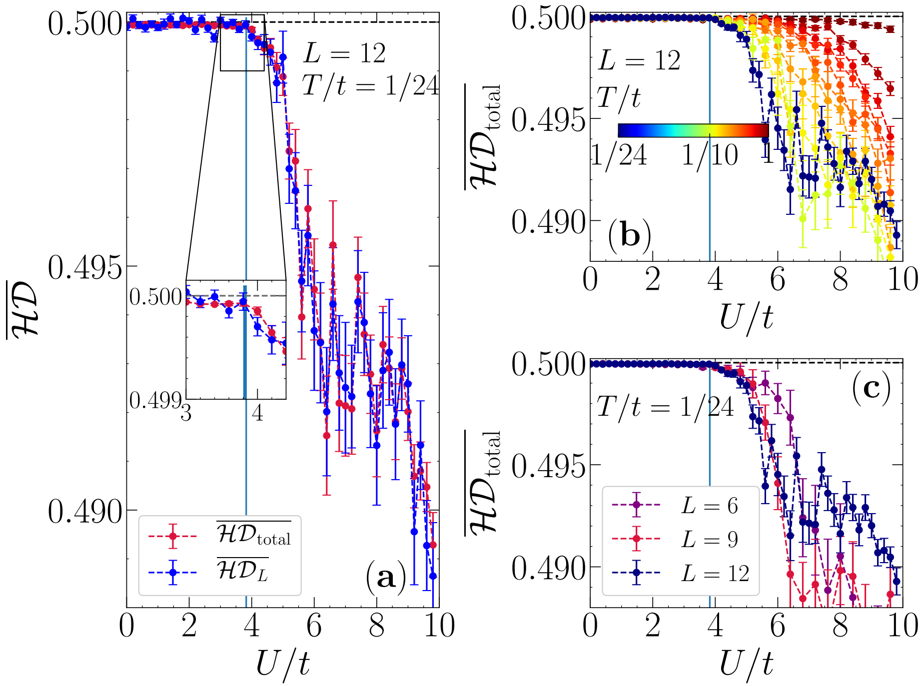
How about quantum systems?

The SU(2) honeycomb Hubbard model



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





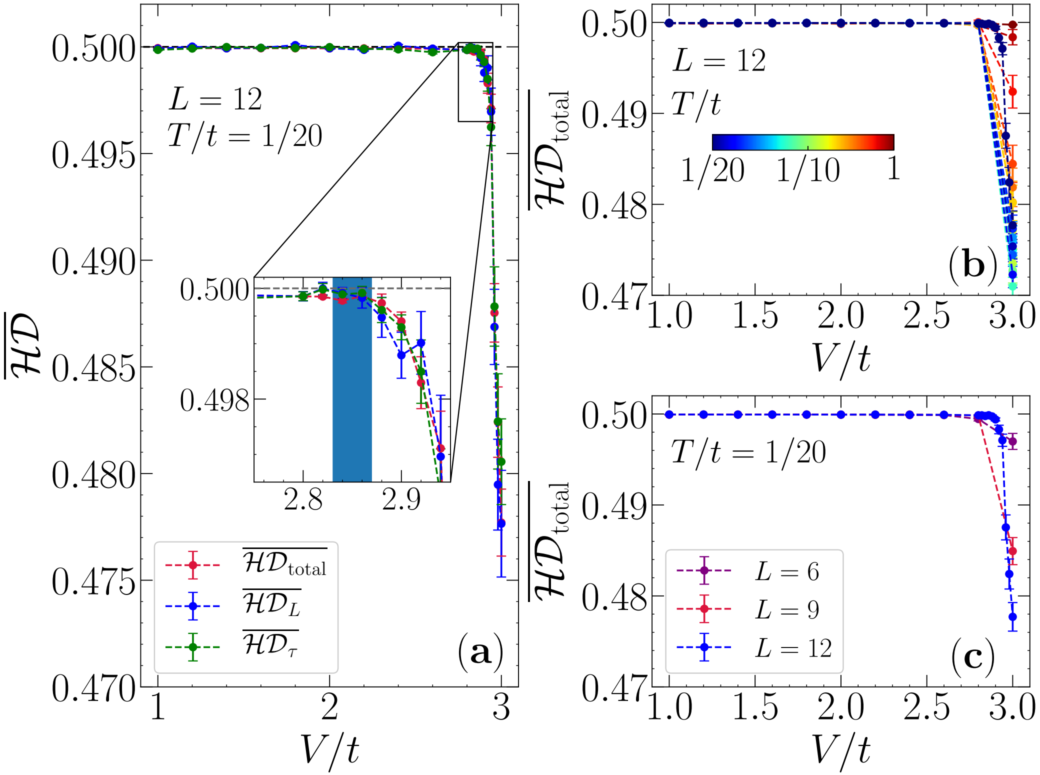
- Finite temperature crossover regime
- Small finite-size effects close to the QCP

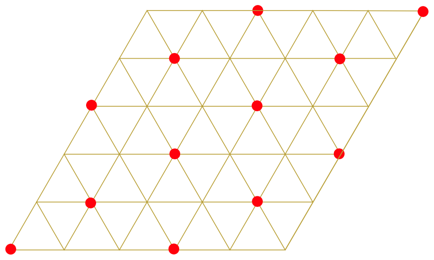
Triangular lattices – frustration leads to a deleterious sign problem

$$\hat{H} = -t \sum_{\langle ij \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

$$\langle \hat{n} \rangle = 1/3$$

Interactions lead to a 1/3-CDW insulator





Questions? How do you know it's a 1/3-CDW insulator?

We don't. Sign problem is terrible.

Interpretation: akin to fidelity susceptibility

$$g = \frac{2}{N_S} \frac{1 - \langle \Psi_0(x) | \Psi_0(x + dx) \rangle}{dx^2}$$

Triangular lattices – frustration leads to a deleterious sign problem

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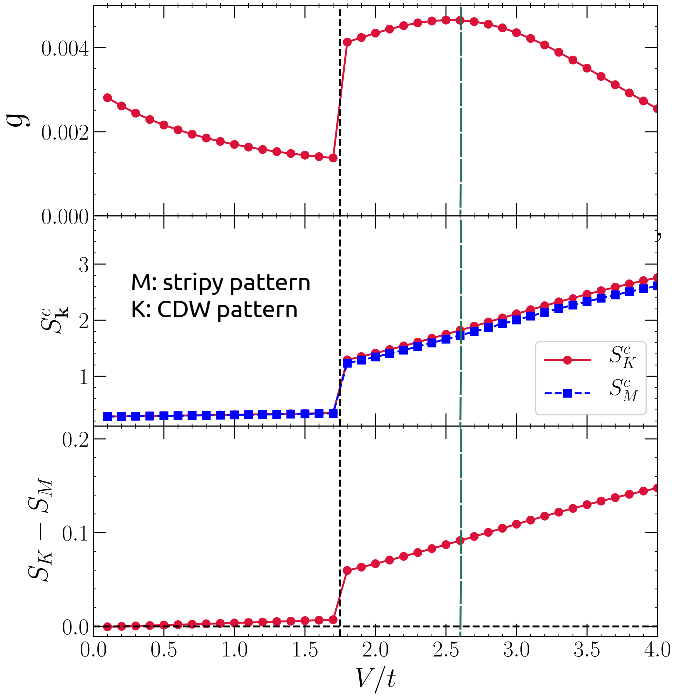
$$\langle \hat{n} \rangle = 1/3$$

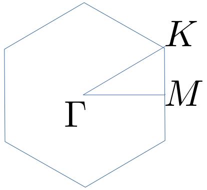
Interactions lead to a 1/3-CDW insulator

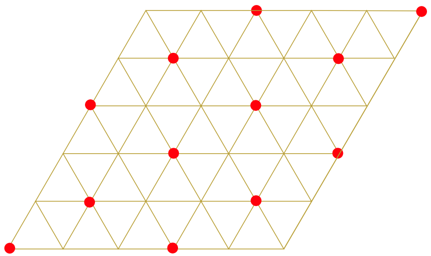
Structure factor:

$$S^c_{\mathbf{k}} = \frac{1}{N_s} \sum_{l,m}^{N_s} e^{i\mathbf{k}\cdot(\mathbf{r}_l - \mathbf{r}_m)} \langle (\hat{n}_l - 1/3)(\hat{n}_m - 1/3) \rangle .$$

Exact diagonalization: 6x6 lattice







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Triangular lattices – The spinful version

$$\hat{H} = -t \sum_{\langle ij \rangle\, \sigma} \left(\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \right) - \mu \sum_{i\sigma} \hat{n}_{i\sigma} + U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) \qquad \langle \hat{n} \rangle = 1$$

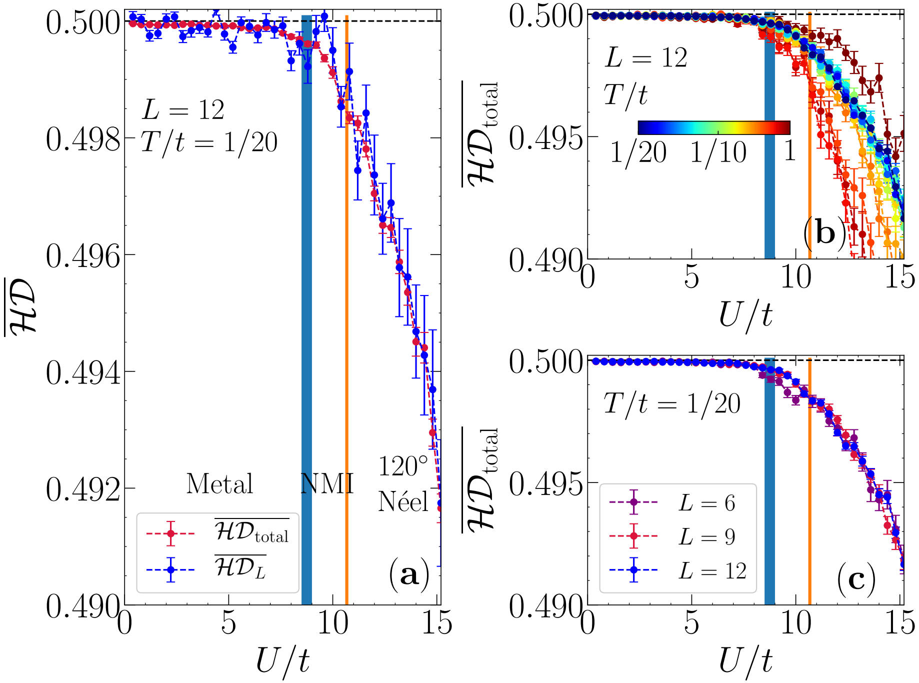
: half-filling

DMRG family of algorithms in cylinders:

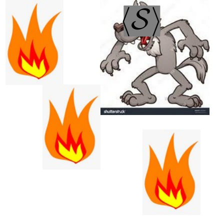
- Szasz, Motruk, Zaletel,Moore PRX 10, 021042 (2020)
- Wietek,Rossi, Šimkovic,Klett,Hansmann ,Ferrero ,Stoudenmire, Schäfer ,Georges PRX 11, 041013 (2021)
- Chen, Chen, Gong, Sheng, Li, Weichselbaum arXiv:2102.05560

- Non-bipartite lattice → Magnetic ordering does not concomitantly occur with insulating Behavior

Our results in 2D lattices:



Triangular lattices – The spinful version – capturing relevant physical information



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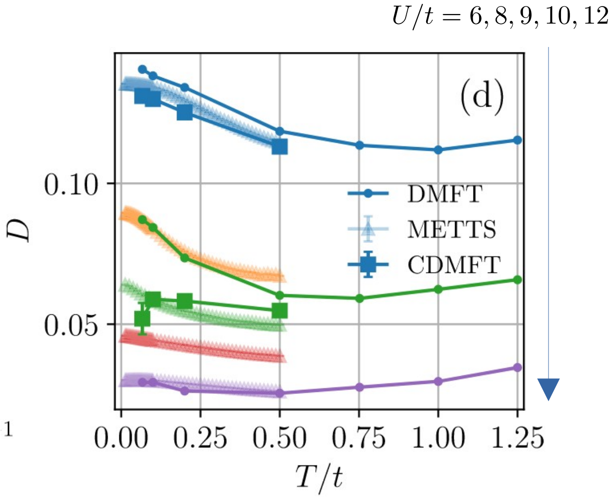
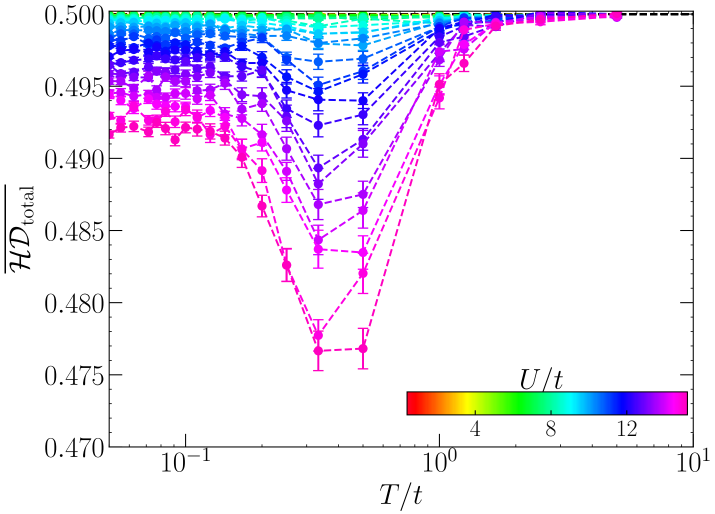
- Interplay of geometric frustration and interactions may lead to ground states with large thermal entropies S

Maxwell relation: $$\left.\frac{\partial S}{\partial U}\right|_T = -\left.\frac{\partial D}{\partial T}\right|_U$$

- Manifestation of the Pomeranchuk effect of increased localization upon heating:



PRX11, 041013 (2021)



Alternate Hubbard-Stratonovich transformations – Hamming distance

SU(2) symmetric transformation

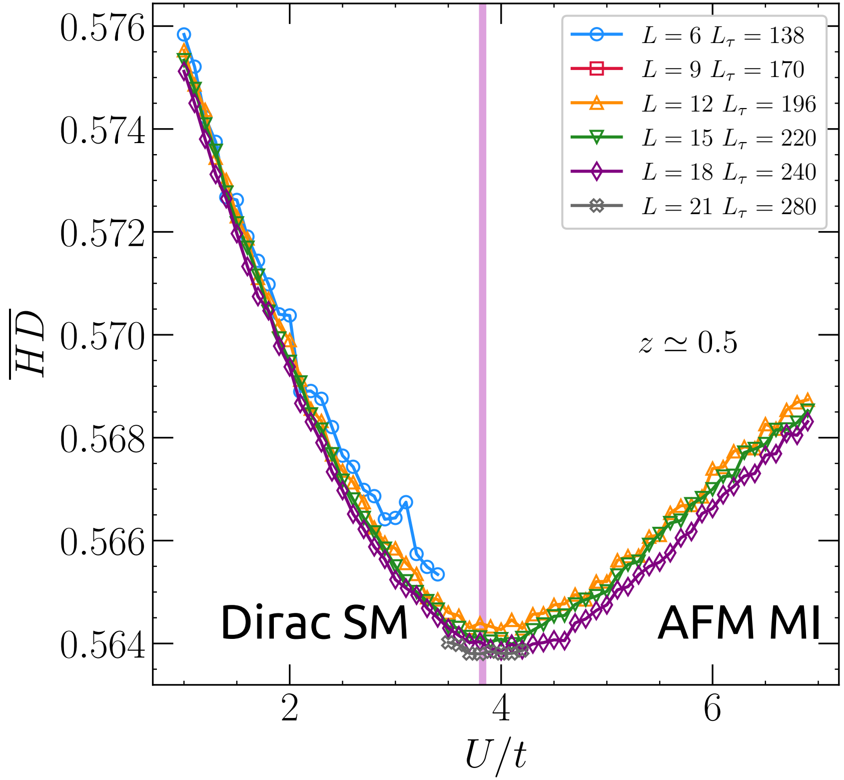
$$e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}-1)^2/2} = \sum_{x_{i\tau}=\pm1,\pm2} \gamma(x_{i\tau}) \prod_{\sigma} e^{\mathrm{i}\sqrt{\Delta\tau U/2}\eta(x_{i\tau})(\hat{n}_{i\sigma}-1/2)} + \mathcal{O}(\Delta\tau^4)$$

$x_{i\tau} = \pm1, \pm2$: 4-valued HS field

Real constants

$$\gamma(\pm1) = 1 + \sqrt{6}/3\ ;\ \eta(\pm1) = \pm\sqrt{2(3-\sqrt{6})}$$
$$\gamma(\pm2) = 1 - \sqrt{6}/3\ ;\ \eta(\pm2) = \pm\sqrt{2(3+\sqrt{6})}$$

SU(2) Hubbard model on the Honeycomb lattice



But why HD (or autocorrelations of the field) capture the physics of the original Hamiltonian?

- Hirsch 1983, 1986:

$$\underbrace{\langle[\hat{n}_{i\uparrow}(\tau) - n_{i\downarrow}(\tau)][\hat{n}_{j\uparrow}(0) - n_{j\downarrow}(0)]\rangle}_{\text{Fermion spin-spin corr.}} = \frac{1}{1-\exp(-\Delta\tau U)} \underbrace{\langle s_{i,\tau} s_{j,0}\rangle}_{\text{Aux. field spin-spin corr.}} \qquad i \neq j, \text{ if } \tau = 0$$

- And similarly for the spinless cases:

$$\langle[\hat{n}_i(\tau) - \hat{n}_j(\tau)][\hat{n}_k(0) - \hat{n}_l(0)]\rangle = \frac{1}{1-e^{-\Delta\tau V}} \langle s_{ij,\tau} s_{kl,0}\rangle$$

Thus fields carry information about the underlying Hamiltonian!

- **When U (or V) → ∞:** one-to-one mapping between aux. field spin-spin correlation and physical correlations
  (provided that Δτ is goes to zero slower than the atomic limit is approached)
- Spin or charge texture on the atomic limit is reflected on the texture of the fields which are mostly likely sampled on

Summary

Thank you!

→ A systematic study of the Hamming distance at finite-T QMC calculations for itinerant fermion models

→ Evidence that the Hamming distance is remarkably efficient in location QCP even in the presence of the sign problem
(maybe not so in deconfined QCP's though)

Disclaimer:

→ Hamming distance does not quantify physical observables

→ We do not neglect the sign problem, it is built in on the determination of $\langle \hat{n}(\mu) \rangle$

Outlook: many new venues of current/future investigation:

→ Other types of HS transformations (include pair-types) may well display information of other ordered phases

$$e^{-\Delta\tau U(\hat{n}_{i\uparrow}-\frac{1}{2})(\hat{n}_{i\downarrow}-\frac{1}{2})} = \frac{1}{2} e^{-U\Delta\tau/4} \sum_{s_i=\pm 1} e^{\lambda s_i (\hat{\Delta}_i^\dagger + \hat{\Delta}_i)} \qquad \hat{\Delta}_i^\dagger = \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger$$

→ Zero-temperature QMC calculations (Projective QMC) → canonical simulations, no need to find $\langle \hat{n}(\mu) \rangle$

→ ....